Slip and barodiffusion phenomena in slow flows of a gas mixture

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The slip and barodiffusion problems for the slow flows of a gas mixture are investigated on the basis of the linearized moment equations following from the Boltzmann equation. We restrict ourselves to the set of the third-order moment equations and state two general relations (resembling conservation equations) for the moments of the distribution function similar to the conditions used by Loyalka [S. K. Loyalka, Phys. Fluids 14, 2291 (1971)] in his approximation method (the modified Maxwell method). The expressions for the macroscopic velocities of the gas mixture species, the partial viscous stress tensors, and the reduced heat fluxes for the stationary slow flow of a gas mixture in the semi-infinite space over a plane wall are obtained as a result of the exact solution of the linearized moment equations in the 10- and 13-moment approximations. The general expression for the slip velocity and the simple and accurate expressions for the viscous, thermal, diffusion slip, and baroslip coefficients, which are given in terms of the basic transport coefficients, are derived by using the modified Maxwell method. The solutions of moment equations are also used for investigation of the flow and diffusion of a gas mixture in a channel formed by two infinite parallel plates. A fundamental result is that the barodiffusion factor in the cross-section-averaged expression for the diffusion flux contains contributions associated with the viscous transfer of momentum in the gas mixture and the effect of the Knudsen layer. Our study revealed that the barodiffusion factor is equal to the diffusion slip coefficient (correct to the opposite sign). This result is consistent with the Onsager's reciprocity relations for kinetic coefficients following from nonequilibrium thermodynamics of the discontinuous systems.

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I. INTRODUCTION

It is well known that full description of a rarefied gas flow for arbitrary Knudsen numbers (Kn = ℓ/a , where ℓ is the molecular mean free path and *a* is the characteristic length scale of the gas flow) requires solution of the Boltzmann equation [1,2]. When gas is slightly rarefied or the Knudsen number is small, adequate description of the gas flow can be achieved by using a system of fluid dynamics equations and appropriate slip (or jump) boundary conditions for the main macroscopic parameters of the gas. The usual Navier-Stokes equations or the more general moment equations following from the Boltzmann equation can be used as a basis for the problem under study. In so doing the slip conditions can be determined by solving the planar boundary value problems for the Boltzmann equation (e.g., Kramers problem and Couette and Poiseuille flows; see [1–3]).

A rich history of research on the slip phenomena in rarefied gas flows originates from the classic work of Maxwell [4]. In 1879 Maxwell conducted an elementary analysis of stress arising in a moving, heated simple gas and discussed the phenomena of viscous slip, thermal creep, and temperature jump. In 1943 Kramers and Kistemaker [5] discussed the analogous phenomenon of diffusion slip, which occurs in a nonuniform gas mixture. Maxwell's method is based on analyzing the equation of momentum balance at the wall and on the assumption that the distribution function for molecules approaching a wall is the same as the function in the gas far from the wall. This assumption is a serious limitation since the incident molecules interact with the reflected ones and the distribution function of the incident molecules varies significantly in the vicinity of a wall (in a thin Knudsen layer with the thickness of a few mean free paths). Such a variation must be taken into account by solving the Boltzmann equation.

Since then, various approximate and numerical methods for solving the model or the exact Boltzmann equation were widely used for investigating the slip and jump phenomena in gas flows. An extensive list of papers on this topic for the case of a single-component gas can be found in the review [6]. In relation to the subject of our paper we shall restrict ourselves mainly to mentioning the basic works concerned with the study of slip effects in a gas mixture.

The early studies of slip problems in the gas mixture flows on the basis of the Boltzmann equation were performed in Refs. [7-9]. Brock [7] used an improved ansatz for the Chapman-Enskog approximation [10] to the distribution function far from the wall and obtained the expressions for viscous slip and diffusion slip coefficients. Zhdanov [9] treated all the slip phenomena using Grad's 13 moments equations [11], refining the results of Ref. [8], and derived the complete expression for the slip velocity of a binary gas mixture due to gradients of velocity, temperature, composition, and pressure. In all these theories the fundamental Maxwell assumption, concerning the form of the distribution function near a wall, was retained. Despite this drawback, the important conclusions [7–9] on the roles of thermal diffusion corrections to some slip coefficients and redetermination of the barodiffusion factor in the diffusion flux by taking into account the viscous momentum transfer in a gas mixture [12] remain valid to the present day.

A number of works, where theoretical treatments of the slip problems in a binary gas mixture are based on the use of the half-range moment method [13-18], should also be

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mentioned. It has been found, among other things, that the diffusion slip coefficient and the barodiffusion factor are significantly affected by the presence of the Knudsen layer and by gas-surface interaction.

Application of a variational method to the linearized Boltzmann equation is of particular interest among the analytical methods used for treating the slip problems today. Loyalka used the variational techniques and derived simple and accurate expressions for the velocity slip coefficient (viscous slip), thermal slip coefficient (thermal creep), and the temperature jump coefficient for a simple gas [19,20], as well as for viscous slip and diffusion slip coefficients for a gas mixture [21]. Cercignani *et al.* [22] has also given general expressions for the velocity slip in a gas mixture using an intregrodifferential variational principle. The important part, distinguishing these methods of analysis from others, is in using the exact form of the linearized Boltzmann equation and the most generalized potential of intermolecular collision as well as the "gas-surface" interaction laws.

Loyalka also proposed an approximation method for the calculation of slip coefficients [23] by a simple modification of the Maxwell's assumption on the velocity distribution of the gas molecules impinging on the wall. Using the approach, denoted as the "modified Maxwell method," he derived the expressions for the velocity slip and the temperature jump identical to those obtained by variational method. This method was thereafter used to obtain the expressions for the diffusion slip coefficient [24] and rederive the expressions for all slip coefficients (including the thermal creep) for binary and multicomponent gas mixtures [25]. It should be noted that the final results of Loyalka et al. are presented in terms of scalar products involving the pertinent Chapman-Enskog solutions [10] and an operator \hat{A} containing the effects of gas-surface interactions. More recently the general expressions for the slip coefficients in binary gas mixtures have also been obtained using the modified Maxwell method in two papers [26,27], where the Chapman-Enskog expansions of the first and second order for a gas mixture and the Maxwell conditions of molecule reflection at the wall (the diffuse-specular model) were used.

In a series of papers [28-30] Sharipov and Kalempa have calculated the viscous, thermal, and diffusion slip coefficients for a gas mixture based on the McCormack kinetic model of the linearized Boltzmann equation, which was solved by the discrete velocity method. The accurate numerical analysis of slip problems in a gas mixture was carried out in a number of works on the basis of the linearized Boltzmann equation for the hard-sphere model of molecules. Takata et al. [31,32] investigated the thermal, diffusion, and viscous slip phenomena in a gas mixture by the finite-difference method. Garcia and Siewert [33] developed numerical solutions for the three slip problems using the analytical discrete ordinate method. The important advantage of such studies is that the velocity, heat flux, and shear stress profiles in the Knudsen layer and away from the wall are established for each species of particles of a binary gas mixture in addition to computations of slip coefficients.

Another analytical method of investigation of the slip phenomena that is alternative to the methods which used the known Chapman-Enskog solutions is the moment method [11]. In 1949 Grad treated the slip effects in a simple gas [11] by the 13-moment approximation of his method. Moment equations were used then for theoretical treatment of the slip phenomena in a simple polyatomic gas [34] and in a mixture of monatomic gases [8,9].

The aim of the present paper is to propose the full description of the slip problems in slow flows of a gas mixture based on the solutions of the linearized moment equations derived on the basis of the Grad's method. We restrict ourselves to the set of the third-order moment equations and state two general relations (resembling conservation equations) for the moments of the distribution function similar to the conditions used by Loyalka in his approximation method [23]. The stationary slow flow of a gas mixture in the semi-infinite space over a plane wall is considered, assuming that longitudinal small gradients of the partial pressure of the gas mixture species and the temperature gradient exist in the z-axis direction. The expressions for the macroscopic velocities of the species, the partial viscous stress tensors, and reduced heat fluxes as a function of the x coordinate normal to the wall are obtained as the result of the exact solution of the linearized moment equations in the 10- and 13-moment approximations. The modified Maxwell method is then used to obtain the general expressions for the slip velocity and viscous, thermal, diffusion slip, and baroslip coefficients for the case of the diffuse-specular model of molecule scattering at the wall. The simple and accurate expressions for the aforementioned quantities are presented, which are given in terms of the basic transport coefficients and are convenient for practical calculations. The obtained expression for slip velocity differs from the well-known results [25-27] in that it contains some new terms (barodiffusion and baroslip) essential in the presence of the pressure gradient in a gas mixture and correspond to the second-order slip effects.

We also use the solutions of moment equations for analyzing diffusion of a gas mixture in a channel formed by two infinite parallel plates. A fundamental result is that the barodiffusion factor in the cross-section-averaged expression for the diffusion flux contains contributions associated with the viscous transfer of momentum in the gas mixture and the effect of the Knudsen layer. It turns out that the barodiffusion factor is equal to the diffusion slip coefficient (correct to the opposite sign). This result is in full agreement with the Onsager's reciprocity relations for kinetic coefficients following from nonequilibrium thermodynamics of the discontinuous systems [35].

We should note here that the moment equations of the Grad's method have already been used in our previous works [36–38] to obtain values of the mass-averaged velocity, diffusion, and heat fluxes in a gas mixture, averaged over a channel cross section in channels with various geometries, for the case of the moderate small Knudsen number. A special feature of the approach used is that it allows us to relate the values of the averaged fluxes to the values of the gradients of corresponding macroscopic parameters and the values of distribution function moments at the channel wall, which should then be found independently using the current techniques for solving the boundary value problems. A generalization of the moment method for description of rarefied gas flow has also been presented in papers [39–41]. In the approach used, the moments at the channel walls

arising in the expressions for the average fluxes turn out to be functionals of the known solutions for viscosity, heat conductivity, and diffusion derived within the framework of the usual approximation of the Chapman-Enskog method and the Burnett solution, which corresponds to the higher-order approximation of the same method [10]. Note that in contrast to all these approaches an explicit solution of moment equations treated in the present paper allows for examining the velocity profiles and other parameters for each species in a gas mixture inside the channel (including the Knudsen layers) and then determining the average value of appropriate quantities over a channel cross section.

Recently Struchtrup and Torrilhon developed a new approach for obtaining transport equations for rarefied gases, the regularized 13 (R13)-moment equations [42,43], which are an extension of the Grad's set of 13-moment equations. By an expansion in the Knudsen number it was shown that the R13 equations and their boundary conditions can be reduced to the Navier-Stokes-Fourier equations with a second-order jump and slip boundary conditions [44,45]. The most important rarefaction effects, e.g., temperature jump, velocity slip, and formation of Knudsen boundary layers in a simple gas, were investigated using the linearized R13 [46] and R26 [47] equations. In the last few years the regularized moment equations were also derived and analyzed for binary gas mixtures of Maxwell molecules [48,49] and hard spheres [50].

II. INITIAL EQUATIONS

Let the gas mixture occupy a half space x > 0 over the surface located in the coordinate plane y - z with x = 0. We consider a stationary flat flow of gas mixture, assuming that relative gradients of the partial pressure of gas mixture species α ; $k_{\alpha} = p_{\alpha}^{-1} \nabla_z p_{\alpha}$; and the relative temperature gradient, $\tau = T^{-1} \nabla_z T$, exist in the direction *z*. It is assumed that the partial pressure p_{α} and the temperature *T* weakly vary on the characteristic mean free path of the particles ℓ , so that

$$|k_{\alpha}\ell| \ll 1, \quad |\tau\ell| \ll 1. \tag{1}$$

The existence of viscous friction between the gas layers and the presence of a wall leads to macroscopic velocities of the mixture species $u_{\alpha z}$, directed along z, becoming a function of the variable x, which will be determined in further analysis of the problem.

For slow flows of gas mixtures (the flow velocity is much smaller than the characteristic thermal velocity of the molecules) and when the conditions (1) are satisfied, the distribution function for the mixture species can be searched for in the form [1-3]

$$f_{\alpha}(\mathbf{v}_{\alpha}, x, z) = f_{\alpha}^{(0)}(\mathbf{v}_{\alpha}, z)[1 + \phi_{\alpha}(\mathbf{v}_{\alpha}, x)],$$

$$f_{\alpha}^{(0)} = n_{\alpha} \left(\frac{\beta_{\alpha}}{\pi}\right)^{3/2} \exp\left(-\beta_{\alpha}v_{\alpha}^{2}\right),$$
 (2)

$$n_{\alpha} = p_{\alpha}(z)/kT(z), \quad \beta_{\alpha} = m_{\alpha}/2kT(z).$$

Here $f_{\alpha}^{(0)}$ is the local equilibrium Maxwell distribution function, \mathbf{v}_{α} is the peculiar velocity of a particle, n_{α} is the number density of species α , m_{α} is the mass of the particles of species α , and k is the Boltzmann constant. The nonequilibrium correction to the distribution function ϕ_{α} satisfies the linearized Boltzmann equation [2,51] written as

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$$v_{\alpha z}k_{\alpha} + v_{\alpha z}\left(\beta_{\alpha}v_{\alpha}^{2} - \frac{5}{2}\right)\tau + v_{\alpha x}\frac{\partial\phi_{\alpha}}{\partial x} = \sum_{\beta}L_{\alpha\beta}\phi_{\alpha},\quad(3)$$

where $L_{\alpha\beta}\phi_{\alpha}$ is the linearized collision operator of particles of species α and β [51]:

$$L_{\alpha\beta}\phi_{\alpha} = \int f_{\beta}^{(0)} [\phi_{\alpha}' + \phi_{\beta}' - \phi_{\alpha} - \phi_{\beta}] g\sigma_{\alpha\beta}(g,\Omega) d\Omega d\mathbf{v}_{\beta}.$$
 (4)

To solve the posed problem, below we will use the equations for moments of the distribution function following from the kinetic equation (3). We will restrict ourselves to a set of moment equations of the third order [11]. Let us introduce the dimensionless velocity of molecules $\mathbf{c}_{\alpha} = \beta_{\alpha}^{1/2} \mathbf{v}_{\alpha}$ as a new variable. We consecutively multiply Eq. (3) by $\psi_{\alpha}^{(n)}(\mathbf{c}_{\alpha}) f_{\alpha}^{(0)}$, where

$$\psi_{\alpha}^{(1)} = c_{\alpha z}, \quad \psi_{\alpha}^{(2)} = c_{\alpha z} c_{\alpha x}, \quad \psi_{\alpha}^{(3)} = c_{\alpha z} \left(c_{\alpha}^2 - \frac{5}{2}\right).$$
 (5)

As a result, after integrating over the velocities for the considered planar geometry of the problem, we arrive at the moment equations of the form

$$p_{\alpha}k_{\alpha} + \frac{\partial \pi_{\alpha_{ZX}}}{\partial x} = R_{\alpha_{Z}}^{(1)}, \quad p_{\alpha}\beta_{\alpha}^{-1/2}\frac{\partial Q_{\alpha_{Z}}}{\partial x} = R_{\alpha_{ZX}}^{(2)},$$

$$p_{\alpha}\tau + \frac{2}{5}\frac{\partial \Pi_{\alpha_{ZX}}}{\partial x} = R_{\alpha_{Z}}^{(3)}.$$
(6)

The moments of the distribution function on the left-hand side of Eqs. (6) are defined as follows:

$$\pi_{\alpha zx} = 2\pi^{-3/2} p_{\alpha} \int c_{\alpha z} c_{\alpha x} \phi_{\alpha} \exp\left(-c_{\alpha}^{2}\right) d\mathbf{c}_{\alpha}, \qquad (7)$$

$$Q_{\alpha z} = 2\pi^{-3/2} \int c_{\alpha z} c_{\alpha x}^2 \phi_\alpha \exp\left(-c_\alpha^2\right) d\mathbf{c}_\alpha, \qquad (8)$$

$$\Pi_{\alpha zx} = 2\pi^{-3/2} p_{\alpha} \int c_{\alpha z} c_{\alpha x} \left(c_{\alpha}^2 - \frac{5}{2} \right) \phi_{\alpha} \exp\left(-c_{\alpha}^2 \right) d\mathbf{c}_{\alpha}.$$
(9)

Below we will also need to define the mean velocity $u_{\alpha z}$ and the reduced heat flux $h_{\alpha z}$ of species α ,

$$u_{\alpha z} = \pi^{-3/2} \beta_{\alpha}^{-1/2} \int c_{\alpha z} \phi_{\alpha} \exp\left(-c_{\alpha}^{2}\right) d\mathbf{c}_{\alpha}, \qquad (10)$$
$$h_{\alpha z} = \pi^{-3/2} \beta_{\alpha}^{-1/2} p_{\alpha} \int c_{\alpha z} \left(c_{\alpha}^{2} - \frac{5}{2}\right) \phi_{\alpha} \exp\left(-c_{\alpha}^{2}\right) d\mathbf{c}_{\alpha}. \tag{11}$$

General expressions for the moments of the collision integral on the right-hand side of Eqs. (6) can be represented as

$$R_{\alpha}^{(n)} = \sum_{\beta} \int \psi_{\alpha}^{(n)} f_{\alpha}^{(0)} L_{\alpha\beta} \phi_{\alpha} d\mathbf{v}_{\alpha}$$
$$= \sum_{\beta} \int \psi_{\alpha}^{(n)} f_{\alpha}^{(0)} f_{\beta}^{(0)} (\phi_{\alpha}' + \phi_{\beta}' - \phi_{\alpha} - \phi_{\beta}) g$$
$$\times \sigma_{\alpha\beta}(g, \Omega) d\Omega d\mathbf{v}_{\alpha} d\mathbf{v}_{\beta}.$$
(12)

Specific expressions for $R_{\alpha}^{(n)}$ can be written if we use the finite expansion of the distribution function (2) in series over tensorial Hermite polynomials of the molecular velocities. To

achieve this goal, below we will employ the expansion for f_{α} , taken in the 13-moment approximation of the Grad's method [11,12]:

$$f_{\alpha} = n_{\alpha} \left(\frac{\beta_{\alpha}}{\pi}\right)^{3/2} \exp[-\beta_{\alpha} (\mathbf{v}_{\alpha} - \mathbf{u})^{2}]$$

$$\times \left\{ 1 + 2\beta_{\alpha} w_{\alpha z} (v_{\alpha z} - u_{z}) + 2\beta_{\alpha} \frac{\pi_{\alpha z x}}{p_{\alpha}} (v_{\alpha z} - u_{z}) v_{\alpha x} + \frac{4}{5} \beta_{\alpha} \frac{h_{\alpha z}}{p_{\alpha}} (v_{\alpha z} - u_{z}) \left[\beta_{\alpha} (\mathbf{v}_{\alpha} - \mathbf{u})^{2} - \frac{5}{2} \right] \right\}, \quad (13)$$

where $\mathbf{u} = \rho^{-1} \sum_{\alpha} \rho_{\alpha} \mathbf{u}_{\alpha}$ is the mass-averaged mixture velocity; $w_{\alpha z} = u_{\alpha z} - u_z$ is the diffusion velocity of species α . Here $\rho_{\alpha} = m_{\alpha} n_{\alpha}$ is the mass density of species α and $\rho = \sum_{\alpha} \rho_{\alpha}$ is the mixture mass density. Note that we have used the conditions $\mathbf{u} \equiv (0, 0, u_z)$ and $\pi_{\alpha zx} = \pi_{\alpha zx}$ in passing from the conventional form of the expansion for f_{α} [12] to the expression (13).

