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Velocity slip and temperature jump coefficients for gaseous mixtures. IV. Temperature jump coefficient

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Abstract

The temperature jump coefficient was calculated for a binary gaseous mixture on the basis of the McCormack kinetic model of the Boltzmann equation, which was solved by the discrete velocity method. The calculations were carried out for the three mixtures of noble gases: neon–argon, helium–argon and helium–xenon. A strong influence of the intermolecular interaction on the temperature jump coefficient was observed by comparing the results based on the model of rigid spheres with those obtained for a realistic potential.

Keywords: Rarefied gases; Mixtures; Temperature jump; Knudsen layer

1. Introduction

Usually, to calculate a temperature distribution in a gas restricted by a solid surface the Fourier equation is applied with the temperature continuity condition on the gas-surface boundary, i.e. $T_g = T_w$, where T_g is the temperature of the gas near the surface and T_w is the surface temperature. It is correct when the Knudsen number is so small, say $Kn < 0.01$, that the gas rarefaction can be neglected. Note, the Knudsen number is defined as a ratio of the molecular mean-free-path to a characteristic size of the region occupied by gas. If the Knudsen number is not small then the Boltzmann kinetic equation [1–3] must be applied. A numerical solution of this equation requires much computational efforts. However, for a moderately small Knudsen number, i.e. when $Kn < 0.1$, the Fourier equation can be still applied but the gas rarefaction must be taken into account via the temperature jump boundary condition, which reads

$$T_g = T_w + \zeta_T \frac{\mu}{P}\left(\frac{2kT_w}{m}\right)^{1/2} \frac{\partial T}{\partial x'}\bigg|_{x'=0}, \tag{1}$$

where x' is the coordinate normal to the surface directed towards the gas with the origin at the surface, μ is the stress viscosity of the gas, P is the local pressure, m is the molecular mass of the gas, k is the Boltzmann constant. The dimensionless constant ζ_T is the temperature jump coefficient (TJC), which must be calculated applying the Boltzmann equation to the Knudsen layer.

Once the TJC is known, then the Fourier equation with the boundary condition (1) can be used for moderately small Knudsen numbers. Such an approach allows us to take into account a gas rarefaction and, at the

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same time, to avoid a numerical solving of the kinetic Boltzmann equation for every specific problem.

A knowledge of the TJC is necessary in many engineering fields such as aerothermodynamics of space vehicles, vacuum systems, microelectromechanical systems etc. Nowadays, the TJC is so important in practical calculations of heat transfer as the heat conductivity coefficient.

An estimation of the TJC can be found in the book by Kennard [4] who following Maxwell assumed that the incident molecules on a surface have the same distribution function as those in the midst of the gas. In other words, the distribution function does not vary in the Knudsen layer. As a result he obtained, see Eq. (238a) of Ref. [4],

$$\zeta_T = \frac{2-\alpha}{\alpha}\frac{\sqrt{\pi}\gamma}{(\gamma+1)Pr}, \quad Pr = \frac{\mu}{\kappa}c_p, \tag{2}$$

where α is the accommodation coefficient, γ is the specific heat ratio, Pr is the Prandtl number, κ is the thermal conductivity of the gas, and c_p is the specific heat at a constant pressure. For a monatomic gas ($Pr = 2/3$ and $\gamma = 5/3$) with a perfect accommodation ($\alpha = 1$) the expression (2) provides the value

$$\zeta_T = 1.662. \tag{3}$$

However, this is just an estimation because the assumption about the incident molecules is not fulfilled in reality. To calculate the TJC the variation of the distribution function in the Knudsen layer must be taken into account via the Boltzmann equation.

Many works devoted to numerical calculation of the TJC for a single gas, see e.g. Refs. [5–14], were published in the open literature. All of then report a value close to each other but different from the value given by Eq. (3). For instance, applying the S-model with the diffuse scattering the value

$$\zeta_T = 1.954 \tag{4}$$

was obtained in Ref. [14]. So, one can see that the variation of the distribution function in the Knudsen layer influences significantly the TJC. If one wants to obtain reliable results of heat transfer one has to use the rigorously obtained TJC instead of the approximate one given by Eq. (3).

Though in practice one deals with gaseous mixtures more often than with a single gas, there are very few works about this topic. Loyalka [15] obtained some analytical expressions of the TJC applying the moment method to the Boltzmann equation. Onishi [16], Siewert and Valougeorgis [17] solved the Hamel model equation [18]. However, this model does not provide the correct expressions of the transport coefficients and the results [16,17] based on it cannot be considered as reliable. At the same time, the McCormack model [19] yields all transport coefficients for a mixture, i.e. viscosity, thermal conductivity, diffusion, and thermal diffusion. That is why this model was successfully used in our recent publications [20–23]. Recently, Siewert [24] reported some results on the TJC for mixtures, but he considered just the hard sphere model of the intermolecular interaction.