For the problem considered in this paper, in the case of a slow flow of a gas mixture we have $\beta_{\alpha}^{1/2}u_z \ll 1$ and $\exp[-\beta_{\alpha}(\mathbf{v}_{\alpha} - \mathbf{u})^2] \approx \exp(-\beta_{\alpha}v_{\alpha}^2 + 2\beta_{\alpha}u_{\alpha z}v_{\alpha z})$. Then linearization of the expression (13) taking into account the smallness of the quantities $\beta_{\alpha}^{1/2}u_z$, $\beta_{\alpha}^{1/2}w_{\alpha z}$, $\pi_{\alpha zx}/p_{\alpha}$, and $\beta_{\alpha}^{1/2}h_{\alpha z}/p_{\alpha}$ with respect to unity leads to representation of the nonequilibrium correction ϕ_{α} in the following form:

$$\phi_{\alpha} = 2\beta_{\alpha}^{1/2}u_{\alpha z}c_{\alpha z} + 2\frac{\pi_{\alpha z x}}{p_{\alpha}}c_{\alpha x}c_{\alpha z} + \frac{4}{5}\beta_{\alpha}^{1/2}\frac{h_{\alpha z}}{p_{\alpha}}c_{\alpha z}\left(c_{\alpha}^{2} - \frac{5}{2}\right).$$
(14)

Moments of the collision integral $R_{\alpha}^{(n)}$, evaluated using Eq. (14), look like [12,52]

$$R_{\alpha z}^{(1)} = -\sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \alpha_{\alpha\beta} (u_{\alpha z} - u_{\beta z}) - \sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \xi_{\alpha\beta} \left(\frac{h_{\alpha z}}{m_{\alpha} y_{\alpha}} - \frac{h_{\beta z}}{m_{\beta} y_{\beta}} \right),$$
(15)

$$R_{\alpha_{zx}}^{(2)} = -p \sum_{\beta=1}^{N} H_{\alpha\beta} \frac{\pi_{\beta_{zx}}}{y_{\beta}},$$
(16)

$$R_{\alpha z}^{(3)} = -\frac{p}{T} \sum_{\beta=1}^{N} \Lambda_{\alpha\beta} \frac{h_{\beta z}}{y_{\beta}} - p \sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \frac{1}{m_{\alpha}} \xi_{\alpha\beta} (u_{\alpha z} - u_{\beta z}).$$
(17)

Here $y_{\alpha} = n_{\alpha}/n$ is the relative concentration of species α in the mixture; *N* is the number of the mixture species. The coefficients $\alpha_{\alpha\beta}$ and $\xi_{\alpha\beta}$ are written as

$$\alpha_{\alpha\beta} = \frac{p y_{\alpha} y_{\beta}}{\left[D_{\alpha\beta}\right]_{1}}, \quad \xi_{\alpha\beta} = \frac{y_{\alpha} y_{\beta}}{\left[D_{\alpha\beta}\right]_{1}} \mu_{\alpha\beta} \left(\frac{6}{5} C^{*}_{\alpha\beta} - 1\right), \quad (18)$$

where the binary diffusion coefficient $[D_{\alpha\beta}]_1$ (the first Chapman-Cowling approximation [10]) and the dimensionless coefficient $C^*_{\alpha\beta}$ are defined by

$$[D_{\alpha\beta}]_1 = \frac{3}{16} \frac{kT}{n\mu_{\alpha\beta}\Omega_{\alpha\beta}^{11}}, \quad C^*_{\alpha\beta} = \frac{\Omega_{\alpha\beta}^{12}}{3\Omega_{\alpha\beta}^{11}}.$$
 (19)

Here, $\mu_{\alpha\beta} = m_{\alpha}m_{\beta}/(m_{\alpha} + m_{\beta})$ is the reduced mass of the molecules of species α and β ; $\Omega_{\alpha\beta}^{lr}$ are the well-known Ω integrals of Chapman and Cowling [10]. The coefficients $H_{\alpha\beta}$ and $\Lambda_{\alpha\beta}$, expressed using the Ω integrals, are given in Appendix A.

We note that the first of the moment equations (6) represents the momentum balance equation for species α of the mixture. It follows from the law of the conservation of momentum in molecule collisions that we have $\sum_{\alpha} R_{\alpha z}^{(1)} = 0$ for the mixture as a whole. Then summation of the corresponding equations over α leads to the relation

$$\frac{\partial \pi_{zx}}{\partial x} = -\sum_{\alpha} p_{\alpha} k_{\alpha} = -\frac{dp}{dz},$$
(20)

where *p* is the total pressure; π_{zx} is the nondiagonal part of the pressure tensor for the gas mixture. Integration of Eq. (20) gives

$$\pi_{zx} = -x\frac{dp}{dz} + C_1. \tag{21}$$

The second important relation, which we will need below, follows from the second equation (6). Using Eq. (16), one can represent this equation in the form

$$y_{\alpha}\beta_{\alpha}^{-1/2}\frac{\partial Q_{\alpha z}}{\partial x} = -\sum_{\beta=1}^{N}H_{\alpha\beta}\frac{\pi_{\beta zx}}{y_{\beta}}.$$
 (22)

Solving this equation with respect to $\pi_{\alpha zx}$, we find

$$\pi_{\alpha zx} = -y_{\alpha} \sum_{\beta=1}^{N} y_{\beta} \frac{|H|_{\beta\alpha}}{|H|} \beta_{\beta}^{-1/2} \frac{\partial Q_{\beta z}}{\partial x}.$$
 (23)

Here the notation |H| corresponds to the determinant consisting of the elements $H_{\alpha\beta}$, and $|H|_{\beta\alpha}$ is the cofactor of an element $\beta\alpha$ of the determinant. Summing the system of equations (23) over α and changing the summation order under the sum signs lead to the following result:

$$\pi_{zx} = -\sum_{\alpha=1}^{N} \eta_{\alpha} \beta_{\alpha}^{-1/2} \frac{\partial Q_{\alpha z}}{\partial x}, \qquad (24)$$

The quantity η_{α} is defined as

$$\eta_{\alpha} = y_{\alpha} \sum_{\beta=1}^{N} y_{\beta} \frac{|H|_{\beta\alpha}}{|H|}, \qquad (25)$$

and corresponds, as we will see below, to the partial viscosity coefficient of the mixture (the first Chapman-Cowling approximation [10,12,52]).

Integration of Eq. (24) with respect to the relation (21) gives

$$\sum_{\alpha=1}^{N} \eta_{\alpha} \beta_{\alpha}^{-1/2} Q_{\alpha z} = \frac{x^2}{2} \frac{dp}{dz} - C_1 x + C_2.$$
(26)

Equations (21) and (26) represent some general relations (resembling the conservation equations) for the moments of the distribution function, which turn out to be valid for the whole half space, which a gas mixture occupies. In particular, the conditions (21) and (26) take the following form at the

wall (x = 0):

$$\pi_{zx}(0) = C_1, \tag{27}$$

$$\sum_{\alpha=1}^{N} \eta_{\alpha} \beta_{\alpha}^{-1/2} Q_{\alpha z}(0) = C_2.$$
(28)

The constants C_1 and C_2 will be defined below during the analysis of asymptotic solutions of moment equations, which are valid beyond the thin Knudsen layer (i.e., on distances from the wall of the order of several characteristic mean free paths of molecules). Herein the condition (27) becomes crucial when searching for the expressions for the slip velocity of the gas mixture at the wall using the traditional method proposed by Maxwell for the first time [4,9]. Simultaneous use of the conditions (27) and (28) for the same task is equivalent to the Loyalka method [23–25].

For the explicit solution of the system of moment equations and, in particular, for obtaining the solutions valid in the asymptotic region, we will use a closed system of moment equations following from Eq. (6) if the expansion for ϕ_{α} in the form of (14) is also used to evaluate the moments of the distribution function on the left-hand side of these equations. In this case we have

$$\Pi_{\alpha zx} = \pi_{\alpha zx},$$

$$Q_{\alpha z} = \beta_{\alpha}^{1/2} \left(u_z + \frac{2}{5} \frac{q_{\alpha z}}{p_{\alpha}} \right) = \beta_{\alpha}^{1/2} \left(u_{\alpha z} + \frac{2}{5} \frac{h_{\alpha z}}{p_{\alpha}} \right), \quad (29)$$

where the definition of the partial heat flux $q_{\alpha z} = h_{\alpha z} + (5/2)p_{\alpha}w_{\alpha z}$ is introduced. Accounting for the expressions for the right-hand side of Eqs. (15)–(17), the system of moment equations is then written in the following form:

$$\frac{d p_{\alpha}}{dz} + \frac{\partial \pi_{\alpha z x}}{\partial x} = -\sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \alpha_{\alpha\beta} (u_{\alpha z} - u_{\beta z}) - \sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \xi_{\alpha\beta} \left(\frac{h_{\alpha z}}{m_{\alpha} y_{\alpha}} - \frac{h_{\beta z}}{m_{\beta} y_{\beta}}\right), \quad (30)$$

$$y_{\alpha}\frac{\partial u_{z}}{\partial x} + \frac{2}{5p}\frac{\partial q_{\alpha z}}{\partial x} = -\sum_{\beta=1}^{N}H_{\alpha\beta}\frac{\pi_{\beta zx}}{y_{\beta}},$$
(31)

$$y_{\alpha} \frac{dT}{dz} + \frac{2}{5} \frac{T}{p} \frac{\partial \pi_{\alpha zx}}{\partial x} = -\sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \Lambda_{\alpha\beta} \frac{h_{\beta z}}{y_{\beta}} - \sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \frac{T}{m_{\alpha}} \xi_{\alpha\beta} (u_{\alpha z} - u_{\beta z}).$$
(32)

These equations correspond to the well-known linearized moment equations for a multicomponent gas mixture, written in the Grad's 13-moment approximation [11,12,52]. They form a closed system of coupled differential equations for the macroscopic parameters of gas mixture species, which must be solved in the general case for some boundary conditions at the wall (x = 0) and a restriction condition of these quantities when $x \to \infty$. The total number of the moment equations is $3 \times N$. Due to the condition $\sum_{\alpha=1}^{N} \rho_{\alpha} \mathbf{w}_{\alpha} = 0$ (following

from the definition of the mass-averaged velocity **u**), Eq. (30), containing the differences between the velocities of the mixture species $u_{\alpha z} - u_{\beta z} = w_{\alpha z} - w_{\beta z}$, are linearly dependent. Thus the actual number of independent equations in the system (30) necessary for defining the diffusion velocities $w_{\alpha z} = u_{\alpha z} - u_z$ is 3*N*-1. The missing equation for obtaining the expression for u_z can be found as a result of summation of Eq. (30) over α [see Eq. (51) for the binary mixture given in Sec. III B] and then using the solution of Eq. (31).

III. SOLUTION OF MOMENT EQUATIONS

A. Influence of viscous momentum transfer on diffusion in a gas mixture

Solution of Eqs. (30)–(32) is considerably simplified if we neglect the terms with the derivatives of partial moments with respect to the coordinates $\partial \pi_{\alpha zx}/\partial x$ and $\partial q_{\alpha z}/\partial x$ on the left-hand side of these equations. Herein the obtained relations for the total viscous stress tensor π_{zx} and the heat flux q_z [12,52] coincide with known results of the so-called first Chapman-Enskog approximation [10,51]. Within the framework of this method the solution of the kinetic equation is sought in the form of formal expansion in powers of the small parameter ε , which has the order of magnitude of the Knudsen number. Terms with the derivatives of fluxes (or, equivalently, the terms with the second derivatives of the mixture velocity, temperature, and concentration) appear in the corresponding expressions only in the next, the so-called Burnett, order of approximation in the parameter ε .

As has been shown in [12], accounting for the term $\partial \pi_{\alpha zx} / \partial x$ becomes important in the diffusion equations (30) in case of steady-state viscous flows of gas, leading to redefinition of the barodiffusion factor in the expressions for the diffusion fluxes. At the same time, as shown below, the influence of the Knudsen layer near the wall on distribution of macroscopic velocities of the mixture components in the half space above the wall is related to the account of the term $\partial q_{\alpha z} / \partial x$. We will consider a full solution of the system of moment equations, taking into account all terms in the next sections of the paper.

If we neglect the term $\partial q_{\alpha z}/\partial x$ on the left-hand side of Eqs. (31), then the solution of these equations can be represented in the form

$$\pi_{\alpha zx} = -\eta_{\alpha} \frac{\partial u_z}{\partial x}, \quad \pi_{zx} = -\eta \frac{\partial u_z}{\partial x}, \quad \eta = \sum_{\alpha} \eta_{\alpha}, \quad (33)$$

where η_{α} is the partial viscosity coefficient, defined by the expression (25); η is the total viscosity coefficient. For a binary gas mixture,

$$\eta_1 = y_1 \frac{y_1 H_{22} - y_2 H_{12}}{|H|}, \quad \eta_2 = y_2 \frac{y_2 H_{11} - y_1 H_{21}}{|H|},$$
$$|H| = H_{11} H_{22} - H_{12} H_{21}.$$
(34)

The derivative of the partial viscous stress tensor, entering the left-hand sides of Eqs. (30) and (32), can be represented as

$$\frac{\partial \pi_{\alpha zx}}{\partial x} = -\eta_{\alpha} \frac{\partial^2 u_z}{\partial x^2} = -\frac{\eta_{\alpha}}{\eta} \frac{dp}{dz},$$
(35)

where the usual relation $\eta \partial^2 u_z / \partial x^2 = dp/dz$, describing viscous flow of a mixture and following from the relations (20)

and (33), is used. As a result, the left-hand side of Eqs. (30) takes the form

$$pd_{\alpha z}^{\nu} = \frac{dp_{\alpha}}{dz} - \frac{\eta_{\alpha}}{\eta}\frac{dp}{dz} = p\frac{dy_{\alpha}}{dz} + \left(y_{\alpha} - \frac{\eta_{\alpha}}{\eta}\right)\frac{dp}{dz}.$$
 (36)

First, we consider the 10-moment approximation, when the contribution from the moments of the third order or the reduced heat fluxes $h_{\alpha z}$ is neglected in the expansion of the nonequilibrium part of the distribution function (14). Equation (30) is then written as

$$pd_{\alpha z}^{\nu} = -p \sum_{\substack{\beta=1\\\beta\neq\alpha}}^{N} \frac{y_{\alpha}y_{\beta}}{[D_{\alpha\beta}]} (u_{\alpha z} - u_{\beta z}).$$
(37)

An important characteristic of these equations is that they describe the influence of viscous momentum transfer on diffusion in a mixture [12], differing from regular diffusion equations in the Stefan-Maxwell form [53], in which the left-hand side of Eq. (37) has the form

$$pd_{\alpha z} = \frac{dp_{\alpha}}{dz} - \frac{\rho_{\alpha}}{\rho}\frac{dp}{dz} = p\frac{dy_{\alpha}}{dz} + \left(y_{\alpha} - \frac{\rho_{\alpha}}{\rho}\right)\frac{dp}{dz},\qquad(38)$$

where $pd_{\alpha z}$ is the thermodynamic diffusion force [34]. It was shown in [12] that the canonical form of the diffusion equations with $pd_{\alpha z}$ in the form (38) is characteristic only for flows including inertial terms in the motion equations for the mixture components when the viscous friction forces acting on them are neglected. For the steady-state, slow (viscous) mixture flows where viscosity terms should be accounted for, it is natural to represent the diffusion equations as shown in Eq. (37) using $d_{\alpha z}^{\nu}$ (36) instead of $d_{\alpha z}$ (38).