The aim of the present paper is to calculate the TJC as a function of the molar concentration for some mixtures of the noble gases such as helium (He), neon (Ne), argon (Ar), and xenon (Xe). The calculations are based on the discrete velocity method applied to the McCormack model equation [19]. Two intermolecular interaction models are considered: hard spheres and realistic potential.

2. Statement of the problem

To calculate the TJC we consider a binary gaseous mixture occupying a semi-infinite space $x' \geqslant 0$ over an infinite solid surface fixed at $x' = 0$ and having a temperature T_w, which will be used as a reference (or equilibrium) temperature with the notation T_0. The mixture has a small temperature gradient ($\xi_T \ll 1$) normal to the surface, which is constant far from the surface, i.e.

$$T(x') \to T_0\left[1 + \left(\zeta_T + \frac{x'}{\ell_0}\right)\xi_T\right] \quad \text{at} \quad \frac{x'}{\ell_0} \to \infty, \tag{5}$$

where ℓ_0 is a quantity of the order of the mean free path defined as

$$\ell_0 = \frac{\mu v_0}{P_0}, \tag{6}$$

μ is the stress viscosity of the mixture at the equilibrium temperature, P_0 is the equilibrium pressure, v_0 is the characteristic molecular velocity at the temperature T_0,

$$v_0 = \left(\frac{2kT_0}{m}\right)^{1/2}, \tag{7}$$

m is the mean molecular mass of the mixture defined as

$$m = C_0 m_1 + (1 - C_0)m_2. \tag{8}$$

Here, m_α is the molecular mass of species α and C_0 is the equilibrium concentration

$$C_0 = \frac{n_{01}}{n_{01} + n_{02}}, \tag{9}$$

$n_{0\alpha}$ ($\alpha = 1, 2$) is the equilibrium number densities of species α.

So, the asymptotic behavior of the temperature (5) satisfies the boundary condition (1). The fact that the condition (1) is posed at $x' = 0$ seems to contradict to the fact that the TJC is calculated via the asymptotic behavior of the temperature at the infinity $(x'/\ell_0) \to \infty$ according to Eq. (5). The matter is that, the Knudsen layer is thick when compared with the mean free path.

At the same time, it is assumed to be very thin compared with a characteristic size of a region occupied by a mixture. The temperature on the boundary surface is assumed to be equal to that outside of the Knudsen layer. Thus, the condition (1) posed at $x' = 0$ from the macroscopic viewpoint corresponds to the asymptotic behavior of the temperature (5) far from the surface from the kinetic viewpoint.

Unlike the slip coefficients considered in Refs. [21,22], to calculate the TJC we cannot assume the concentration to be constant over the semi-space but we have to take into account a concentration gradient ξ_C far from the surface, which is established due to the temperature gradient ξ_T. So, the asymptotic behavior of the concentration has the form

$$C_\infty(x') = C_0\left(1 + \frac{x'}{\ell_0}\xi_C\right) \quad \text{at} \quad \frac{x'}{\ell_0} \to \infty. \tag{10}$$

This concentration gradient is established so as the thermal diffusion is compensated by the ordinary diffusion. As a result, both species of the mixture are at rest. Assuming the ordinary diffusion to be equal to the thermal diffusion the relation between the concentration gradient ξ_C and the temperature gradient ζ_T is obtained

$$\xi_C = (C_0 - 1)a_T\xi_T, \tag{11}$$

where a_T is the thermal diffusion factor given in Appendix A.

When the temperature and concentration gradients are established the normal heat flux can be calculated as

$$q_x = -\kappa\frac{T_0}{\ell_0}\xi_T, \tag{12}$$

where κ is the thermal conductivity coefficient of the mixture given in Appendix A, which takes into account the concentration gradient. Because of the heat conservation law the heat flux q_x does not vary in the whole space.

We are going to calculate the coefficient ζ_T for some mixtures of the noble gases as function of the equilibrium concentration C_0.

3. Input equation

For further derivations it is convenient to introduce the following dimensionless quantities:

$$x = \frac{x'}{\ell_0}, \quad \mathbf{c}_\alpha = \left(\frac{m_\alpha}{2kT_0}\right)^{1/2}\mathbf{v}_\alpha, \tag{13}$$

where $\mathbf{v}_\alpha$ is the molecular velocity of species α.

Since we assumed the temperature gradient to be small, the distribution function $f_\alpha(\mathbf{r}, \mathbf{c})$ of each species α can be linearized as

$$f_\alpha(\mathbf{r}, \mathbf{c}) = f_\alpha^M(x, \mathbf{c})[1 + h_\alpha(x, \mathbf{c})\xi_T], \tag{14}$$

where f_α^M is the local Maxwellian corresponding to the state of the mixture at the infinity, i.e.,

$$f_\alpha^M(x, \mathbf{c}) = n_{\infty\alpha}(x)\left[\frac{m_\alpha}{2\pi kT_\infty(x)}\right]^{3/2}\exp\left[-\frac{c_\alpha^2}{T_\infty(x)/T_0}\right], \tag{15}$$

$$T_\infty(x) = T_0[1 + x\xi_T], \tag{16}$$

$$n_{\infty\alpha} = n_{0\alpha}[1 - x\xi_T(1 + \eta_\alpha)], \tag{17}$$

$$\eta_1 = (1 - C_0)a_T, \quad \eta_2 = -C_0a_T. \tag{18}$$

Note, Eq. (17) takes into account the fact that the pressure of the mixture does not vary far from the surface, while the concentration has the gradient given by Eq. (11).

The perturbation functions h_α obey the two coupled Boltzmann equations [1,2], which for the problem in question read

$$c_{\alpha x}\frac{\partial h_\alpha}{\partial x} = \ell_0\left(\frac{m_\alpha}{2kT_0}\right)^{1/2}\sum_{\beta=1}^{2}\widehat{L}_{\alpha\beta}h_\alpha - c_{\alpha x}\left(c_\alpha^2 - \frac{5}{2} - \eta_\alpha\right), \quad \alpha = 1, 2. \tag{19}$$

$\widehat{L}_{\alpha\beta}h_\alpha$ is the linearized collision operator between species α and β. Like the previous works [20–23], here we also apply the McCormack model kinetic equation [19], which provides reliable results but requires modest computational efforts. For the problem under question the collision operator is written as

$$\begin{aligned}\widehat{L}_{\alpha\beta}h_\alpha = {} & -\gamma_{\alpha\beta}h_\alpha + \gamma_{\alpha\beta}\upsilon_\alpha - \left(\frac{m_\alpha}{m}\right)^{1/2}\nu_{\alpha\beta}^{(2)}\left(q_\alpha - \frac{m_\alpha}{m_\beta}q_\beta\right)c_{\alpha x} \\ & + \left[\gamma_{\alpha\beta}\tau_\alpha - 2\frac{m_{\alpha\beta}}{m_\beta}(\tau_\alpha - \tau_\beta)\nu_{\alpha\beta}^{(1)}\right]\left(c_\alpha^2 - \frac{3}{2}\right) \\ & + 2[(\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(3)})\Pi_{\alpha xx} + \nu_{\alpha\beta}^{(4)}\Pi_{\beta xx}] \\ & \times\left[c_{\alpha x}^2 - \frac{1}{2}(c_{\alpha y}^2 + c_{\alpha z}^2)\right] + \frac{8}{10}\left(\frac{m_\alpha}{m}\right)^{1/2} \\ & \times\left[(\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(5)})q_\alpha + \nu_{\alpha\beta}^{(6)}\left(\frac{m_\beta}{m_\alpha}\right)^{1/2}q_\beta\right] \\ & \times c_{\alpha x}\left(c_\alpha^2 - \frac{5}{2}\right),\end{aligned} \tag{20}$$

where $m_{\alpha\beta}$ is the reduced mass defined by Eq. (A.15). The quantities $\nu_{\alpha\beta}^{(k)}$ are given in Appendix A. The dimensionless moments of the distribution function are given as

$$\upsilon_\alpha(x) = \frac{1}{\pi^{3/2}}\int\exp(-c_\alpha^2)h_\alpha(x, \mathbf{c}_\alpha)\mathrm{d}\mathbf{c}_\alpha, \tag{21}$$

$$\tau_\alpha(x) = \frac{1}{\pi^{3/2}}\int\exp(-c_\alpha^2)h_\alpha(x, \mathbf{c}_\alpha)\left(\frac{2}{3}c_\alpha^2 - 1\right)\mathrm{d}\mathbf{c}_\alpha, \tag{22}$$

$$\Pi_{\alpha xx}(x) = \frac{1}{\pi^{3/2}} \int \exp(-c_\alpha^2) h_\alpha(x, \mathbf{c}_\alpha) \left(c_{\alpha x}^2 - \frac{1}{3} c_\alpha^2 \right) \mathrm{d}\mathbf{c}_\alpha, \tag{23}$$

$$q_\alpha(x) = \frac{1}{\pi^{3/2}} \left(\frac{m}{m_\alpha} \right)^{1/2} \int \exp(-c_\alpha^2) h_\alpha(x, \mathbf{c}_\alpha) c_{\alpha x} c_\alpha^2 \, \mathrm{d}\mathbf{c}_\alpha. \tag{24}$$

Applying the Chapman–Enskog method to the McCormack model we obtain the same expressions of the transport coefficients as those obtained from the exact Boltzmann equation [1,2]. The explicit expressions of the coefficients are given in Appendix A.