Using Eqs. (37) and (36) in the case of a binary gas mixture, we obtain the following expression for the difference between the velocities of species 1 and 2 in a viscous gas flow $U_z^v = u_{1z} - u_{2z}$, which corresponds to the 10-moment approximation (called "the first approximation" from here onwards):

$$\begin{bmatrix} U_z^v \end{bmatrix}_1 = -\frac{\begin{bmatrix} D_{12} \end{bmatrix}_1}{y_1 y_2} d_{1z}^v = -\frac{\begin{bmatrix} D_{12} \end{bmatrix}_1}{y_1 y_2} \left(\frac{dy_1}{dz} + \begin{bmatrix} \alpha_p^v \end{bmatrix}_1 y_1 y_2 \frac{1}{p} \frac{dp}{dz} \right).$$
(39)

The binary diffusion coefficient $[D_{12}]_1$ corresponds to the result of the first Chapman-Cowling approximation (19), and the barodiffusion factor in a viscous flow $[\alpha_p^v]_1$ is defined as [12]

$$\left[\alpha_{p}^{\nu}\right]_{1} = \left(y_{1} - \frac{\eta_{1}}{\eta}\right)\frac{1}{y_{1}y_{2}} = \frac{1}{\eta}\left(\frac{\eta_{2}}{y_{2}} - \frac{\eta_{1}}{y_{1}}\right).$$
(40)

We note that using $d_{\alpha z}$ (38) for $d_{\alpha z}^{v}$ on the left-hand side of Eq. (37) leads to the expression identical to Eq. (39) for U_z with the familiar barodiffusion factor for the binary gas mixture, which is consistent with the first Chapman-Enskog approximation [10]:

$$[\alpha_p]_1 = \left(y_1 - \frac{\rho_1}{\rho}\right) \frac{1}{y_1 y_2} = \frac{m_2 - m_1}{(m)_y},$$

$$(m)_y = m_1 y_1 + m_2 y_2.$$
(41)

Now we consider the 13-moment approximation for a binary mixture, in which the contribution from the reduced heat fluxes $h_{\alpha z}$ is additionally accounted for in the expansion of the distribution function (14). Solution of system (32) in this case yields

$$h_{1z} = -\lambda_1 \frac{dT}{dz} - (\kappa_{11} - \kappa_{12}) \frac{\partial \pi_{1zx}}{\partial x} + \kappa_{12} \frac{dp}{dz} - \varsigma_1 U_z, \quad (42a)$$

$$h_{2z} = -\lambda_2 \frac{dI}{dz} - (\kappa_{21} - \kappa_{22}) \frac{\partial \pi_{1zx}}{\partial x} + \kappa_{22} \frac{dp}{dz} - \varsigma_2 U_z, \quad (42b)$$

where

$$\lambda_{1} = y_{1} \frac{y_{1}\Lambda_{22} - y_{2}\Lambda_{12}}{|\Lambda|}, \quad \lambda_{2} = y_{2} \frac{y_{2}\Lambda_{11} - y_{1}\Lambda_{21}}{|\Lambda|}, \quad (43)$$

$$\kappa_{11} = \frac{2}{5} \frac{T}{p} y_{1} \frac{\Lambda_{22}}{|\Lambda|}, \quad \kappa_{12} = -\frac{2}{5} \frac{T}{p} y_{1} \frac{\Lambda_{12}}{|\Lambda|}, \quad \kappa_{21} = -\frac{2}{5} \frac{T}{p} y_{2} \frac{\Lambda_{11}}{|\Lambda|}, \quad (44)$$

$$\varsigma_{1} = y_{1} \xi_{12} T \left(\frac{\Lambda_{22}}{m_{1}} + \frac{\Lambda_{12}}{m_{2}}\right) \frac{1}{|\Lambda|}, \quad (44)$$

$$\varsigma_{2} = -y_{2} \xi_{12} T \left(\frac{\Lambda_{11}}{m_{2}} + \frac{\Lambda_{21}}{m_{1}}\right) \frac{1}{|\Lambda|}, \quad (45)$$

For Eqs. (42) we additionally used the relation (20).

Substituting the relations (42) into the set (30) in the case of the binary gas mixture, we arrive at the expression for the difference between the velocities of the species, U_z^v (the second approximation [12]), in the form

$$\begin{bmatrix} U_{z}^{v} \end{bmatrix}_{2} = -\frac{[D_{12}]_{2}}{y_{1}y_{2}} \left(\frac{dy_{1}}{dz} + [\alpha_{p}^{v}]_{2}y_{1}y_{2}\frac{1}{p}\frac{dp}{dz} + [\alpha_{T}]_{1}y_{1}y_{2}\frac{1}{T}\frac{dT}{dz} \right).$$
(46)

Here $[D_{12}]_2 = [D_{12}]_1/(1 - \Delta_{12})$, where Δ_{12} is the secondorder correction to the binary diffusion coefficient, and $[\alpha_T]_1$ is the thermal diffusion factor; they are defined as follows:

$$\Delta_{12} = \frac{1}{p} \mu_{12} \left(\frac{6}{5} C_{12}^* - 1 \right) \left(\frac{\zeta_1}{m_1 y_1} - \frac{\zeta_2}{m_2 y_2} \right),$$

$$y_1 y_2 [\alpha_T]_1 = -\frac{1}{p} (\zeta_1 + \zeta_2).$$
(47)

The expressions for Δ_{12} and $[\alpha_T]_1$, after substituting the coefficients ζ_1 and ζ_2 (45) into them, are in full agreement with the Chapman-Cowling results [10,51,53] (the second approximation for the binary diffusion coefficient and the first nonvanishing approximation for the thermal diffusion factor). For the barodiffusion factor in a mixture viscous flow in the second-order approximation we obtain [12]

$$\left[\alpha_p^v\right]_2 = \left[\alpha_p^v\right]_1 (1 - \Delta_p) - \frac{2}{5} [\alpha_T]_1, \tag{48}$$

$$\Delta_{p} = -\frac{2}{5} \frac{1}{p} \left(\frac{5_{2}}{y_{2}} - \frac{\varsigma_{1}}{y_{1}} \right) = \frac{2}{5} \left\{ \frac{m_{2} - m_{1}}{(m)_{y}} y_{1} y_{2} [\alpha_{T}]_{1} + \frac{m_{2} + m_{1}}{(m)_{y}} \frac{\Delta_{12}}{(6/5)C_{12}^{*} - 1} \right\}.$$
(49)

Useful expressions, which are necessary for evaluating the quantities η_{α} , λ_{α} and $[\alpha_p]_1$, $[\alpha_T]_1$, Δ_{12} , are given in Appendix B.

B. Binary gas mixture: 10-moment approximation

The general solutions of the moment equations (30)–(32) are discussed in the following sections for a binary gas mixture. We start with considering the 10-moment approximation. The corresponding system of equations becomes in this case as follows:

$$\frac{dp_1}{dz} + \frac{\partial \pi_{1zx}}{\partial x} = -\alpha_{12}U_z,$$
(50)

$$\frac{dp}{dz} + \frac{\partial \pi_{zx}}{\partial x} = 0, \tag{51}$$

$$H_{11}\frac{\pi_{1zx}}{y_1} + H_{12}\frac{\pi_{2zx}}{y_2} = -y_1\frac{\partial u_{1z}}{\partial x},$$

$$H_{21}\frac{\pi_{1zx}}{y_1} + H_{22}\frac{\pi_{2zx}}{y_2} = -y_2\frac{\partial u_{2z}}{\partial x}.$$
 (52)

Here

$$U_z = u_{1z} - u_{2z}, \quad \pi_{zx} = \pi_{1zx} + \pi_{2zx}.$$

We note that Eq. (51) is obtained as a result of summation of system (30) over α ($\alpha = 1,2$) considering that the righthand side of the equation vanishes in the process. We express the quantities $u_{\alpha z}$ ($\alpha = 1,2$) using the mass-averaged velocity u_z and the difference between the velocities of the mixture species, U_z :

$$u_{1z} = u_{z} + w_{1z} = u_{z} + a_{2}U_{z},$$

$$u_{2z} = u_{z} + w_{2z} = u_{z} - a_{1}U_{z},$$

$$a_{1} = \frac{m_{1}y_{1}}{(m)_{y}}, \quad a_{2} = \frac{m_{2}y_{2}}{(m)_{y}}.$$
(53)

The solution of a system (52) for π_{1zx} and π_{2zx} can then be represented in the form

$$\pi_{1zx} = -\eta_1 \frac{\partial u_z}{\partial x} - \gamma_1 \frac{\partial U_z}{\partial x}, \quad \pi_{2zx} = -\eta_2 \frac{\partial u_z}{\partial x} - \gamma_2 \frac{\partial U_z}{\partial x}, \quad (54)$$

where the partial viscosity coefficients η_{α} are defined by the relations (34), and the coefficients γ_{α} ($\alpha = 1,2$) are written as

$$\gamma_{1} = y_{1} \frac{y_{1}a_{2}H_{22} + y_{2}a_{1}H_{12}}{|H|},$$

$$\gamma_{2} = -y_{2} \frac{y_{2}a_{1}H_{11} + y_{1}a_{2}H_{21}}{|H|}.$$
(55)

For the viscous stress tensor of the mixture as a whole we obtain

$$\pi_{zx} = -\eta \frac{\partial u_z}{\partial x} - \gamma \frac{\partial U_z}{\partial x},$$

$$\eta = \eta_1 + \eta_2, \quad \gamma = \gamma_1 + \gamma_2 = a_2 \eta_1 - a_1 \eta_2. \quad (56)$$

As opposed to the results obtained by using regular kinetic theory [10,51], the viscous stress tensor of the mixture π_{zx} in the considered case appears to be a function depending not only on the derivative of the mass-averaged mixture velocity, but also on the derivative of the diffusion velocity or (in the case of the binary mixture) on the derivative of

the difference between the velocities of the mixture species. In the framework of, e.g., the Chapman-Enskog method, such dependence appears only in the so-called Burnett approximation for the gas mixture [10,54].

Differentiating Eq. (56) with respect to x and using Eq. (51), we arrive at the equation

$$\eta \frac{\partial^2 u_z}{\partial x^2} + \gamma \frac{\partial^2 U_z}{\partial x^2} = \frac{dp}{dz},\tag{57}$$

which differs from the regular Navier-Stokes equation for steady-state viscous flow of the gas mixture by including the term which depends on the second derivative of the difference between the velocities of the mixture species.

Now we obtain the equation to determine U_z using Eq. (50). We find the derivative $\partial \pi_{1_z x} / \partial x$ in this expression by differentiating the first equation of the set (54) with respect to x and excluding the second derivative of the mass-averaged velocity using Eq. ([57]). We get the following as a result:

$$\frac{\partial \pi_{1zx}}{\partial x} = -\frac{\eta_1}{\eta} \frac{dp}{dz} - \gamma_{12} \frac{\partial^2 U_z}{\partial x^2},$$

$$\gamma_{12} = \gamma_1 - \frac{\eta_1}{\eta} \gamma = \frac{1}{\eta} (\gamma_1 \eta_2 - \gamma_2 \eta_1) = \frac{y_1^2 y_2^2}{\eta |H|}.$$
 (58)

Substituting the first equation (58) into Eq. (50), we arrive at the equation

$$\frac{\partial^2 U_z}{\partial x^2} = s_0^2 \left(U_z - \left[U_z^v \right]_1 \right).$$
⁽⁵⁹⁾

The quantity $[U_z^v]_1$ is defined by the relation (39), and the parameter s_0^2 is written as

$$s_0^2 = \frac{p|H|\eta}{y_1 y_2[D_{12}]_1}, \quad |H|\eta = y_1^2 H_{22} + y_2^2 H_{11} - 2y_1 y_2 H_{12}.$$
(60)

Solution of Eq. (59) with the boundary condition $u_{\alpha z} = u_{\alpha z}(0)$, when x = 0, and the finiteness of U_z when $x \to \infty$, is

$$U_z = \left[U_z^v\right]_1 [1 - \exp(-s_0 x)] + U_z(0) \exp(-s_0 x).$$
(61)

Estimates show that the parameter s_0^{-1} has the order of magnitude of the mean free path of particles in a gas mixture. Let us consider, for example, a gas mixture when the molar concentration of one of the components tends towards zero $(y_1 \rightarrow 1, y_2 \rightarrow 0)$. In this case the determinant $|H| \approx H_{11}H_{22}$, where $H_{11} \approx 1/[\eta_{11}]_1$, $H_{22} \approx C_{12}y_2/[\eta_{22}]_1$, and C_{12} is the numerical factor depending on the mass of particles and details of particles interaction with each other (its expression is cumbersome and thus is omitted here). Considering as an example the case of a gas mixture comprising particles with close masses and average interaction cross sections ($m_1 \sim m_2$, $[\eta_{11}]_1 \sim [\eta_{22}]_1 \sim \eta$, and $C_{12} \sim 1$), we find $|H| \sim y_2 \eta^{-2}$ and $s_0^2 \sim p/\eta D_{12}$. Taking into account that $\eta \sim \rho \ell \langle v \rangle$ and $(\rho D_{12}/\eta) \sim 1$, where $\rho = pm/kT$ is the mass density, $\langle v \rangle \sim$ $(kT/m)^{1/2}$ is the mean thermal velocity of molecules and ℓ is the mean free path of molecules, we obtain $s_0 \sim \ell^{-1}$. It can be demonstrated that this estimate for s_0 remains valid even in the case of gas mixtures having particles with disparate masses and interaction cross sections, if we assume $\ell = \ell_p$ [see Eq. (126)]. Specific calculations of the quantity $s_0\ell_p$ for a series of gas mixtures given in Table II (see Sec. V) show that $s_0\ell_p \sim 1-2$.

The quantity $\delta = 1/s_0$ actually defines the thickness of some thin Knudsen layer at the wall, outside the boundaries of which the hydrodynamic solutions for the mixture flow are valid. The latter means that for $s_0 x \gg 1$, or for distances from the wall on the order of several mean free paths, the value U_z tends to its asymptotic value $U_z^{as} = [U_z^v]_1$.

The expression for the mass-averaged velocity of the mixture u_z can be obtained by putting the derivative $\partial^2 U_z / \partial x^2$ calculated using Eq. (61) into Eq. (57). As a result, we have

$$\eta \frac{\partial^2 u_z}{\partial x^2} = \frac{dp}{dz} + \gamma s_0^2 \left[U_z^{as} - U_z(0) \right] \exp\left(-s_0 x\right).$$
(62)

Integration of Eq. (62) gives

$$\eta \frac{\partial u_z}{\partial x} = -\gamma s_0 \left[U_z^{as} - U_z(0) \right] \exp\left(-s_0 x\right) + x \frac{dp}{dz} + A_1, \quad (63)$$

$$\eta u_{z} = \gamma \left[U_{z}^{as} - U_{z}(0) \right] \exp\left(-s_{0}x \right) + \frac{x^{2}}{2} \frac{dp}{dz} + A_{1}x + A_{2}.$$
(64)

Using the boundary condition $u_z = u_z(0)$ when x = 0, we find

$$A_2 = \eta u_z(0) - \gamma \left[U_z^{as} - U_z(0) \right].$$
(65)

As for the constant A_1 , its definition depends on two specific setups of the problem.

(1) Let the full pressure of the mixture p be constant (dp/dz = 0). Then from Eq. (63) it follows that when $s_0x \rightarrow \infty$, the gradient of the mass-averaged velocity of the mixture $\partial u_z/\partial x$ is constant. This case corresponds, for example, to the usual setup of the problem for the Couette flow [1,2]. In the absence of the pressure gradient we have

$$A_1 = \eta \left(\frac{\partial u_z}{\partial x}\right)_{sx \to \infty} = \eta \frac{\partial u_z^{as}}{\partial x}.$$
 (66)

As a result, for this case,

$$u_z = u_z(0) + x \frac{\partial u_z^{as}}{\partial x} - \frac{\gamma}{\eta} \left[U_z^{as} - U_z(0) \right] [1 - \exp\left(-s_0 x\right)].$$
(67)

(2) Let the longitudinal component of the total pressure gradient of the mixture differ from zero $(dp/dz \neq 0)$. This case corresponds, for example, to the well-known Poiseuille flow between two parallel surfaces separated by the distance *d*. We can then use the symmetry of the velocity field with respect to the channel walls, fulfilling the conditions

$$(\partial u_{\tau}/\partial x)_{x=d/2} = 0.$$

Using Eq. (63), we obtain in this case $A_1 = -(d/2)dp/dz$.