The relations of the dimensionless moments (21)–(24) to the corresponding dimensional quantities are as follows:

$$\frac{n_\alpha(x) - n_{\infty\alpha}(x)}{n_{0\alpha}\xi_\mathrm{T}} = \upsilon_\alpha(x), \quad \alpha = 1, 2, \tag{25}$$

$$\frac{T(x) - T_\infty(x)}{T_0 \xi_\mathrm{T}} = \tau(x) = C_0 \tau_1(x) + (1 - C_0)\tau_2(x), \tag{26}$$

$$\frac{P_{xx}(x)}{2P_0\xi_\mathrm{T}} = C_0 \Pi_{1xx}(x) + (1 - C_0)\Pi_{2xx}(x), \tag{27}$$

$$\frac{q_x}{P_0 v_0 \xi_\mathrm{T}} = C_0 q_1(x) + (1 - C_0) q_2(x), \tag{28}$$

where $n_\alpha(x)$ is the number density of species α, $T(x)$ is the temperature of the mixture and $P_{xx}(x)$ is the diagonal element of the pressure tensor of the mixture. In Eq. (20) we considered the isotropy in the plane yz, i.e.

$$\Pi_{\alpha yy} = \Pi_{\alpha zz}, \tag{29}$$

and the fact that the stress tensor is traceless, i.e.

$$\Pi_{\alpha xx} + \Pi_{\alpha yy} + \Pi_{\alpha zz} = 0. \tag{30}$$

With the help of Eqs. (12) and (28) the quantities q_1 and q_2 can be related to each other as

$$C_0 q_1(x) + (1 - C_0) q_2(x) = -\frac{m\kappa}{2k\mu}. \tag{31}$$

Using this equality we may reduce the number of unknown moments in the collision operator given by Eq. (20).

The parameters $\gamma_{\alpha\beta}$ are proportional to the collision frequency between species α and β and appear only in the combinations

$$\gamma_1 = \gamma_{11} + \gamma_{12}, \quad \gamma_2 = \gamma_{21} + \gamma_{22}. \tag{32}$$

Thus, it is sufficient to define γ_1 and γ_2 for which we use the same expressions as in the previous works [20–23], i.e.

$$\gamma_\alpha = \frac{P_{0\alpha}}{\mu_\alpha}, \tag{33}$$

where $P_{0\alpha}$ is the equilibrium partial pressure and μ_α is the partial viscosity given by Eq. (A.4).

We assumed the impermeability condition on the surface with the diffuse scattering of gaseous particles. Mathematically, it means that

$$h_\alpha(0, \mathbf{c}_\alpha) = \frac{2}{\pi} \int_{c'_{\alpha x} < 0} c'_{\alpha x} h_\alpha(0, c'_{\alpha x}) \exp(-c'^2_\alpha) \mathrm{d}\mathbf{c}'_\alpha \quad \text{for } c_{\alpha x} \geqslant 0. \tag{34}$$

According to the experimental data [25,26] and the theoretical results [14] the interaction of helium and neon with a glass surface differs from the diffuse one. However, our aim is to study the dependence of the TJC on the chemical composition of the mixture. That is why we restrict ourselves just by the diffuse reflection for all species.

Far from the surface i.e. $x \to \infty$, the perturbation functions are assumed to be spatial uniform, i.e.

$$\frac{\partial h_\alpha}{\partial x} = 0 \quad \text{at } x \to \infty. \tag{35}$$

The system of kinetic equations (19) with the boundary conditions (34) and (35) was solved by the discrete velocity method [27]. Once the equation is solved and the temperature profile is known then the TJC is calculated as

$$\zeta_\mathrm{T} = \lim_{x \to \infty} \tau(x), \tag{36}$$

which follows from Eqs. (5) and (26).

The TJC was calculated with the relative numerical error less than 0.1%. The numerical accuracy was estimated by comparing the results for different grid parameters.

The numerical calculations were carried out for the same mixtures considered in the previous works [21–23], namely, Ne–Ar, He–Ar and He–Xe. These mixtures have quite different molecular mass ratios and allow us to study the dependence of the TJC on this parameter.

The omega integrals $\Omega_{\alpha\beta}^{(ij)}$ determining the functions $v^{(k)}$ depend on the intermolecular potential. For the hard spheres they can be calculated analytically, see Eq. (A.16). The molecular diameters d_α of every species α being part of the integrals were calculated via the experimental data on the viscosities μ_α of the single gases He, Ne, Ar and Xe at the temperature $T = 300$ K given in Ref. [28]. The ratios of the diameters d_2/d_1 obtained from the viscosities are as follows: 1.406, 1.665, and 2.226 for the mixtures, Ne–Ar, He–Ar, and He–Xe, respectively.

However, in Refs. [22,23] it was found that the thermal and diffuse slip coefficients are very sensitive to the intermolecular potential and the same is expected for the TJC. To study this influence upon the TJC the so-called realistic potential was considered too. It means that the empirical expressions of the omega integrals $\Omega_{\alpha\beta}^{(ij)}$ given in Ref. [28] were used. These expressions determine the transport coefficients of the mixtures and reproduce them within an experimental error. The integrals were calculated assuming the temperature equal to 300 K.

4. Numerical results and discussion

The results of the numerical calculations for the three mixtures Ne–Ar, He–Ar and He–Xe are presented in Tables 1–3, respectively. The data corresponding to the rigid sphere model are given in the second columns of Tables 1–3. These values coincide with those reported by Siewert [24] obtained by the analytical discrete ordinate method. The results corresponding to the realistic potential are given in the fourth columns of Tables 1–3. Our results are compared with those obtained by Loyalka [15] applying the moment method to the Boltzmann equation. His results are given in the third and fifth columns of Tables 1–3 for the rigid sphere model and for the realistic potential, respectively. From these data we may conclude the following:

(i) At the limits corresponding to a single gas, i.e. $C_0 = 0$ and $C_0 = 1$, the TJC is exactly the same as that obtained from the S-model in Ref. [14] and given by Eq. (4). This is a natural result because the McCormack model is reduced to the S-model in the case of a single gas.

(ii) Like the thermal slip coefficient calculated in the previous work [22], the TJC is very sensitive to the intermolecular interaction potential. The difference between the TJC for the rigid sphere and that for the realistic potential reaches 3%, 12% and 26% for the mixtures Ne–Ar, He–Ar and He–Xe, respectively, i.e. the difference increases by increasing the molecular mass ratio m_2/m_1. For the rigid spheres the TJC has a non-monotone dependence on the concentration. It has a minimum near $C_0 = 0.5$ and a maximum near $C_0 = 0.9$. For the realist potential the TJC is always larger than that of a single gas. Thus, the intermolecular potential changes qualitatively the dependence of the TJC on the mixture concentration.

Table 1
Temperature jump coefficient ζ_T of the mixture Ne–Ar vs concentration C_0

C_0	ζ_T			
	Rigid spheres		Realistic potential	
	Present	Ref. [15]	Present	Ref. [15]
0.0	1.954	1.931	1.954	1.931
0.01	1.953	1.930	1.956	1.933
0.1	1.948	1.924	1.970	1.945
0.2	1.943	1.918	1.982	1.952
0.3	1.941	1.914	1.988	1.957
0.4	1.940	1.912	1.991	1.959
0.5	1.940	1.912	1.991	1.959
0.6	1.941	1.913	1.988	1.956
0.7	1.943	1.916	1.982	1.953
0.8	1.946	1.920	1.974	1.947
0.9	1.949	1.925	1.965	1.940
0.95	1.952	1.928	1.960	1.936
0.99	1.954	1.930	1.955	1.932
1.0	1.954	1.931	1.954	1.931

Table 2
Temperature jump coefficient ζ_T of the mixture He–Ar vs concentration C_0

C_0	ζ_T			
	Rigid spheres		Realistic potential	
	Present	Ref. [15]	Present	Ref. [15]
0.0	1.954	1.931	1.954	1.931
0.01	1.941	1.918	1.953	1.930
0.1	1.845	1.829	1.953	1.930
0.2	1.783	1.777	1.962	1.941
0.3	1.755	1.755	1.976	1.958
0.4	1.753	1.754	1.995	1.977
0.5	1.777	1.770	2.017	1.996
0.6	1.819	1.802	2.040	2.015
0.7	1.876	1.853	2.062	2.034
0.8	1.943	1.917	2.078	2.049
0.9	2.000	1.975	2.069	2.043
0.95	2.004	1.979	2.036	2.012
0.99	1.971	1.948	1.977	1.954
1.0	1.954	1.931	1.954	1.931

Table 3
Temperature jump coefficient ζ_T of the mixture He–Xe vs concentration C_0