As has been pointed out above, the parameter s_0 has the same order of magnitude as $1/\delta$, where δ is the thickness of the Knudsen layer equal to several characteristic mean free paths of the molecules. On the boundary of this layer, when $x \sim \delta$ because of the conditions $d \gg \delta$, the x^2 term of the expression (64) is negligible compared to the linear term (for this case we can assume that the velocity profile, which is parabolic in the main part of the channel, is approximately linear in the vicinity of the wall). For this case, the previously obtained expression for u_z (67) then becomes valid in the flow region near the wall,

if we substitute $(\partial u_z^{as}/\partial x)$ with $(-d/2\eta)dp/dz$ for the case of the flow between two parallel surfaces.

We obtain the expressions for the macroscopic velocities of each species by using the relations (53) and Eqs. (61) and (67):

$$u_{1z} = u_{1z}(0) + x \frac{\partial u_z^{as}}{\partial x} + \frac{\eta_2}{\eta} [U_z^{as} - U_z(0)] [1 - \exp(-s_0 x)],$$
(68a)

$$u_{2z} = u_{2z}(0) + x \frac{\partial u_z^{as}}{\partial x} - \frac{\eta_1}{\eta} [U_z^{as} - U_z(0)] [1 - \exp(-s_0 x)].$$
(68b)

It is also useful to present the expressions for the partial viscous stress tensors, which will be used below. To do this, we employ the expressions (54), (61), and (67). As a result, for the case when dp/dz = 0 we have

$$\pi_{1zx} = -\eta_1 \frac{\partial u_z^{as}}{\partial x} - \gamma_{12} s_0 [U_z^{as} - U_z(0)] \exp(-s_0 x), \quad (69a)$$

$$\pi_{2zx} = -\eta_2 \frac{\partial u_z^{as}}{\partial x} + \gamma_{12} s_0 [U_z^{as} - U_z(0)] \exp(-s_0 x). \quad (69b)$$

For the case of the flow between two parallel surfaces $(dp/dz \neq 0)$, we can again substitute $(\partial u_z^{as}/\partial x)$ with $(-d/2\eta)dp/dz$ in the flow region near the wall.

C. Binary gas mixture: 13-moment approximation

Now we consider the solution to the system of moment equations (30)–(32) in the 13-moment approximation. For a binary gas mixture the corresponding system of equations takes the form

$$\frac{dp_1}{dz} + \frac{\partial \pi_{1zx}}{\partial x} = -\alpha_{12}U_z - \xi_{12} \left(\frac{h_{1z}}{m_1 y_1} - \frac{h_{2z}}{m_2 y_2}\right),$$
(70)

$$\frac{dp}{dz} + \frac{\partial \pi_{zx}}{\partial x} = 0, \tag{71}$$

$$H_{11}\frac{\pi_{1zx}}{y_1} + H_{12}\frac{\pi_{2zx}}{y_2} = -y_1\frac{\partial u_{1z}}{\partial x} - \frac{2}{5p}\frac{\partial h_{1z}}{\partial x},$$
 (72a)

$$H_{21}\frac{\pi_{1zx}}{y_1} + H_{22}\frac{\pi_{2zx}}{y_2} = -y_2\frac{\partial u_{2z}}{\partial x} - \frac{2}{5p}\frac{\partial h_{2z}}{\partial x},$$
(72b)

$$\Lambda_{11} \frac{h_{1z}}{y_1} + \Lambda_{12} \frac{h_{2z}}{y_2} = -y_1 \frac{dT}{dz} - \frac{2}{5} \frac{T}{p} \frac{\partial \pi_{1zx}}{\partial x} - \frac{T}{m_1} \xi_{12} U_z,$$
(73a)

$$\Lambda_{21} \frac{h_{1z}}{y_1} + \Lambda_{22} \frac{h_{2z}}{y_2} = -y_2 \frac{dT}{dz} - \frac{2}{5} \frac{T}{p} \frac{\partial \pi_{2zx}}{\partial x} + \frac{T}{m_2} \xi_{12} U_z.$$
(73b)

Solving the system (72) with respect to π_{1zx} and π_{2zx} , and using the relations (53), we find

$$\pi_{1zx} = -\eta_1 \frac{\partial u_z}{\partial x} - \gamma_1 \frac{\partial U_z}{\partial x} - \chi_{11} \frac{\partial h_{1z}}{\partial x} - \chi_{12} \frac{\partial h_{2z}}{\partial x}, \quad (74a)$$

$$\pi_{2zx} = -\eta_2 \frac{\partial u_z}{\partial x} - \gamma_2 \frac{\partial U_z}{\partial x} - \chi_{21} \frac{\partial h_{1z}}{\partial x} - \chi_{22} \frac{\partial h_{2z}}{\partial x}, \quad (74b)$$

where the coefficients η_{α} and γ_{α} ($\alpha = 1,2$) are defined by the expressions (25) and (55), and for the coefficient $\chi_{\alpha\beta}$ we have

$$\chi_{11} = \frac{2}{5} \frac{y_1}{p} \frac{H_{22}}{|H|}, \quad \chi_{12} = -\frac{2}{5} \frac{y_1}{p} \frac{H_{12}}{|H|},$$

$$\chi_{21} = -\frac{2}{5} \frac{y_2}{p} \frac{H_{21}}{|H|}, \quad \chi_{22} = \frac{2}{5} \frac{y_2}{p} \frac{H_{11}}{|H|}.$$
 (75)

The solution of the system (73) for $h_{\alpha z}$ has been considered previously and is defined by the expressions in (42).

Now we turn to Eq. (70). Substituting h_{1z} and h_{2z} (42) into it, after some algebra using the previously obtained relations (47), we find

$$U_{z} = -\frac{[D_{12}]_{2}}{y_{1}y_{2}} \left[\frac{dy_{1}}{dz} + (y_{1} - b_{2}) \frac{1}{p} \frac{dp}{dz} + y_{1}y_{2}[\alpha_{T}]_{1} \frac{1}{T} \frac{dT}{dz} + (1 + b_{1} - b_{2}) \frac{1}{p} \frac{\partial \pi_{1zx}}{\partial x} \right],$$
(76)

where

$$b_1 = -\frac{2}{5} \frac{1}{p} \frac{\varsigma_1}{y_1}, \quad b_2 = -\frac{2}{5} \frac{1}{p} \frac{\varsigma_2}{y_2}.$$
 (77)

Note that according to Eq. (49), we have $b_2 - b_1 = \Delta_p$.

Determining the quantity $\partial \pi_{1zx}/\partial x$ on the right-hand side of Eq. (76) is a bit more difficult than in the case of the 10-moment approximation. We begin by converting the expressions for $\pi_{\alpha zx}$ (74). Differentiating the relations for $h_{\alpha z}$ (42) with respect to x, we find

$$\frac{\partial h_{1z}}{\partial x} = -(\kappa_{11} - \kappa_{12})\frac{\partial^2 \pi_{1zx}}{\partial x^2} - \varsigma_1 \frac{\partial U_z}{\partial x},$$
$$\frac{\partial h_{2z}}{\partial x} = -(\kappa_{21} - \kappa_{22})\frac{\partial^2 \pi_{1zx}}{\partial x^2} - \varsigma_2 \frac{\partial U_z}{\partial x}.$$
(78)

Substituting these expressions into Eq. (74), we have

$$\pi_{1zx} = -\eta_1 \frac{\partial u_z}{\partial x} - \alpha_1 \frac{\partial U_z}{\partial x} + \beta_1 \frac{\partial^2 \pi_{1zx}}{\partial x^2},$$

$$\pi_{2zx} = -\eta_2 \frac{\partial u_z}{\partial x} - \alpha_2 \frac{\partial U_z}{\partial x} + \beta_2 \frac{\partial^2 \pi_{1zx}}{\partial x^2},$$
 (79)

Here

$$\begin{aligned} \alpha_1 &= \gamma_1 - (\varsigma_1 \chi_{11} + \varsigma_2 \chi_{12}), \quad \alpha_2 &= \gamma_2 - (\varsigma_1 \chi_{21} + \varsigma_2 \chi_{22}), \\ \beta_1 &= \chi_{11}(\kappa_{11} - \kappa_{12}) + \chi_{12}(\kappa_{21} - \kappa_{22}), \\ \beta_2 &= \chi_{21}(\kappa_{11} - \kappa_{12}) + \chi_{22}(\kappa_{21} - \kappa_{22}). \end{aligned}$$

The value $\partial^2 \pi_{1zx} / \partial x^2$ in Eqs. (79) can be expressed using the derivative $\partial U_z / \partial x$, which is obtained by differentiating Eq. (76) with respect to *x*:

$$\frac{\partial^2 \pi_{1zx}}{\partial x^2} = -\theta_{12} \frac{\partial U_z}{\partial x}, \quad \theta_{12} = \frac{p y_1 y_2}{[D_{12}]_2} \frac{1}{1 - \Delta_p}, \quad (80)$$

Then the expressions for the partial viscous stress tensors (79) take the following form:

$$\pi_{1zx} = -\eta_1 \frac{\partial u_z}{\partial x} - f_1 \frac{\partial U_z}{\partial x}, \quad \pi_{2zx} = -\eta_2 \frac{\partial u_z}{\partial x} - f_2 \frac{\partial U_z}{\partial x},$$
(81)

where

1

$$f_1 = \alpha_1 + \beta_1 \theta_{12}, \quad f_2 = \alpha_2 + \beta_2 \theta_{12}$$

The total viscous stress tensor of the mixture is written as

$$\pi_{zx} = -\eta \frac{\partial u_z}{\partial x} - f \frac{\partial U_z}{\partial x},\tag{82}$$

where

$$f = f_1 + f_2 = (\alpha_1 + \alpha_2) + (\beta_1 + \beta_2)\theta_{12}.$$

We note that considering the previously obtained expressions for α_{α} , β_{α} , and θ_{12} , the last expression can be transformed into

$$f = a_2\eta_1 - a_1\eta_2 + b_1\eta_1 + b_2\eta_2 + c_2\eta_1 - c_1\eta_2, \quad (83)$$

where the coefficients c_{α} are defined as

$$c_{1} = \frac{4}{25} \frac{T}{p^{2}} \theta_{12} \frac{\Lambda_{11} + \Lambda_{21}}{|\Lambda|}, \quad c_{2} = \frac{4}{25} \frac{T}{p^{2}} \theta_{12} \frac{\Lambda_{22} + \Lambda_{12}}{|\Lambda|}.$$
(84)

We obtain the expression for $\partial \pi_{1zx} / \partial x$ by differentiating the first of Eqs. (81) with respect to *x*:

$$\frac{\partial \pi_{1zx}}{\partial x} = -\eta_1 \frac{\partial^2 u_z}{\partial x^2} - f_1 \frac{\partial^2 U_z}{\partial x^2}.$$
(85)

The second derivative, $\partial^2 u_z / \partial x^2$, on the right-hand side of this equation is excluded by using the relation for the total viscous stress tensor (82), which after differentiation with respect to x accounting for Eq. (71) yields

$$\eta \frac{\partial^2 u_z}{\partial x^2} + f \frac{\partial^2 U_z}{\partial x^2} = \frac{dp}{dz}.$$
(86)

As a result, we have

$$\frac{\partial \pi_{1zx}}{\partial x} = -\frac{\eta_1}{\eta} \frac{dp}{dz} - f_{12} \frac{\partial^2 U_z}{\partial x^2},\tag{87}$$

where

$$f_{12} = f_1 - \frac{\eta_1}{\eta} f = \frac{1}{\eta} (f_1 \eta_2 - f_2 \eta_1), \tag{88}$$

Substituting $\partial \pi_{1zx}/\partial x$ (87) into the right-hand side of Eq. (76), we arrive at the differential equation for determining U_z , which coincides with the previously obtained Eq. (59),

$$\frac{\partial^2 U_z}{\partial x^2} = s^2 \left(U_z - U_z^{as} \right),\tag{89}$$

where $U_z^{as} = [U_z^v]_2$ is given by the expression (46), and the parameter s^2 is written as

$$s^2 = \frac{\theta_{12}}{f_{12}}.$$
 (90)

Considering the specific expressions for the coefficients η_{α} , δ_{α} , β_{α} , and θ_{12} , the expression for f_{12} (88) after some algebra can be presented in the form

$$f_{12} = \gamma_{12}(1 + c_{12} - \Delta_p), \quad c_{12} = c_1 + c_2.$$
 (91)

As a result,

$$s^{2} = s_{0}^{2} \frac{(1 - \Delta_{12})}{(1 - \Delta_{p})(1 + c_{12} - \Delta_{p})}$$
$$= \frac{p|H|\eta}{y_{1}y_{2}[D_{12}]_{2}} \frac{1}{(1 - \Delta_{p})(1 + c_{12} - \Delta_{p})}.$$
(92)

The estimates of the coefficient c_{12} for a series of gas mixtures show that it is of the order of unity, and the corrections Δ_{12} and Δ_p are small compared to unity; thus the order of magnitude of the parameter *s* is in fact determined by the magnitude of the parameter s_0 [the formula (60)].

The solution of Eq. (89) with the boundary condition $U_z = U_z(0)$ when x = 0 and the finiteness of U_z when $x \to \infty$ has the form

$$U_z = U_z^{as} [1 - \exp(-sx)] + U_z(0) \exp(-sx).$$
(93)

When $sx \to \infty$, we have $U_z \to U_z^{as}$ where $U_z^{as} = [U_z^v]_2$.

We obtain the equation for determining the mass-averaged velocity of the mixture u_z by substituting the derivative $\partial^2 U_z/\partial x^2$ into Eq. (86), so that

$$\eta \frac{\partial^2 u_z}{\partial x^2} = \frac{dp}{dz} + f s^2 \big[U_z^{as} - U_z(0) \big] \exp(-sx).$$
(94)

Note that this equation has the same form as the previously obtained Eq. (62), if we substitute the parameters γ and s_0 with f and s, respectively. The corresponding solution for u_z takes the form

$$u_z = u_z(0) + x \frac{\partial u_z^{as}}{\partial x} - \frac{f}{\eta} \left[U_z^{as} - U_z(0) \right] [1 - \exp(-sx)].$$
(95)

The mean velocities of the mixture species $u_{\alpha z}$ are defined using the relations (53) and Eq. (95):

$$u_{1z} = u_{1z}(0) + x \frac{\partial u_z^{as}}{\partial x} - \left(\frac{f}{\eta} - a_2\right)$$
$$\times \left[U_z^{as} - U_z(0)\right] [1 - \exp(-sx)], \qquad (96a)$$

$$u_{2z} = u_{2z}(0) + x \frac{\partial u_z^{as}}{\partial x} - \left(\frac{f}{\eta} + a_1\right)$$
$$\times \left[U_z^{as} - U_z(0)\right] [1 - \exp(-sx)]. \tag{96b}$$

Taking into account the expression for f (83) and the relations for the coefficients b_{α} and c_{α} , we obtain

$$-\left(\frac{f}{\eta}-a_{2}\right) = \frac{\eta_{2}}{\eta}+\delta_{b}+\delta_{c},$$

$$-\left(\frac{f}{\eta}+a_{1}\right) = -\frac{\eta_{1}}{\eta}+\delta_{b}+\delta_{c},$$

$$\delta_{b} = -\left(\left[\alpha_{p}^{\nu}\right]_{1}\Delta_{p}+\frac{2}{5}[\alpha_{T}]_{1}\right)y_{1}y_{2},$$

$$\delta_{c} = \frac{4}{25}\frac{T}{p^{2}}\theta_{12}\left(\frac{\eta_{2}}{\eta}\frac{\Lambda_{11}+\Lambda_{21}}{|\Lambda|}-\frac{\eta_{1}}{\eta}\frac{\Lambda_{22}+\Lambda_{12}}{|\Lambda|}\right).$$
(97)

The expressions for the partial viscous stress tensors π_{azx} have the same form as the previously obtained Eqs. (69) with $U_z^{as} = [U_z^v]_2$ and with the coefficients γ_{12} and s_0 substituted, correspondingly, with f_{12} and s. For the total viscous stress tensor π_{zx} we have

$$\pi_{zx} = -\eta \frac{\partial u_z^{as}}{\partial x}.$$
(98)

In regard to the expressions for h_{1z} and h_{2z} , they follow from the previously obtained relations (42) after substituting into them the expressions for U_z (93) and the derivatives $\partial \pi_{1zx} / \partial x$ defined by Eq. (87). As a result,

$$h_{1z} = -\lambda_1 \frac{dT}{dz} + \xi_1 \frac{dp}{dz} - \varsigma_1 [U_z^v]_2 + g_1 [U_z(0) - [U_z^v]_2] \exp(-sx), \qquad (99a)$$
$$h_{2z} = -\lambda_2 \frac{dT}{dz} + \xi_2 \frac{dp}{dz} - \varsigma_2 [U_z^v]_2$$

$$+g_{2}[U_{z}(0) - [U_{z}^{v}]_{2}]\exp(-sx), \qquad (99b)$$

where the coefficients λ_{α} and ζ_{α} are defined by Eqs. (43) and (45), and for the coefficients ξ_{α} and g_{α} we have

$$\xi_{1} = \frac{1}{\eta} (\kappa_{11}\eta_{1} + \kappa_{12}\eta_{2}), \quad \xi_{2} = \frac{1}{\eta} (\kappa_{21}\eta_{1} + \kappa_{22}\eta_{2}),$$

$$g_{1} = f_{12}s^{2}(\kappa_{11} - \kappa_{12}) - \varsigma_{1}, \quad g_{2} = f_{12}s^{2}(\kappa_{21} - \kappa_{22}) - \varsigma_{2}.$$
(100)

IV. SLIP VELOCITY AT THE WALL

A. General setup of the problem

The expressions for the macroscopic parameters of the mixture species obtained above contain the terms that are proportional to $\exp(-sx)$, which corresponds to the contribution of the thin Knudsen layer, having the thickness of the order of $\delta = 1/s$. Beyond this layer or when $sx \to \infty$ the indicated terms vanish. This means that at distances from the wall of the order of several mean free paths of molecules the asymptotic value of the mass-averaged velocity of the binary mixture u_z behaves as a linear function of x, having the form

$$u_z^{as} = u_z(0) - \frac{f}{\eta} \left[U_z^{as} - U_z(0) \right] + x \frac{\partial u_z^{as}}{\partial x} = u_z^{as}(0) + x \frac{\partial u_z^{as}}{\partial x}.$$
(101)

Below we will assume the velocity u_z^{as} to be the slip velocity of the gas mixture at the wall, $u_z^{as}(0)$, linearly extrapolated to the wall (x = 0). The value $u_z^{as}(0)$ is connected to the true values of the mean velocities of species at the wall by the relation

$$u_{z}^{as}(0) = u_{z}(0) - \frac{f}{\eta} \left[U_{z}^{as} - U_{z}(0) \right]$$
$$= \left(a_{1} + \frac{f}{\eta} \right) u_{1z}(0) + \left(a_{2} - \frac{f}{\eta} \right) u_{2z}(0) - \frac{f}{\eta} U_{z}^{as}.$$
(102)

Recall that $U_z^{as} = [U_z^v]_2$.