C_0	ζ_T			
	Rigid spheres		Realistic potential	
	Present	Ref. [15]	Present	Ref. [15]
0.0	1.954	1.931	1.954	1.931
0.01	1.943	1.920	1.990	1.965
0.1	1.884	1.871	2.203	2.156
0.2	1.873	1.876	2.330	2.279
0.3	1.893	1.908	2.413	2.369
0.4	1.934	1.955	2.472	2.439
0.5	1.992	2.009	2.515	2.492
0.6	2.067	2.070	2.544	2.523
0.7	2.158	2.144	2.556	2.530
0.8	2.263	2.236	2.540	2.509
0.9	2.347	2.318	2.458	2.428
0.95	2.312	2.284	2.339	2.311
0.99	2.090	2.065	2.085	2.060
1.0	1.954	1.931	1.954	1.931

(iii) Comparing our results with those obtained by Loyalka in Ref. [15] applying the moment method to the Boltzmann equation we conclude that both methods provide the same qualitative behavior of the TJC. Quantitatively, there is a difference between our results and those obtained in Ref. [15]. The maximum difference between the values obtained by the two methods is about 1% for the rigid sphere model and 2% for the realistic potential for all mixtures considered here. So, we can say that the results obtained by two different methods for both potentials are in a good agreement with each other, i.e. the TJC is not sensitive to the method of solution.

(iv) Small quantity of the heavy component in a mixture changes significantly the value of the TJC. For instance, the mixture He–Xe with the concentration $C_0 = 0.99$ contains just 1% of Xe, while the TJC of this mixture differs from that for a single gas for 7%.

To show how much is the variation of the moments in the Knudsen layer we introduce the following two quantities:

$$\upsilon(x) = \frac{n(x) - n_\infty(x)}{n_0 \xi_\mathrm{T}} = C_0 \upsilon_1(x) + (1 - C_0)\upsilon_2(x), \tag{37}$$

$$\chi(x) = \frac{C(x) - C_\infty(x)}{C_0 \xi_\mathrm{T}} = \upsilon_1(x) - \upsilon(x). \tag{38}$$

The quantity $\upsilon(x)$ is the deviation of the total number density, i.e. $n(x) = n_1(x) + n_2(x)$ from its asymptotic behavior $n_\infty(x)$ given as

$$n_\infty(x) = n_{\infty 1}(x) + n_{\infty 2}(x) = n_0(1 - x\xi_\mathrm{T}), \tag{39}$$

where Eq. (17) has been used. The quantity $\chi(x)$ corresponds to the concentration deviation from its asymptotic behavior given by Eq. (10). The temperature deviation $\tau(x)$ has been defined above by Eq. (26).

The deviations $\tau(x)$, $\upsilon(x)$ and $\chi(x)$ for some values of the concentration are given in Tables 4–6 for the mixtures Ne–Ar, He–Ar and He–Xe, respectively. The second and third columns correspond to a single gas. From these data we can see that in all cases

$$\lim_{x\to\infty} \tau(x) = -\lim_{x\to\infty} \upsilon(x). \tag{40}$$

Physically, it means that no pressure deviation from its equilibrium value P_0 far from the surface. However, near the surface $\tau + \upsilon \neq 0$, i.e. there is a small deviation of the pressure from P_0. The variations of both temperature and density in the Knudsen layer are significant and depend on the chemical composition of mixture. That is why the neglect of the density distribution variation in the Knudsen layer made in the book [4] leads to the significant error. The concentration deviation χ in

Table 4
Temperature, density and concentration deviations for the mixture Ne–Ar (realistic potential)

x	$C_0 = 0$		$C_0 = 0.1$			$C_0 = 0.5$			$C_0 = 0.9$		
	τ	$-\upsilon$	τ	$-\upsilon$	$-\chi$	τ	$-\upsilon$	$-\chi$	τ	$-\upsilon$	$-\chi$
0.0	1.280	1.432	1.284	1.436	0.101	1.288	1.441	0.059	1.283	1.435	0.012
0.1	1.434	1.564	1.435	1.567	0.087	1.440	1.571	0.050	1.434	1.565	0.010
0.2	1.508	1.624	1.512	1.628	0.079	1.517	1.633	0.045	1.511	1.626	0.009
0.5	1.643	1.727	1.648	1.733	0.065	1.655	1.740	0.035	1.646	1.732	0.006
1.0	1.756	1.811	1.763	1.819	0.051	1.772	1.829	0.026	1.761	1.817	0.004
2.0	1.857	1.883	1.867	1.894	0.033	1.880	1.908	0.015	1.864	1.891	0.002
5.0	1.936	1.939	1.949	1.954	0.011	1.967	1.972	0.004	1.945	1.950	0.000
10.0	1.952	1.952	1.968	1.968	0.002	1.988	1.988	0.000	1.963	1.963	0.000
20.0	1.954	1.954	1.970	1.970	0.000	1.991	1.991	0.000	1.965	1.965	0.000