The problem of finding the mass-averaged slip velocity is actually reduced to finding the value of $u_z^{as}(0)$, for which the solution of the moment equations outside the Knudsen layer $(sx \to \infty)$ would coincide with the solution of the linearized Boltzmann equation (3) with the predefined true kinetic conditions at the wall.

To solve the slip velocity problem, it is convenient to introduce the distribution functions in the vicinity of the wall, corresponding to the reflected ($c_{\alpha x} > 0$) and the inci-

dent ($c_{\alpha x} < 0$) molecules. The boundary conditions for the nonequilibrium correction ϕ_{α} to the distribution function at the wall can be expressed in the form [1,2]

$$\phi_{\alpha}(\mathbf{c}_{\alpha},0) = \hat{A}_{\alpha}\phi_{\alpha}(\mathbf{c}_{\alpha}',0), \quad (c_{\alpha x} > 0, \ c_{\alpha x}' < 0), \quad (103)$$

where \hat{A}_{α} is the operator of molecule scattering at the wall, defined in the general case as [25]

$$\hat{A}_{\alpha}\phi_{\alpha}(\mathbf{c}',0) = \int \frac{f_{\alpha}^{(0)}(c')|c'_{x}|}{f_{\alpha}^{(0)}(c)c_{x}} P_{\alpha}(\mathbf{c}'\to\mathbf{c})\phi_{\alpha}(\mathbf{c}',0)d\mathbf{c}'.$$
 (104)

The kernel of the scattering operator $P_{\alpha}(\mathbf{c}' \rightarrow \mathbf{c})$ represents the probability density of molecule scattering at the wall.

For simplicity, below we will restrict ourselves to the known Maxwell conditions of molecule reflection at the wall (the diffuse-specular model), when the scattering operator $P_{\alpha}(\mathbf{c}' \rightarrow \mathbf{c})$ takes the form

$$P_{\alpha}(\mathbf{c}' \to \mathbf{c}) = (1 - \kappa_{\alpha})\delta(c'_{\alpha x} + c_{\alpha x})\delta(c'_{\alpha y} - c_{\alpha y})\delta(c'_{\alpha z} - c_{\alpha z}) + \kappa_{\alpha}\frac{2\sqrt{\pi\beta_{\alpha}}}{n_{\alpha}}c_{\alpha x}f_{\alpha}^{(0)}(\mathbf{c}_{\alpha})\eta(-c'_{x}).$$
(105)

Here $\delta(x)$ is the Dirac delta function, $\eta(x)$ is the Heaviside step function $[\eta(x) = 1, x > 0$ and $\eta(x) = 0, x < 0]$, and κ_{α} is the accommodation coefficient (the fraction of particles of species α that have experienced the diffusion reflection at the wall). In this case [1,2]

$$\begin{split} \bar{A}_{\alpha}\phi_{\alpha}(\mathbf{c}',0) \\ &= (1-\kappa_{\alpha})\phi_{\alpha}(-c_{x},c_{y},c_{z},0) + \kappa_{\alpha}\frac{2\pi^{1/2}}{n_{\alpha}}\beta_{\alpha}^{1/2} \\ &\times \int d\mathbf{c}'\eta(-c_{x}')f_{\alpha}^{(0)}(\mathbf{c}')|c_{x}'|\phi_{\alpha}(\mathbf{c}',0). \end{split}$$
(106)

We define the functions ϕ_{α}^{+} for the molecules reflected from the wall $(c_{\alpha x} > 0)$ and ϕ_{α}^{-} for the molecules incident on the wall $(c_{\alpha x} < 0)$, so that $\phi_{\alpha} = \phi_{\alpha}^{+} \eta(c_{\alpha x}) + \phi_{\alpha}^{-} \eta(-c_{\alpha x})$. The boundary condition corresponding to the previously adopted model then takes the form

$$\phi_{\alpha}^{+}(c_{\alpha x}, c_{\alpha y}, c_{\alpha z}, 0) = (1 - \kappa_{\alpha})\phi_{\alpha}^{-}(-c_{\alpha x}, c_{\alpha y}, c_{\alpha z}, 0), \quad c_{\alpha x} > 0,$$
(107)

since the diffusely scattered molecules obey the Maxwell distribution [one can easily see that the integral on the right-hand side of Eq. (106) vanishes for the correction ϕ_{α} given by Eq. (14)].

Two important relations, (27) and (28), obtained previously and following from the general moment equations (6), will be used below for obtaining the expression for the slip velocity. The constant C_1 in the relation (27) is defined by comparing the expression for π_{zx} (21), which is valid for the whole flow region (including the Knudsen layer), with Eq. (98). It follows that

$$C_1 = -\eta \frac{\partial u_z^{as}}{\partial x}.$$

The condition (27) then takes the form

$$\pi_{zx}(0) = -\eta \frac{\partial u_z^{as}}{\partial x}.$$
 (108)

We find the integration factor C_2 in Eq. (28) by using the definition

$$Q_{\alpha z} = Q_{\alpha z}^{as} = \beta_{\alpha}^{1/2} \left(u_{\alpha z}^{as} + \frac{2}{5} \frac{h_{\alpha z}^{as}}{p_{\alpha}} \right), \quad \text{when } sx \to \infty,$$

which follows from Eq. (29). In this case Eq. (26) can be written as

$$\sum_{\alpha=1}^{N} \eta_{\alpha} \left[u_{\alpha z}^{as} + \frac{2}{5} \frac{h_{\alpha z}^{as}}{p_{\alpha}} \right] = \frac{x^2}{2} \frac{dp}{dz} - C_1 x + C_2.$$
(109)

Assuming that x = 0, we express the constant C_2 by using the values $u_{\alpha z}^{as}(0)$ and $h_{\alpha z}^{as}(0)$ at the wall. As a result, the condition (28) takes the form

$$\sum_{\alpha=1}^{N} \eta_{\alpha} \beta_{\alpha}^{-1/2} Q_{\alpha z}(0) = \sum_{\alpha=1}^{N} \eta_{\alpha} \left[u_{\alpha z}^{as}(0) + \frac{2}{5} \frac{h_{\alpha z}^{as}(0)}{p_{\alpha}} \right].$$
(110)

It follows from Eq. (53) that

$$u_{1z}^{as}(0) = u_z^{as}(0) + w_{1z}^{as}(0) = u_z^{as}(0) + a_2 U_z^{as}(0),$$

$$u_{2z}^{as}(0) = u_z^{as}(0) + w_{2z}^{as}(0) = u_z^{as}(0) - a_1 U_z^{as}(0), \quad (111)$$

where $U_{z}^{as}(0) = [U_{z}^{v}]_{2}$.

For a binary mixture, it is convenient to represent the condition (110) in the form

$$\sum_{\alpha=1}^{N} \eta_{\alpha} \beta_{\alpha}^{-1/2} \mathcal{Q}_{\alpha z}(0) = \eta u_{z}^{as}(0) + (a_{2}\eta_{1} - a_{1}\eta_{2}) [U_{z}^{v}]_{2} + \frac{2}{5} \sum_{\alpha=1}^{2} \eta_{\alpha} \frac{h_{\alpha z}^{as}(0)}{p_{\alpha}}.$$
 (112)

The expressions for $h_{\alpha}^{as}(0)$ follow from Eqs. (99):

$$h_{1z}^{as}(0) = -\lambda_1 \frac{dT}{dz} + \xi_1 \frac{dp}{dz} - \varsigma_1 [U_z^v]_2, \qquad (113a)$$

$$h_{2z}^{as}(0) = -\lambda_2 \frac{dT}{dz} + \xi_2 \frac{dp}{dz} - \varsigma_2 [U_z^v]_2.$$
(113b)

The modified Maxwell method [23] will be used below for obtaining the general expression for the slip velocity at the wall.

B. Modified Maxwell method

As has been pointed out in the Introduction, the initial Maxwell's approach was used in the early studies of slip problems in gas mixture flows. It is assumed that in this method the distribution function of particles coming to the wall coincides with its asymptotic expression, which is valid far from the wall; that is

$$\phi_{\alpha}^{-}(\mathbf{c}_{\alpha},0) = \phi_{\alpha}^{as}(\mathbf{c}_{\alpha},0), \quad c_{\alpha x} < 0.$$
(114)

For this case in the 13-moment approximation we have

$$p_{\alpha}^{as}(\mathbf{c}_{\alpha},0) = 2\beta_{\alpha}^{1/2}c_{\alpha z}\left(u_{z}^{as}(0) + w_{\alpha z}^{as}(0)\right) + 2\frac{\pi_{\alpha z x}^{as}(0)}{p_{\alpha}}c_{\alpha z}c_{\alpha x} + \frac{4}{5}\beta_{\alpha}^{1/2}\frac{h_{\alpha z}^{as}(0)}{p_{\alpha}}c_{\alpha z}\left(c_{\alpha}^{2} - \frac{5}{2}\right).$$
(115)

It should be noted that the choice of the distribution function for incident particles in the vicinity of the wall in the form (115) does not satisfy, as can be easily shown, the previously obtained general condition (112). In this context Loyalka [23] proposed a modification of the Maxwell method by varying some constant *a* instead of $u_z^{as}(0)$ in the expression for ϕ_{α}^{-} to provide the fulfillment of his condition, which is equivalent to Eq. (112). This approximation method can also be justified by comparing its results with the more rigorous variational approach considered in Refs. [19–21].

First we use the condition (108). Considering the relation $\pi_{zx} = \sum_{\alpha} \pi_{\alpha zx}$ and the definition for $\pi_{\alpha zx}$ (7), this condition for the case of a binary gas mixture can be represented as

$$2\pi^{-3/2} \sum_{\alpha=1}^{2} p_{\alpha} \left[\int_{-\infty}^{0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_{x} c_{z} \phi_{\alpha}^{-}(\mathbf{c}, 0) \right]$$
$$\times \exp(-c^{2}) dc_{x} dc_{y} dc_{z} + \int_{0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_{x} c_{z} \phi_{\alpha}^{+}(\mathbf{c}, 0)$$
$$\times \exp(-c^{2}) dc_{x} dc_{y} dc_{z} = -\eta \frac{\partial u_{z}^{as}}{\partial x}.$$
(116)

Using Eq. (115) for $\phi_{\alpha}^{-}(\mathbf{c}_{\alpha},0)$ with a constant *a* instead of $u_{z}^{as}(0)$ and the boundary condition (107) for evaluating the integrals on the left-hand side of Eq. (116), we arrive at the relation

$$-\pi^{-1/2} \sum_{\alpha=1}^{2} \beta_{\alpha}^{1/2} p_{\alpha} \kappa_{\alpha} \left(a + w_{\alpha z}^{as}(0) \right) + \frac{1}{2} \sum_{\alpha=1}^{2} \kappa_{\alpha} \pi_{\alpha z x}^{as}(0)$$
$$-\frac{1}{5} \pi^{-1/2} \sum_{\alpha=1}^{2} \beta_{\alpha}^{1/2} \kappa_{\alpha} h_{\alpha z}^{as}(0) = -\eta \frac{\partial u_{z}^{as}}{\partial x}.$$
 (117)

The quantities $w_{\alpha}^{as}(0)$ and $h_{\alpha z}^{as}(0)$ for $\alpha = 1,2$ are defined by the relations (111) and (113). Using Eq. (69) we also have

$$\pi_{\alpha_{zx}}^{as}(0) = -\eta_{\alpha} \frac{\partial u_{z}^{as}}{\partial x}, \quad \alpha = 1, 2.$$
(118)

We find the expression for a by rearranging Eq. (117):

$$a = \left(\frac{\pi kT}{2}\right)^{1/2} \frac{1}{p} \frac{\sum_{\alpha=1}^{2} (2 - \kappa_{\alpha})\eta_{\alpha}}{(m^{1/2}\kappa)_{y}} \frac{\partial u_{z}^{as}}{\partial x} + \frac{1}{5p} \frac{\sum_{\alpha=1}^{2} m_{\alpha}^{1/2} \kappa_{\alpha} \lambda_{\alpha}}{(m^{1/2}\kappa)_{y}} \frac{dT}{dz} - \frac{1}{5p} \frac{\sum_{\alpha=1}^{2} m_{\alpha}^{1/2} \kappa_{\alpha} \xi_{\alpha}}{(m^{1/2}\kappa)_{y}} \frac{dp}{dz} - \left[\frac{m_{2}m_{1}^{1/2} \kappa_{1} - m_{1}m_{2}^{1/2} \kappa_{2}}{(m^{1/2}\kappa)_{y}(m)_{y}} + \delta\right] y_{1} y_{2} [U_{z}^{v}]_{2}, \quad (119)$$

where the correction δ is defined as

$$\delta = -\frac{1}{5p} \frac{m_1^{1/2} \kappa_1 \varsigma_1 + m_2^{1/2} \kappa_2 \varsigma_2}{(m^{1/2} \kappa)_y y_1 y_2}.$$
 (120)

The expressions for the coefficients ζ_{α} and ξ_{α} are defined by the relations (45) and (100). The reduced notations $(m^{1/2}\kappa)_y = m_1^{1/2}y_1\kappa_1 + m_2^{1/2}y_2\kappa_2$ and $(m)_y = m_1y_1 + m_2y_2$ are also used in Eqs. (119) and (120). Now we use the condition (112), which after substituting in the definition of $Q_{\alpha z}$ from (8) can be rewritten as

$$2\pi^{-3/2} \sum_{\alpha=1}^{2} \eta_{\alpha} \beta_{\alpha}^{-1/2} \\ \times \left[\int_{-\infty}^{0} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_{x}^{2} c_{z} \phi_{\alpha}^{-}(\mathbf{c}, 0) \exp(-c^{2}) dc_{x} dc_{y} dc_{z} \right. \\ \left. + \int_{0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c_{x}^{2} c_{z} \phi_{\alpha}^{+}(\mathbf{c}, 0) \exp(-c^{2}) dc_{x} dc_{y} dc_{z} \right] \\ = \eta u_{z}^{as}(0) + (a_{2}\eta_{1} - a_{1}\eta_{2}) \left[U_{z}^{v} \right]_{2} + \sum_{\alpha=1}^{2} \eta_{\alpha} \frac{h_{\alpha z}^{as}(0)}{p_{\alpha}}.$$
(121)

Evaluating the corresponding integrals, we find

$$u_{z}^{as}(0) = \frac{1}{2}a \sum_{\alpha=1}^{2} (2 - \kappa_{\alpha}) \frac{\eta_{\alpha}}{\eta} + \pi^{-1/2} \sum_{\alpha=1}^{2} \beta_{\alpha}^{-1/2} (2 - \kappa_{\alpha})$$
$$\times \frac{\eta_{\alpha}^{2}}{p_{\alpha}\eta} \frac{\partial u_{z}^{as}}{\partial x} - \frac{1}{5} \sum_{\alpha=1}^{2} \kappa_{\alpha} \frac{\eta_{\alpha}}{\eta} \frac{h_{\alpha z}^{as}}{p_{\alpha}}$$
$$+ \frac{1}{2} \left(a_{1}\kappa_{2} \frac{\eta_{2}}{\eta} - a_{2}\kappa_{1} \frac{\eta_{1}}{\eta} \right) [U_{z}^{v}]_{2}.$$
(122)

To obtain the final result, it is necessary to substitute the constant *a* from Eq. (119) into Eq. (122). Using the relations (113) for $h_{\alpha z}^{as}(0)$, we can present the expression for the slip velocity of the mixture at the wall $u_z^{as}(0)$ in the following general form:

$$u_{z}^{as}(0) = A_{p} \frac{\partial u_{z}^{as}}{\partial x} + A_{T} \frac{dT}{dz} - B_{p} \frac{1}{p} \frac{dp}{dz} - \sigma_{12}^{(v)} y_{1} y_{2} [U_{z}^{v}]_{2},$$
(123)

where

$$y_{1}y_{2}[U_{z}^{v}]_{2} = -[D_{12}]_{2}\left(\frac{dy_{1}}{dz} + [\alpha_{p}^{v}]_{2}y_{1}y_{2}\frac{1}{p}\frac{dp}{dz} + [\alpha_{T}]_{1}y_{1}y_{2}\frac{1}{T}\frac{dT}{dz}\right).$$
(124)

The coefficients A_p , A_T , and $\sigma_{12}^{(v)}$ are called the viscous, thermal, and diffusion slip coefficients; the coefficient B_p can be called the baroslip coefficient. For further calculations, it is convenient to introduce the dimensionless slip coefficients σ_p , σ_T , and σ'_p , using the relations

$$A_{p} = \sigma_{p}l_{p}, \quad A_{T} = \left[\frac{k}{2(m)_{y}T}\right]^{1/2} \sigma_{T}l_{p},$$
$$B_{p} = \left[\frac{(m)_{y}}{2kT}\right]^{1/2} \sigma_{p}'l_{p}.$$
(125)

Here l_p is the effective mean free path of molecules in a mixture, defined as

$$l_p = \left(\frac{2kT}{(m)_y}\right)^{1/2} \frac{\eta}{p},\tag{126}$$

where $(m)_y = \rho/n = m_1 y_1 + m_2 y_2$; η is the viscosity coefficient.

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The expression for $u_z^{as}(0)$ then takes the form

$$u_{z}^{as}(0) = \sigma_{p} \frac{\eta}{p} \left[\frac{2kT}{(m)_{y}} \right]^{1/2} \frac{\partial u_{z}^{as}}{\partial x} + \sigma_{T} \frac{\eta}{\rho} \frac{1}{T} \frac{dT}{dz} - \sigma_{p}' \frac{\eta}{\rho} \frac{1}{p} \frac{dp}{dz} + \sigma_{12}^{(v)} [D_{12}]_{2} \left(\frac{dy_{1}}{dz} + \left[\alpha_{p}^{v} \right]_{2} y_{1} y_{2} \frac{1}{p} \frac{dp}{dz} + \left[\alpha_{T} \right]_{1} y_{1} y_{2} \frac{1}{T} \frac{dT}{dz} \right).$$
(127)

General expressions for the coefficients σ_p , σ_T , and σ'_p are written as

$$\sigma_p = \frac{\pi^{1/2}}{2} \left\{ \frac{(m)_y^{1/2}}{2(m^{1/2}\kappa)_y} \left[\sum_{\alpha=1}^2 (2-\kappa_\alpha) \frac{\eta_\alpha}{\eta} \right]^2 + \frac{2}{\pi} \sum_{\alpha=1}^2 (2-\kappa_\alpha) \frac{(m)_y^{1/2}}{m_\alpha^{1/2} y_\alpha} \left(\frac{\eta_\alpha}{\eta} \right)^2 \right\},\tag{128}$$

$$\sigma_T = \frac{1}{5} \frac{(m)_y}{k} \left[\sum_{\alpha=1}^2 \left(1 - \frac{\kappa_\alpha}{2} \right) \frac{\eta_\alpha}{\eta^2 (m^{1/2} \kappa)_y} \left(\sum_{\alpha=1}^2 m_\alpha^{1/2} \kappa_\alpha \lambda_\alpha \right) + \sum_{\alpha=1}^2 \kappa_\alpha \frac{\eta_\alpha \lambda_\alpha}{\eta^2 y_\alpha} \right],\tag{129}$$

$$\sigma'_{p} = \frac{1}{5} \frac{(m)_{y}}{k} \left[\sum_{\alpha=1}^{2} \left(1 - \frac{\kappa_{\alpha}}{2} \right) \frac{\eta_{\alpha}}{\eta^{2} (m^{1/2} \kappa)_{y}} \left(\sum_{\alpha=1}^{2} m_{\alpha}^{1/2} \kappa_{\alpha} \xi_{\alpha} \right) + \sum_{\alpha=1}^{2} \kappa_{\alpha} \frac{\eta_{\alpha} \xi_{\alpha}}{\eta^{2} y_{\alpha}} \right].$$
(130)

For the coefficient of the diffusion slip $\sigma_{12}^{(v)}$ we have

$$\sigma_{12}^{(v)} = \left[\frac{m_2 m_1^{1/2} \kappa_1 - m_1 m_2^{1/2} \kappa_2}{(m^{1/2} \kappa)_y(m)_y} + \delta\right] \sum_{\alpha=1}^2 \left(1 - \frac{\kappa_\alpha}{2}\right) \frac{\eta_\alpha}{\eta} + \frac{1}{2} \left[\frac{1}{(m)_y} \left(\frac{m_2 \kappa_1}{y_1} \frac{\eta_1}{\eta} - \frac{m_1 \kappa_2}{y_2} \frac{\eta_2}{\eta}\right) + \Delta\right],\tag{131}$$

where the correction δ is defined by Eq. (120) and the correction Δ has the form

$$\Delta = -\frac{2}{5} \frac{1}{p y_1 y_2} \left(\kappa_1 \frac{\eta_1}{\eta} \frac{\zeta_1}{y_1} + \kappa_2 \frac{\eta_2}{\eta} \frac{\zeta_2}{y_2} \right).$$
(132)

When studying gas mixture flows in a series of specific problems, it is more appropriate to deal with the molar-averaged mixture velocity $u_z^m = y_1u_{1z} + y_2u_{2z}$ instead of the mass-averaged velocity $u_z = a_1u_{1z} + a_2u_{2z}$. The connection between these parameters in case of a binary mixture has the form

$$u_z^m = u_z + \frac{m_2 - m_1}{(m)_y} y_1 y_2 (u_{1z} - u_{2z}).$$
(133)

It can be noted that in such transition only the term related to the diffusion slip is redefined when writing the expression for the molar-averaged slip velocity u_z^m , so that instead of the coefficient $\sigma_{12}^{(v)}$ (131) the coefficient σ_{12} appears, which is defined as

$$\sigma_{12} = \sigma_{12}^{(v)} + \frac{m_1 - m_2}{(m)_y}.$$
(134)

For the specific case when $\kappa_1 = \kappa_2 = \kappa$ the corresponding slip coefficients take the form

$$\sigma_p = \frac{2-\kappa}{\kappa} \frac{\pi^{1/2}}{2} (m)_y^{1/2} \left\{ \left(1-\frac{\kappa}{2}\right) \frac{1}{(m^{1/2})_y} + \frac{2}{\pi} \kappa \left[\frac{1}{m_1^{1/2} y_1} \left(\frac{\eta_1}{\eta}\right)^2 + \frac{1}{m_2^{1/2} y_2} \left(\frac{\eta_2}{\eta}\right)^2 \right] \right\},\tag{135}$$

$$\sigma_T = \frac{1}{5} \frac{(m)_y}{k} \left[\left(1 - \frac{\kappa}{2} \right) \frac{m_1^{1/2} \lambda_1 + m_2^{1/2} \lambda_2}{\eta(m^{1/2})_y} + \kappa \left(\frac{\eta_1 \lambda_1}{\eta^2 y_1} + \frac{\eta_2 \lambda_2}{\eta^2 y_2} \right) \right],\tag{136}$$

$$\sigma'_{p} = \frac{1}{5} \frac{(m)_{y}}{k\eta} \left[\left(1 - \frac{\kappa}{2} \right) \frac{m_{1}^{1/2} \xi_{1} + m_{2}^{1/2} \xi_{2}}{(m^{1/2})_{y}} + \kappa \left(\frac{\eta_{1} \xi_{1}}{\eta_{y_{1}}} + \frac{\eta_{2} \xi_{2}}{\eta_{y_{2}}} \right) \right],$$
(137)

$$\sigma_{12}^{(v)} = \left(1 - \frac{\kappa}{2}\right) \left[\frac{m_2 m_1^{1/2} - m_1 m_2^{1/2}}{(m^{1/2})_y(m)_y} + \delta\right] + \frac{\kappa}{2} \left[\frac{1}{(m)_y} \left(\frac{m_2}{y_1} \frac{\eta_1}{\eta} - \frac{m_1}{y_2} \frac{\eta_2}{\eta}\right) + \delta'\right].$$
(138)

The reduced notation $(m^{1/2})_y = m_1^{1/2}y_1 + m_2^{1/2}y_2$ will be used in the foregoing equations. The coefficient of the diffusion slip σ_{12} is written in this case as

$$\sigma_{12} = \left(1 - \frac{\kappa}{2}\right) \left[\frac{m_1^{1/2} - m_2^{1/2}}{(m^{1/2})_y} + \delta\right] + \frac{\kappa}{2} \left(\frac{\eta_1}{y_1} - \frac{\eta_2}{y_2} + \delta'\right).$$
(139)

The correction coefficients δ and δ' are conveniently expressed by $[\alpha_T]_1$ and Δ_{12} as a result of the solution of Eqs. (47):

$$\delta = \frac{1}{5} \left\{ \frac{m_1^{3/2} y_1 + m_2^{3/2} y_2}{(m^{1/2})_y(m)_y} [\alpha_T]_1 + \frac{m_2^{1/2} - m_1^{1/2}}{(m^{1/2})_y(m)_y} \times (m_1 + m_2) \frac{\Delta_{12}}{(6/5)C_{12}^* - 1} \right\},$$
(140)

$$\delta' = \frac{\Delta}{\kappa} = \left[\alpha_p^v\right]_1 \Delta_p + \frac{2}{5} [\alpha_T]_1.$$
(141)

It is easy to note, that, considering Eqs. (40) and (48), the expression for the coefficient σ_{12} can be also represented in the form

$$\sigma_{12} = \left(1 - \frac{\kappa}{2}\right) \left[\frac{m_1^{1/2} - m_2^{1/2}}{(m^{1/2})_y} + \delta\right] - \frac{\kappa}{2} \left[\alpha_p^v\right]_2.$$
 (142)

V. DISCUSSION OF RESULTS

First we consider the case of a mixture flow at constant pressure (dp/dz = 0), when the expression (127) for the slip velocity takes the form

$$u_{z}^{as}(0) = \sigma_{p} \frac{\eta}{p} \left[\frac{2kT}{(m)_{y}} \right]^{1/2} \frac{\partial u_{z}^{as}}{\partial x} + \sigma_{T}^{*} \frac{\eta}{\rho T} \frac{dT}{dz} + \sigma_{12}^{(v)} [D_{12}]_{2} \frac{dy_{1}}{dz},$$
(143)

where

$$\sigma_T^* = \sigma_T + \sigma_{12}^{(v)} \frac{\rho[D_{12}]_2}{\eta} [\alpha_T]_1 y_1 y_2.$$
(144)

As one can see, taking thermal diffusion into account leads to the redefinition of the thermal slip coefficient in a gas mixture.

In the presence of the pressure gradient in a gas mixture $(dp/dz \neq 0)$ barodiffusion and baroslip effects must be taken into account. As an example, we consider the nonisothermal flow of a gas mixture in a channel formed by two parallel infinite plates. Using Eq. (127) and taking into account the relation $\partial u_z^{as}/\partial x = -(d/2\eta)dp/dz$, which becomes valid in the flow region near the wall (see Sec. III B), we have

$$u_{z}^{as}(0) = -\sigma_{p}^{*} \frac{d}{2} \left[\frac{2kT}{(m)_{y}} \right]^{1/2} \frac{1}{p} \frac{dp}{dz} + \sigma_{T}^{*} \frac{\eta}{\rho T} \frac{dT}{dz} + \sigma_{12} [D_{12}]_{2} \frac{dy_{1}}{dz},$$
(145)

where

$$\sigma_p^* = \sigma_p + 2\frac{l_p}{d}\sigma_p' - \frac{l_p}{d}\sigma_{12}[\alpha_p^v]_2 \frac{\rho[D_{12}]_2}{\eta}y_1y_2. \quad (146)$$

The mass-averaged mixture velocity averaged over the channel cross section can be written as

$$\langle u_z \rangle = -\frac{d^2}{12\eta} \frac{dp}{dz} + u_z^{as}(0), \qquad (147)$$

or taking Eq. (145) into account,

$$\langle u_z \rangle = -\frac{d^2}{12\eta} \frac{dp}{dz} \left(1 + 6\sigma_p^* \frac{l_p}{d} \right) + \sigma_T^* \frac{\eta}{\rho T} \frac{dT}{dz} + \sigma_{12}^{(v)} [D_{12}]_2 \frac{dy_1}{dz}.$$
(148)

The slip coefficients σ_T^* and $\sigma_{12}^{(w)}$ in the expression (148) seem identical to those in the case of a gas mixture flow at constant pressure. As for the coefficient σ_p^* , new terms related to the contributions of baroslip and barodiffusion appear. Since $(\rho D_{12}/\eta) \sim 1$, this contribution corresponds to the contribution of the following terms in the expansion in the small Knudsen number Kn = l_p/d , i.e., corresponds to the so-called slip effects of the second order.

Let us consider the case of a single-component gas. Assuming $m_1 = m_2 = m$ and $y_1 \rightarrow 0$ in the expressions (129)–(132), we find

$$\sigma_{p}^{*} = \sigma_{p} + 2\frac{l_{p}}{d}\sigma_{p}^{\prime}, \quad \sigma_{p} = \frac{2-\kappa}{\kappa}\frac{\pi^{1/2}}{2} \bigg[1 + \bigg(\frac{2}{\pi} - \frac{1}{2}\bigg)\kappa \bigg],$$

$$\sigma_{T}^{*} = \sigma_{T} = \frac{3}{4}\bigg(1 + \frac{\kappa}{2}\bigg),$$

$$\sigma_{p}^{\prime} = \frac{1}{5}\sigma_{T} = \frac{3}{20}\bigg(1 + \frac{\kappa}{2}\bigg), \quad \sigma_{12}^{(v)} = 0.$$
(149)

The relation $\lambda = (15k/4m)\eta$ was used in writing the expression for σ_T , where λ and η are, respectively, the thermal conductivity and viscosity coefficients of a simple gas calculated in the first approximation of Chapman-Cowling [10]. For the fully diffusive scattering of molecules at the wall ($\kappa = 1$) we have $\sigma_p = 1.0073$, $\sigma_T = 1.125$, and $\sigma'_p = 0.225$. The expressions for σ_p and σ_T (149) correspond to the results of Loyalka obtained either by implementing the variational method [19,20] or with the aid of the modified Maxwell method [23].

We note that the baroslip effect related to the coefficient σ'_p also appears when considering the plane Poiseuille flow of a simple gas. For simplicity we consider the case when such flow is isothermal (dT/dz = 0). We then have

$$\langle u_z \rangle = -\frac{d^2}{12\eta} \frac{dp}{dz} (1 + 6\sigma_p \mathrm{Kn} + 12\sigma'_p \mathrm{Kn}^2).$$
(150)

It is worth mentioning that correct evaluation of the secondorder slip is beyond the scope of the 13-moment approximation used in the present study. This conclusion is solidified by calculations using higher approximations of the moment method (for instance, the Grad's 20-moment approximation [36] or the expansion in half-space Hermite polynomials [55]). More accurate results are also obtained by applying the variational method to the linearized Boltzmann equation with account for the Burnett solutions of the Chapman-Enskog method. Herein the Bhatnagar-Gross-Krook (BGK) model was used for the Burnett term in Ref. [56], whereas the hard-spheres (HS) model was employed with the exact Burnett term in

Author	A_1	A_2	Approach			
Lang [56]	1.0073	0.5000	Var. (the BGK model for the Burnett term)			
Zhdanov and Zaznoba [36]	1.0073	0.4167	20-moment			
Loyalka and Hickey [57]	1.1019	0.4490	Var. (HS-exact Burnett)			
Cercignani and Lorenzani [58]	1.1209	0.2347	Var. (HS)			
Gibelly [55]	1.1144	0.4952	Half-range moments, (HS)			

TABLE I. Velocity slip coefficients A_1 and A_2 .

Refs. [57,58]. The general expression for $\langle u_z \rangle$ is written in the case of a simple gas in the form

$$\langle u_z \rangle = -\frac{d^2}{12\eta} \frac{dp}{dz} (1 + 6A_1 \text{Kn} + 12A_2 \text{Kn}^2).$$
 (151)

In Table I we compare the values of the coefficients A_1 and A_2 for $\kappa = 1$, obtained by different methods. As one can see, these results correspond well to each other (except for the result of Ref. [58] for the coefficient A_2) and to the coefficients obtained in the 20-moment approximation [36]. It should be noted that the coefficient $A_2 = \sigma'_p$ obtained in the 13-moment approximation (as well as the result in Ref. [58]) is about two times smaller.