Table 5
Temperature, density and concentration deviations for the mixture He–Ar (realistic potential)

x	$C_0 = 0$		$C_0 = 0.1$			$C_0 = 0.5$			$C_0 = 0.9$		
	τ	$-\upsilon$	τ	$-\upsilon$	$-\chi$	τ	$-\upsilon$	$-\chi$	τ	$-\upsilon$	$-\chi$
0.0	1.280	1.432	1.273	1.424	0.029	1.292	1.443	0.052	1.344	1.501	0.019
0.1	1.434	1.564	1.499	1.551	0.015	1.433	1.565	0.046	1.493	1.630	0.018
0.2	1.508	1.624	1.494	1.610	0.010	1.506	1.624	0.043	1.570	1.692	0.016
0.5	1.643	1.727	1.627	1.713	0.005	1.641	1.731	0.037	1.710	1.802	0.013
1.0	1.756	1.811	1.741	1.797	0.004	1.761	1.822	0.030	1.833	1.894	0.009
2.0	1.857	1.883	1.844	1.872	0.006	1.877	1.908	0.020	1.947	1.978	0.005
5.0	1.936	1.939	1.929	1.934	0.007	1.982	1.988	0.007	2.042	2.048	0.001
10.0	1.952	1.952	1.949	1.950	0.003	2.011	2.012	0.001	2.065	2.066	0.000
20.0	1.954	1.954	1.953	1.953	0.000	2.017	2.017	0.001	2.069	2.069	0.000

Table 6
Temperature, density and concentration deviations for the mixture He–Xe (realistic potential)

x	$C_0 = 0$		$C_0 = 0.1$			$C_0 = 0.5$			$C_0 = 0.9$		
	τ	$-\upsilon$	τ	$-\upsilon$	$-\chi$	τ	$-\upsilon$	$-\chi$	τ	$-\upsilon$	$-\chi$
0.0	1.280	1.432	1.351	1.510	0.208	1.552	1.733	0.133	1.593	1.780	0.024
0.1	1.434	1.564	1.506	1.644	0.189	1.707	1.867	0.123	1.750	1.916	0.024
0.2	1.508	1.624	1.585	1.708	0.182	1.790	1.935	0.118	1.833	1.984	0.023
0.5	1.643	1.727	1.730	1.822	0.173	1.947	2.062	0.107	1.990	2.107	0.020
1.0	1.756	1.811	1.858	1.919	0.167	2.099	2.178	0.095	2.134	2.217	0.015
2.0	1.857	1.883	1.984	2.014	0.154	2.256	2.300	0.075	2.276	2.322	0.010
5.0	1.936	1.939	2.111	2.116	0.112	2.426	2.436	0.038	2.410	2.421	0.003
10.0	1.952	1.952	2.168	2.169	0.058	2.494	2.495	0.012	2.450	2.452	0.000
20.0	1.954	1.954	2.197	2.196	0.013	2.514	2.514	0.001	2.458	2.458	0.000

the Knudsen layer is small and tends to zero at the infinity.

5. Conclusions

The temperature jump coefficient was calculated as a function of the molar concentration for the three mixtures of the noble gases: Ne–Ar, He–Ar, and He–Xe. The calculations were carried out for two molecular models: hard spheres and realistic potential. It was found that the temperature jump coefficient is strongly sensitive to the intermolecular potential. So, reliable results on this coefficient can be obtained just on the basis of the realistic potential, while an application of the hard sphere model can give a qualitatively different dependence of the coefficient on the mixture concentration.

Comparison of the present results with those obtained by a different method showed that the temperature jump coefficient is weakly sensitive to the method of solution.

For the mixture with a high ratio of the molecular masses, e.g. He–Xe, this coefficient differs significantly from that for a single gas. That is why it is very important to use the reliable and rigorously obtained result on the temperature jump coefficient instead of that given by Eq. (2), which was obtained as an estimation in Ref. [4].

The variations of the temperature and number density in the Knudsen layer are significant and cannot be neglected.