Let us now discuss the expressions for the slip coefficients in the case of a binary gas mixture. We emphasize that the general expressions for all slip coefficients in a gas mixture were found in the paper by Lang and Müller [25] on the basis of the Loyalka method using the so-called Knudsen accommodation coefficients of tangential momentum, introduced by Kuscer (see Ref. [17] in the paper [25]) for describing the interactions between the molecules and the wall. Comparing our results to the formulas obtained in [25], we see that in the case when all accommodation coefficients for each mixture component are equal to each other, our expressions for σ_p, σ_T , and σ_T^* formally become equivalent to the results obtained by Lang and Müller. We note that the explicit expressions for the coefficients of partial viscosity η_{α} and thermal conductivity λ_{α} included in the expressions for the viscous and thermal slip coefficients are not present in [25]. The expressions for these quantities convenient for practical calculations and corresponding to the Grad's 13-moment approximation or the first approximation

TABLE II. Values of the transport coefficients and of the diffusion slip coefficients for a selection of binary gas mixture.

Parameters	$N_2 - H_2$ $y_1 = 0.99$	N_2-Ar $y_1 = 0.5$	$N_2 - O_2$ $y_1 = 0.5$	$N_2 - CO_2$ $y_1 = 0.5$
$\eta_1 (10^{-5} \mathrm{Pas})$	1.7323	0.8756	0.8874	0.7578
$\eta_2 (10^{-5}{ m Pas})$	0.0051	1.1114	0.9949	0.8432
$\eta (10^{-5}{ m Pas})$	1.7374	1.9870	1.8823	1.6010
$[D_{12}]_1(10^{-5} \mathrm{m}^2 \mathrm{s}^{-1})$	7.3599	1.8710	1.9819	1.4778
$[\alpha_T]_1$	0.2461	-0.0614	-0.0228	-0.0757
Δ_{12}	0.0265	0.0037	0.0039	0.0026
$s_0 (10^8 \mathrm{m}^{-1})$	0.1735	0.1865	0.1854	0.2316
$\ell_p (10^{-8} \mathrm{m})$	7.1845	7.4256	7.4856	5.8120
$s_0 \ell_p$	1.2464	1.3850	1.3879	1.3460
σ_{12}^{v} [Eq. (131)]	-0.1899	0.1306	0.0381	0.2586
$c_{Dsl}(1)$	-0.1896	0.1307	0.0380	0.2589
$c_{Dsl}(2)$	-0.1959	0.1331	0.0390	0.2621

for the expansion in the Sonine polynomials within the framework of the Chapman-Enskog method are given in Appendix B of the present work. From our point of view, the expressions for the diffusion slip coefficients $\sigma_{12}^{(v)}$ (131) and (138) have some advantages over the expressions regularly used for calculations, given, for example, in [21,25], since the correcting terms in them are explicitly expressed through the thermal diffusion factor $[\alpha_T]_1$ and the second-order correction Δ_{12} (see Appendix B or Refs. [51,53]).

The general expressions for the slip coefficients in a binary gas mixture obtained with aid of the Loyalka method for the case of the diffuse-specular model of molecule scattering at the wall were also discussed in Refs. [26,27]. To obtain these coefficients the results of, respectively, the first- and second-order Chapman-Enskog approximations for the kinetic coefficients [10], expressed using rather cumbersome linear combinations of the so-called Chapman-Cowling Ω integrals, were used. We have carried out the calculations of the coefficients $\sigma_p, \sigma_T, \sigma_T^*$, and $\sigma_{12}^{(v)}$ using our results obtained above for a series of mixtures, which were taken for calculations in Ref. [27] within the hard-sphere model of molecules and the Lennard-Jones (12-6) potential model. It was shown that the calculation results of the present study are in agreement with the results [27] obtained by using the first-order Chapman-Enskog approximation. As an illustration, we give in Table II the values of the diffusion slip coefficients $\sigma_{12}^{(v)}$ that have been computed for a selection of binary gas mixture (N₂-H₂, N₂-Ar, N₂-O₂, N₂-CO₂) using the Lennard-Jones (12-6) potential model for the case when p =1 atm, T = 293 K, and $\kappa_1 = \kappa_2 = 1$. Similarly to Ref. [27] the relevant parameters for the potential model were taken from Refs. [51,53]. Table II also contains calculated values of the transport coefficients, which are necessary for calculations of the diffusion slip coefficients $\sigma_{12}^{(v)}$. For comparison the values of the similar dimensionless diffusion slip coefficients $c_{Dsl}(1)$ and $c_{Dsl}(2)$, which have been computed in Refs. [27,3] using the first- and second-order Chapman-Enskog approximations, are also given in Table II. Note that the relative difference between the first- and second-order derived values is no more than 3.2%.

VI. DIFFUSION OF A GAS MIXTURE IN A PLANE CHANNEL

We note that the initial set of moment equations (6) can also be used to study diffusion in a gas mixture flow in a channel. Let us consider the flow of a gas mixture in a channel formed by two parallel, infinite plates. For convenience, a new variable x' = x - d/2, where d is the distance between the plates, will be used. Thus the coordinate x = 0 appearing in the previous



FIG. 1. The coordinate system for the problem.

consideration corresponds to the position of the lower plate (x' = -d/2) (see Fig. 1).

We will use Eq. (89) for the difference between the velocities of the mixture species $U_z = u_{1z} - u_{2z}$, which follows from the system of equations (70)–(73) in the 13-moment approximation. This equation, after substituting the new variable, is written as

$$\frac{\partial^2 U_z}{\partial x'^2} = s^2 \left(U_z - U_z^{as} \right), \quad U_z^{as} = \left[U_z^v \right]_2. \tag{152}$$

Solving this equation, taking into account the symmetry of the boundary conditions for the diffusion velocities,

$$U_z(-d/2) = U_z(d/2), \quad \left. \frac{\partial U_z}{\partial x'} \right|_{x'=0} = 0, \quad (153)$$

yields the following:

$$U_{z} = U_{z}(d/2) \frac{\cosh(sx')}{\cosh(sd/2)} + U_{z}^{as} \left[1 - \frac{\cosh(sx')}{\cosh(sd/2)} \right].$$
(154)

Let us consider this quantity averaged over the channel cross section:

$$\langle U_z \rangle = \frac{1}{d} \int_{-d/2}^{d/2} U_z(x') dx'.$$

Using Eq. (154), we find

$$\langle U_z \rangle = U_z^{as} \left[1 - \frac{2}{sd} \tanh(sd/2) \right] + U_z(d/2) \frac{2}{sd} \tanh(sd/2).$$
(155)

Using the condition $th(sd/2) \rightarrow 1$ when $sd \gg 1$, we have

$$\langle U_z \rangle = U_z^{as} + U_z(d/2) \frac{2}{sd}.$$
 (156)

It is important to mention here that $\langle U_z \rangle$ does not coincide with the regular value $U_z^{as} = [U_z^v]_2$ obtained by examining diffusion in a viscous flow of the mixture. The analysis conducted below shows that the quantity $U_z(d/2)$ in the additional term of the expression (156) contains the pressure gradient term with the coefficient proportional to the parameter *sd*. As a result, the second term in this expression contributes comparably to the quantity proportional to the pressure gradient in the expression (124) for $[U_z^v]_2$, which leads to the redefinition of the barodiffusion factor in the expression for $\langle U_z \rangle$. This actually means that the expression for the cross-section-averaged diffusion flux contains the contribution from the Knudsen layers. This fact was pointed out for the first time in the work by Breton [15], where the method of half-space moments was used for obtaining the fluxes of the mixture components in a flat channel. The corresponding analysis utilizing the method of full moments with the model of collision integral in the McCormack's form was also carried out in the work [59].

For evaluating $U_z(d/2)$ one can use the expressions obtained in Secs. III and IV. By considering that the values of the parameters $u_{\alpha z}$, $\pi_{\alpha z x}$, and $h_{\alpha z}$ at the wall (x = 0) in the slip problem, described above, coincide with the values of these quantities at the lower wall of the channel (x' = -d/2), we have

$$u_{\alpha z}(d/2) = u_{\alpha z}(-d/2), \quad h_{\alpha z}(d/2) = h_{\alpha z}(-d/2),$$

$$\pi_{\alpha z x}(d/2) = -\pi_{\alpha z x}(-d/2).$$
(157)

Below for simplicity we will restrict our consideration to the 10-moment approximation, since the contribution of the Knudsen layer to the value of the barodiffusion factor is already fully observed in this approximation. It is convenient then to define the quantity $U_z(d/2)$ using the expression for the partial viscous stress tensor π_{1zx} (69a), which takes the following form at the wall (x = 0):

$$\pi_{1zx}|_{x=0} = -\eta_1 \frac{\partial u_z^{as}}{\partial x} - \gamma_{12} s_0 \{ \left[U_z^v \right]_1 - \left. U_z \right|_{x=0} \}, \quad (158)$$

where $[U_z^v]_1$ is defined by Eq. (39). Expressing $U_z|_{x=0} = U_z(d/2)$ from Eq. (158) and using the relation $\partial u_z^{as}/\partial x = -(d/2\eta)dp/dz$, we have

$$U_{z}(d/2) = \frac{1}{\gamma_{12}s_{0}} \left[\pi_{1zx}(-d/2) - \frac{\eta_{1}}{\eta} \frac{d}{2} \frac{dp}{dz} \right] + \left[U_{z}^{v} \right]_{1}, \quad (159)$$

where $\pi_{1zx}(-d/2) = \pi_{1zx}|_{x=0}$.

It is convenient to transpose the coefficient $\gamma_{12}s_0$, writing it in the form $\gamma_{12}s_0^2/s_0$ and using the expression for s_0^2 (60). As a result, when $sd \gg 1$ the expression (156) is rewritten as

$$\langle U_z \rangle = \left[U_z^v \right]_1 + \frac{2}{d} \frac{[D_{12}]_1}{p y_1 y_2} \left[\pi_{1zx} (-d/2) - \frac{\eta_1}{\eta} \frac{d}{2} \frac{dp}{dz} \right].$$
(160)

The value $\pi_{1zx}(-d/2)$ at the lower plate is calculated using the relation

$$\pi_{1zx}|_{x=0} = 2\pi^{-3/2} p_1 \left[\int_{-\infty}^0 \int_{-\infty}^\infty \int_{-\infty}^\infty c_x c_z \times \phi_{\alpha}^-(\mathbf{c}, 0) \exp(-c^2) dc_x dc_y dc_z + \left[\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty c_x c_z \phi_{\alpha}^+(\mathbf{c}, 0) \times \exp\left(-c^2\right) dc_x dc_y dc_z \right].$$
(161)

Applying the 10-moment approximation and the modified Maxwell method, one can use the expression (115) for $\phi_1^-(\mathbf{c},0)$, in which the term that includes $h_{\alpha}^{as}(0)$ is omitted and the varied constant *a* is introduced instead of $u_z^{as}(0)$. Additionally, using

the boundary condition (107) for $\phi_{\alpha}^{+}(\mathbf{c}_{\alpha}, 0)$ and evaluating the corresponding integrals on the right-hand side of Eq. (161), we find

$$\pi_{1zx}|_{x=0} = -\pi^{-1/2} \beta_1^{1/2} p_1 \kappa_1 \left\{ a + \frac{m_2 y_2}{(m)_y} \left[U_z^v \right]_1 \right\} + \frac{1}{2} \kappa_1 \frac{\eta_1}{\eta} \frac{d}{2} \frac{dp}{dz},$$
(162)

The constant *a* has the form of the right-hand side of the expression (119), in which the terms corresponding to the 10-moment approximation are retained. In the case $\kappa_1 = \kappa_2 = \kappa$, we have

$$a = -\left(\frac{\pi kT}{2}\right)^{1/2} \frac{1}{p} \frac{2-\kappa}{\kappa} \frac{1}{(m^{1/2})_y} \frac{d}{dz} \frac{dp}{dz} - \frac{m_2 m_1^{1/2} - m_1 m_2^{1/2}}{(m^{1/2})_y (m)_y} y_1 y_2 [U_z^v]_1.$$
(163)

We have used the relation (118) and the condition $\partial u_z^{as}/\partial x = -(d/2\eta)dp/dz$, when writing Eqs. (162) and (163), so that

$$\pi_{1_{zx}}^{as}(0) = -\eta_1 \frac{\partial u_z^{as}}{\partial x} = \frac{\eta_1}{\eta} \frac{d}{2} \frac{dp}{dz}.$$

Simple analysis shows that after substituting the obtained expression for $\pi_{1zx}(-d/2) = \pi_{1zx}|_{x=0}$ into Eq. (160), one has to retain only those terms that are proportional to (d/2)dp/dz in the square brackets of this expression, since the remaining terms give a contribution that is proportional to the ratio (ℓ/d) , which is small compared to the contribution from the first term $[U_z^v]_1$ in Eq. (160). As a result, the expression for $\langle U_z \rangle$ can be expressed as

$$\langle U_z \rangle = -\frac{[D_{12}]_1}{y_1 y_2} \left\{ \frac{dy_1}{dz} + \left[\alpha_p^v \right]_1 y_1 y_2 \frac{1}{p} \frac{dp}{dz} - \left(1 - \frac{\kappa}{2} \right) \left[\frac{m_1^{1/2} y_1}{(m^{1/2})_y} - \frac{\eta_1}{\eta} \right] \frac{1}{p} \frac{dp}{dz} \right\}$$

or, rearranging it to its final form,

$$\langle U_z \rangle = -\frac{[D_{12}]_1}{y_1 y_2} \left\{ \frac{dy_1}{dz} + [\bar{\alpha}_p]_1 y_1 y_2 \frac{1}{p} \frac{dp}{dz} \right\}, \quad (164)$$

where

$$[\bar{\alpha}_p]_1 = \left(1 - \frac{\kappa}{2}\right) \frac{m_2^{1/2} - m_1^{1/2}}{(m^{1/2})_y} + \frac{\kappa}{2} [\alpha_p^v]_1.$$
(165)

It is well known that according to the principles of nonequilibrium thermodynamics of the discontinuous systems [34] we can write the relations between the cross-section-averaged fluxes in the channels and the gradients of thermodynamic parameters for isothermal flow of a binary gas mixture $(\nabla_z T = 0)$ as

$$\left\langle u_{z}^{m}\right\rangle = -\Lambda_{mm}\frac{1}{T}\frac{dp}{dz} - \Lambda_{m1}\frac{p}{T}\frac{dy_{1}}{dz},$$
(166)

$$\langle U_z \rangle = -\Lambda_{1m} \frac{1}{T} \frac{dp}{dz} - \Lambda_{11} \frac{p}{T} \frac{dy_1}{dz}, \qquad (167)$$

where u_z^m is the molar-averaged mixture velocity related to the mass-averaged velocity u_z through Eq. (133). Comparison

of the pair of equations (166) and (167) with the pair of equations (148) and (164) leads to the following relations:

$$\Lambda_{mm} = \frac{d^2 T}{12\eta} \left(1 + \sigma_p \frac{l_p}{d} \right), \quad \Lambda_{11} = \frac{T}{p} \frac{[D_{12}]_1}{y_1 y_2},$$
$$\Lambda_{m1} = -\frac{T}{p} [\sigma_{12}]_1 [D_{12}]_1, \quad \Lambda_{1m} = \frac{T}{p} [\bar{\alpha}_p]_1 [D_{12}]_1. \quad (168)$$

For simplicity, the terms in the expression for Λ_{mm} , quadratic in the Knudsen number, are omitted. The value $[\sigma_{12}]_1$ is in agreement with the diffusion slip coefficient (139) calculated in a 10-moment approximation when $\delta = \delta' = 0$. Note that the cross coefficients Λ satisfy the Onsager's reciprocity relations ($\Lambda_{1m} = \Lambda_{m1}$), from which it follows that $[\bar{\alpha}_p]_1 = -[\sigma_{12}]_1$. Hence the barodiffusion factor is equal (with the opposite sign) to the diffusion slip coefficient. It is evident that the similar relation is valid in any approximations. Direct evaluation of $[\bar{\alpha}_p]_2$ was performed in Refs. [35,36] by using the method when the initial moment equations are averaged over the channel cross section. It was found that in the 13-moment approximation,

$$[\bar{\alpha}_p]_2 = -[\sigma_{12}]_2 = \left(1 - \frac{\kappa}{2}\right) \left[\frac{m_2^{1/2} - m_1^{1/2}}{(m^{1/2})_y} - \delta\right] + \frac{\kappa}{2} [\alpha_p^v]_2.$$
(169)

VII. CONCLUSIONS

Our study revealed that the use of the linearized moment equations following from the Boltzmann equation leads to a reliable description of the slip phenomena in a gas mixture. The expressions for the macroscopic velocities of gas mixture species, the partial viscous stress tensors, and reduced heat fluxes as a function of the x coordinate normal to the flat wall are obtained as the result of exact solution of the linearized moment equations in the 10-moment and 13-moment approximations. The obtained expressions contain the terms that are proportional to $\exp(-sx)$, which corresponds to the contribution of the thin Knudsen layer, having the thickness on the order of $\delta = 1/s$ equal to several characteristic mean free paths of the molecules. Beyond this layer or when $sx \to \infty$ the asymptotic value of the mass-averaged velocity of the binary mixture u_z^{as} behaves as a linear function in x. The value of the velocity u_z^{as} , linearly extrapolated to the wall, is defined as the slip velocity of the gas mixture at the wall, $u_z^{as}(0)$. The modified Maxwell method (the approximation Loyalka method) is then used to obtain the general relation for the slip velocity and for the viscous, thermal, and diffusion slip coefficients for the case of the diffuse-specular model of molecule scattering at the wall. The simple, accurate expressions for the latter quantities are presented, which are given in terms of the basic transport coefficients and are convenient for practical calculations. The obtained relation for the slip velocity differs from the well-known results [22,27], which were derived by using the first-order (non-Burnett) Chapman-Enskog expansions, in that it contains some new terms (barodiffusion and baroslip), which are essential in the presence of the pressure gradient in gas mixture and corresponds to the second-order slip effects.