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Appendix A. Expressions of the transport coefficients

The transport coefficients used to state the problem, namely, viscosity μ, thermal conductivity κ and thermal diffusion factor a_T, can be obtained from the Boltzmann equation applying the Chapman–Enskog method [1,2]. Their expressions are as follows:

$$\mu = \mu_1 + \mu_2, \tag{A.1}$$

$$\kappa = \kappa_1 + \kappa_2, \tag{A.2}$$

$$a_T = -\frac{5}{4}\frac{n\nu_{12}^{(2)}}{n_2}\left[a_{T1} - \left(\frac{m_1}{m_2}\right)^2 a_{T2}\right], \tag{A.3}$$

$$\mu_\alpha = P_\alpha(\Psi_\beta + \nu_{\alpha\beta}^{(4)})(\Psi_\alpha\Psi_\beta - \nu_{\alpha\beta}^{(4)}\nu_{\beta\alpha}^{(4)})^{-1}, \tag{A.4}$$

$$a_{T\alpha} = \left[\Phi_\beta + \left(\frac{m_\alpha}{m_\beta}\right)^{1/2}\nu_{\alpha\beta}^{(6)}\right](\Phi_\alpha\Phi_\beta - \nu_{\alpha\beta}^{(6)}\nu_{\beta\alpha}^{(6)})^{-1}, \tag{A.5}$$

$$\Psi_\alpha = \nu_{\alpha\alpha}^{(3)} - \nu_{\alpha\alpha}^{(4)} + \nu_{\alpha\beta}^{(3)}, \tag{A.6}$$

$$\Phi_\alpha = \nu_{\alpha\alpha}^{(5)} - \nu_{\alpha\alpha}^{(6)} + \nu_{\alpha\beta}^{(5)}, \tag{A.7}$$

$$\kappa_\alpha = \frac{5}{2}\frac{P_\alpha k}{m_\alpha}a_{T\alpha}. \tag{A.8}$$

$\beta \neq \alpha$ in Eqs. (A.4)–(A.7).

$$\nu_{\alpha\beta}^{(1)} = \frac{16}{3}\frac{m_{\alpha\beta}}{m_\alpha}n_\beta\Omega_{\alpha\beta}^{(11)}, \tag{A.9}$$

$$\nu_{\alpha\beta}^{(2)} = \frac{64}{15}\left(\frac{m_{\alpha\beta}}{m_\alpha}\right)^2 n_\beta\left(\Omega_{\alpha\beta}^{(12)} - \frac{5}{2}\Omega_{\alpha\beta}^{(11)}\right), \tag{A.10}$$

$$\nu_{\alpha\beta}^{(3)} = \frac{16}{5}\frac{m_{\alpha\beta}^2}{m_\alpha m_\beta}n_\beta\left(\frac{10}{3}\Omega_{\alpha\beta}^{(11)} + \frac{m_\beta}{m_\alpha}\Omega_{\alpha\beta}^{(22)}\right), \tag{A.11}$$

$$\nu_{\alpha\beta}^{(4)} = \frac{16}{5}\frac{m_{\alpha\beta}^2}{m_\alpha m_\beta}n_\beta\left(\frac{10}{3}\Omega_{\alpha\beta}^{(11)} - \Omega_{\alpha\beta}^{(22)}\right), \tag{A.12}$$

$$\nu^{(5)}_{\alpha\beta} = \frac{64}{15}\left(\frac{m_{\alpha\beta}}{m_\alpha}\right)^3 \frac{m_\alpha}{m_\beta} n_\beta \left[\Omega^{(22)}_{\alpha\beta} + \left(\frac{15}{4}\frac{m_\alpha}{m_\beta} + \frac{25}{8}\frac{m_\beta}{m_\alpha}\right)\Omega^{(11)}_{\alpha\beta} - \frac{1}{2}\frac{m_\beta}{m_\alpha}\left(5\Omega^{(12)}_{\alpha\beta} - \Omega^{(13)}_{\alpha\beta}\right)\right], \tag{A.13}$$

$$\nu^{(6)}_{\alpha\beta} = \frac{64}{15}\left(\frac{m_{\alpha\beta}}{m_\alpha}\right)^3 \left(\frac{m_\alpha}{m_\beta}\right)^{3/2} n_\beta \left[-\Omega^{(22)}_{\alpha\beta} + \frac{55}{8}\Omega^{(11)}_{\alpha\beta} - \frac{5}{2}\Omega^{(12)}_{\alpha\beta} + \frac{1}{2}\Omega^{(13)}_{\alpha\beta}\right], \tag{A.14}$$

$$m_{\alpha\beta} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}. \tag{A.15}$$

$\Omega^{(ij)}_{\alpha\beta}$ are the Chapman–Cowling integrals [2], which depend on the intermolecular interaction potential. For the rigid spheres model these integrals read

$$\Omega^{(ij)}_{\alpha\beta} = \frac{(j+1)!}{8}\left[1 - \frac{1+(-1)^i}{2(i+1)}\right]\left(\frac{\pi k T}{2m_{\alpha\beta}}\right)^{1/2}(d_\alpha + d_\beta)^2, \tag{A.16}$$

where d_α is the molecular diameter of specie α. For the realistic potential the Chapman–Cowling integrals are calculated from the expressions given in Ref. [28].

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