The solutions of moment equations are also found to be useful for analyzing the flow and diffusion of a gas mixture

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in channels with various geometry for the case of moderately small Knudsen numbers. The fundamental result is that the barodiffusion factor in the cross-section-averaged diffusion flux contains the contributions associated with the viscous transfer of momentum in the gas mixture and with the effect of the Knudsen layer.

Note that the moment equations of higher order (for example, the equations of the 20-moment approximation) or the regularized 13-moment and 26-moment equations can be used for more correct description of the second-order slip phenomena and Knudsen layer effects on the diffusion and heat fluxes of a gas mixture in the channels. Such investigations are, however, left to future work.

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APPENDIX A

1. Coefficients H, Λ

$$H_{\alpha\alpha} = \frac{y_{\alpha}^{2}}{[\eta_{\alpha\alpha}]_{1}} + \sum_{\beta \neq \alpha} \frac{2y_{\alpha}y_{\beta}}{[\eta_{\alpha\beta}]_{1}} \frac{m_{\alpha}m_{\beta}}{(m_{\alpha} + m_{\beta})^{2}} \left(\frac{5}{3A_{\alpha\beta}^{*}} + \frac{m_{\beta}}{m_{\alpha}}\right),$$

$$H_{\alpha\beta} = -\frac{2y_{\alpha}y_{\beta}}{[\eta_{\alpha\beta}]_{1}} \frac{m_{\alpha}m_{\beta}}{(m_{\alpha} + m_{\beta})^{2}} \left(\frac{5}{3A_{\alpha\beta}^{*}} - 1\right), \quad \beta \neq \alpha. \quad (A1)$$

$$\Lambda_{\alpha\alpha} = \frac{y_{\alpha}^{2}}{[\lambda_{\alpha\alpha}]_{1}} + \sum_{\beta \neq \alpha} \frac{y_{\alpha}y_{\beta}}{2A_{\alpha\beta}^{*}(m_{\alpha} + m_{\beta})^{2}[\lambda_{\alpha\beta}]_{1}}$$

$$\times \left(\frac{15}{2}m_{\alpha}^{2} + \frac{25}{4}m_{\beta}^{2} - 3m_{\beta}^{2}B_{\alpha\beta}^{*} + 4m_{\alpha}m_{\beta}A_{\alpha\beta}^{*}\right),$$

$$\Lambda_{\alpha\beta} = \frac{m_{\alpha}m_{\beta}}{(m_{\alpha} + m_{\beta})^{2}} \frac{y_{\alpha}y_{\beta}}{2A_{\alpha\beta}^{*}[\lambda_{\alpha\beta}]_{1}} \left(\frac{55}{4} - 3B_{\alpha\beta}^{*} - 4A_{\alpha\beta}^{*}\right),$$

$$\beta \neq \alpha. \quad (A2)$$

 Viscosity and thermal conductivity coefficients of a simple gas comprising particles α (the first approximation)

$$[\eta_{\alpha\alpha}]_{1} = \frac{5}{16} \frac{(\pi m_{\alpha} k T)^{1/2}}{\pi \sigma_{\alpha\alpha}^{2} \Omega_{\alpha\alpha}^{(2,2)*}},$$

$$[\lambda_{\alpha\alpha}]_{1} = \frac{15}{4} \frac{k}{m_{\alpha}} [\eta_{\alpha\alpha}]_{1} = \frac{75}{64} k \frac{(\pi k T/m_{\alpha})^{1/2}}{\pi \sigma_{\alpha\alpha}^{2} \Omega_{\alpha\alpha}^{(2,2)*}}.$$
 (A3)

Coefficients, associated with interaction of disparate molecules (β ≠ α)

$$\begin{split} &[\eta_{\alpha\beta}]_1 = \frac{5}{3} \mu_{\alpha\beta} \frac{n[D_{\alpha\beta}]_1}{A_{\alpha\beta}^*} = \frac{5}{16} \frac{(2\pi \mu_{\alpha\beta} kT)^{1/2}}{\pi \sigma_{\alpha\beta}^2 \Omega_{\alpha\beta}^{(2,2)*}} \\ &[\lambda_{\alpha\beta}]_1 = \frac{15}{8} \frac{k}{\mu_{\alpha\beta}} [\eta_{\alpha\beta}]_1, \end{split}$$

$$[D_{\alpha\beta}]_{1} = \frac{3}{16n} \left[\frac{2\pi kT}{\mu_{\alpha\beta}} \right]^{1/2} \frac{1}{\pi \sigma_{\alpha\beta}^{2} \Omega_{\alpha\beta}^{(1,1)*}},$$
$$\mu_{\alpha\beta} = \frac{m_{\alpha}m_{\beta}}{m_{\alpha} + m_{\beta}}.$$
(A4)

4. Reduced Ω integrals

$$\Omega_{\alpha\beta}^{(lr)*} = \frac{\Omega_{\alpha\beta}^{lr}}{\left[\Omega_{\alpha\beta}^{lr}\right]_{h.sph}}.$$
(A5)

5. Chapman-Cowling's Ω integrals

$$\Omega_{\alpha\beta}^{lr} = \left(\frac{2\pi kT}{\mu_{\alpha\beta}}\right)^{1/2} \int_0^\infty \int_0^\pi \zeta^{2r+3} e^{-\zeta^2} (1 - \cos^\ell \chi) \\ \times \sigma_{\alpha\beta}(\zeta, \chi) \sin \chi d\chi d\zeta.$$
(A6)

6. Ω Integrals for the hard-sphere model

$$\left[\Omega_{\alpha\beta}^{lr}\right]_{h.sph} = \left(\frac{kT}{2\pi\mu_{\alpha\beta}}\right)^{1/2} \frac{1}{2}(r+1)! \left[1 - \frac{1 + (-1)^{\ell}}{2(\ell+1)}\right] \pi \sigma_{\alpha\beta}^2.$$
(A7)

7. Ratios of Ω^* integrals

$$A_{\alpha\beta}^{*} = \frac{\Omega_{\alpha\beta}^{(2,2)*}}{\Omega_{\alpha\beta}^{(1,1)*}}, \quad B_{\alpha\beta}^{*} = \frac{5\Omega_{\alpha\beta}^{(2,2)*} - 4\Omega_{\alpha\beta}^{(1,3)*}}{\Omega_{\alpha\beta}^{(1,1)*}},$$
$$C_{\alpha\beta}^{*} = \frac{\Omega_{\alpha\beta}^{(1,2)*}}{\Omega_{\alpha\beta}^{(1,1)*}}.$$
(A8)

8. Hard-sphere model of molecules

$$A^*_{\alpha\beta} = B^*_{\alpha\beta} = C^*_{\alpha\beta} = 1$$

APPENDIX B

1. Partial viscosity coefficients

$$\eta_{1} = \frac{y_{1}H_{22} - y_{2}H_{12}}{|H|} y_{1} = \frac{(1 + Z_{1\eta})}{X_{\eta} + Y_{\eta}} y_{1},$$

$$\eta_{2} = \frac{y_{2}H_{11} - y_{1}H_{21}}{|H|} y_{2} = \frac{(1 + Z_{2\eta})}{X_{\eta} + Y_{\eta}} y_{2},$$

$$Z_{1\eta} = \frac{3}{5}A_{12}^{*} \left[\frac{(m_{1} + m_{2})^{2}}{2m_{1}m_{2}} \frac{[\eta_{12}]_{1}}{[\eta_{22}]_{1}} y_{2} + \left(\frac{m_{1} + m_{2}}{m_{2}} y_{1} - 1\right) \right],$$

$$Z_{2\eta} = \frac{3}{5}A_{12}^{*} \left[\frac{(m_{1} + m_{2})^{2}}{2m_{1}m_{2}} \frac{[\eta_{12}]_{1}}{[\eta_{11}]_{1}} y_{1} + \left(\frac{m_{1} + m_{2}}{m_{1}} y_{2} - 1\right) \right],$$

$$X_{\eta} = \frac{y_{1}^{2}}{[\eta_{11}]_{1}} + \frac{y_{2}^{2}}{[\eta_{22}]_{1}} + \frac{2y_{1}y_{2}}{[\eta_{12}]_{1}},$$

$$Y_{\eta} = \frac{3}{5}A_{12}^{*} \left[\frac{y_{1}^{2}}{[\eta_{11}]_{1}} \frac{m_{1}}{m_{2}} + \frac{y_{2}^{2}}{[\eta_{22}]_{1}} \frac{m_{2}}{m_{1}} + \frac{2y_{1}y_{2}}{[\eta_{12}]_{1}} \frac{(m_{1} + m_{2})^{2}}{[\eta_{11}]_{1}[\eta_{22}]_{1}} \right].$$
(B1)

2. Total viscosity coefficient

$$\eta = \eta_1 + \eta_2 = \frac{1 + Z_{\eta}}{X_{\eta} + Y_{\eta}},$$

$$Z_{\eta} = Z_{1\eta} y_1 + Z_{2\eta} y_2 = \frac{3}{5} A_{12}^* \left(\frac{m_1}{m_2} y_1^2 + \frac{m_2}{m_1} y_2^2 + 2y_1 y_2 \left\{ \frac{(m_1 + m_2)^2}{4m_1 m_2} \left(\frac{[\eta_{12}]_1}{[\eta_{11}]_1} + \frac{[\eta_{12}]_1}{[\eta_{22}]_1} \right) - 1 \right\} \right).$$
(B2)

3. Partial thermal conductivity coefficients

$$\begin{split} \lambda_{1} &= \frac{y_{1}\Lambda_{22} - y_{2}\Lambda_{12}}{|\Lambda|} y_{1} = \frac{(1 + Z_{1\lambda})}{X_{\lambda} + Y_{\lambda}} y_{1}, \\ \lambda_{2} &= \frac{y_{2}\Lambda_{11} - y_{1}\Lambda_{21}}{|\Lambda|} y_{2} = \frac{(1 + Z_{2\lambda})}{X_{\lambda} + Y_{\lambda}} y_{2}, \\ Z_{1\lambda} &= y_{1}U^{(1)} + y_{2}U_{1}^{(Z)}, \quad Z_{2\lambda} = y_{2}U^{(2)} + y_{1}U_{2}^{(Z)}, \\ U^{(1)} &= \frac{4}{15}A_{12}^{*} - \frac{1}{12}\left(\frac{12}{5}B_{12}^{*} + 1\right)\frac{m_{1}}{m_{2}} + \frac{1}{2}\frac{(m_{1} - m_{2})^{2}}{m_{1}m_{2}}, \\ U^{(2)} &= \frac{4}{15}A_{12}^{*} - \frac{1}{12}\left(\frac{12}{5}B_{12}^{*} + 1\right)\frac{m_{2}}{m_{1}} + \frac{1}{2}\frac{(m_{2} - m_{1})^{2}}{m_{1}m_{2}}, \\ U_{1}^{(Z)} &= \frac{4}{15}A_{12}^{*}\left[\frac{(m_{1} + m_{2})^{2}}{2m_{1}m_{2}}\frac{[\lambda_{12}]_{1}}{[\lambda_{22}]_{1}} - 1\right] - \frac{1}{12}\left(\frac{12}{5}B_{12}^{*} + 1\right), \\ U_{2}^{(Z)} &= \frac{4}{15}A_{12}^{*}\left[\frac{(m_{1} + m_{2})^{2}}{2m_{1}m_{2}}\frac{[\lambda_{12}]_{1}}{[\lambda_{11}]_{1}} - 1\right] - \frac{1}{12}\left(\frac{12}{5}B_{12}^{*} + 1\right), \\ X_{\lambda} &= \frac{y_{1}^{2}}{[\lambda_{11}]_{1}} + \frac{2y_{1}y_{2}}{[\lambda_{12}]_{1}} + \frac{y_{2}^{2}}{[\lambda_{22}]_{1}}, \\ Y_{\lambda} &= \frac{y_{1}^{2}}{[\lambda_{11}]_{1}}U^{(1)} + \frac{2y_{1}y_{2}}{[\lambda_{12}]_{1}}U^{(Y)} + \frac{y_{2}^{2}}{[\lambda_{22}]_{1}}U^{(2)}, \\ U^{(Y)} &= \frac{4}{15}A_{12}^{*}\left(\frac{(m_{1} + m_{2})^{2}}{4m_{1}m_{2}}\frac{[\lambda_{12}]_{1}^{2}}{[\lambda_{11}]_{1}[\lambda_{22}]_{1}} - \frac{1}{12}\left(\frac{12}{5}B_{12}^{*} + 1\right) \\ &- \frac{5}{32A_{12}^{*}}\left(\frac{12}{5}B_{12}^{*} - 5\right)\frac{(m_{1} - m_{2})^{2}}{m_{1}m_{2}}. \end{split}$$
(B3)

4. Total thermal conductivity coefficients

$$\lambda = \lambda_1 + \lambda_2 = \frac{1 + Z_{\lambda}}{X_{\lambda} + Y_{\lambda}},$$

$$Z_{\lambda} = Z_{1\lambda}y_1 + Z_{2\lambda}y_2$$

$$= y_1^2 U^{(1)} + y_1 y_2 (U_1^{(Z)} + U_2^{(Z)}) + y_2^2 U^{(2)}.$$
 (B4)

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5. Barodiffusion factor

a. First approximation

$$\begin{bmatrix} \alpha_p^v \end{bmatrix}_1 = \frac{Z_{2\eta} - Z_{1\eta}}{1 + Z_\eta} = \frac{3}{5} A_{12}^* \frac{(m_1 + m_2)^2}{2m_1 m_2} \frac{K_1 y_1 - K_2 y_2}{1 + Z_\eta},$$

$$K_1 = \frac{[\eta_{12}]_1}{[\eta_{11}]_1} - \frac{2m_1}{m_1 + m_2},$$

$$K_2 = \frac{[\eta_{12}]_1}{[\eta_{22}]_1} - \frac{2m_2}{m_1 + m_2}.$$
(B5)

b. Second approximation

$$\begin{split} \left[\alpha_{p}^{v}\right]_{2} &= \left[\alpha_{p}^{v}\right]_{1}(1-\Delta_{p}) - \frac{2}{5}[\alpha_{T}]_{1}, \\ \Delta_{p} &= \frac{2}{5} \left\{\frac{m_{2}-m_{1}}{(m)_{y}} y_{1} y_{2}[\alpha_{T}]_{1} + \frac{m_{2}+m_{1}}{(m)_{y}} \frac{\Delta_{12}}{(6/5)C_{12}^{*}-1}\right\}, \\ (m)_{y} &= m_{1} y_{1} + m_{2} y_{2}. \end{split}$$
(B6)

6. Thermal diffusion factor

$$\begin{aligned} [\alpha_T]_1 &= \frac{1}{n[D_{12}]_1} \frac{\mu_{12}}{k} \left(\frac{6}{5}C_{12}^* - 1\right) \left(\frac{\lambda_2}{m_2 y_2} - \frac{\lambda_1}{m_1 y_1}\right) \\ &= \frac{5}{6} \frac{1}{[\lambda_{12}]_1} \frac{S^{(1)}y_1 - S^{(2)}y_2}{X_\lambda + Y_\lambda} \left(\frac{6}{5}C_{12}^* - 1\right), \\ S^{(1)} &= \frac{m_1 + m_2}{2m_2} \frac{[\lambda_{12}]_1}{[\lambda_{11}]_1} - \frac{15}{4A_{12}^*} \frac{m_2 - m_1}{2m_1} - 1, \\ S^{(2)} &= \frac{m_1 + m_2}{2m_1} \frac{[\lambda_{12}]_1}{[\lambda_{22}]_1} - \frac{15}{4A_{12}^*} \frac{m_1 - m_2}{2m_2} - 1. \end{aligned}$$
(B7)

7. Second-order correction to binary diffusion coefficient

$$\Delta_{12} = \frac{5}{12} \frac{W}{X_{\lambda} + Y_{\lambda}} \left(\frac{6}{5}C_{12}^{*} - 1\right)^{2},$$

$$W = \frac{y_{1}^{2}}{[\lambda_{11}]_{1}} \frac{m_{1}}{m_{2}} + \frac{2y_{1}y_{2}}{[\lambda_{12}]_{1}} \left[1 + \frac{15}{8A_{12}^{*}} \frac{(m_{1} - m_{2})^{2}}{m_{1}m_{2}}\right]$$

$$+ \frac{y_{2}^{2}}{[\lambda_{22}]_{1}} \frac{m_{2}}{m_{1}}.$$
(B8)

The expressions for the total viscosity and thermal conductivity coefficients, thermal diffusion factor, and the secondorder correction to the binary diffusion coefficient coincide with those presented in the book [53] (see also [51,52]).

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