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TEMPERATURE JUMP IN RAREFIED GASEOUS SYSTEMS

Denize Kalempa
Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, 81531-990, Curitiba, Brazil
`kalempa@fisica.ufpr.br`

Felix Sharipov
Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, 81531-990, Curitiba, Brazil
`sharipov@fisica.ufpr.br`

Abstract. *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. It is correct when the Knudsen number, defined as the ratio between the molecular mean free path and a characteristic scale of the gas flow, is so small that the gas rarefaction can be neglected. If the Knudsen number is not small then the Boltzmann equation must be applied. A numerical solution of this equation requires much computational efforts. However, for a moderately small Knudsen number, the Fourier equation can be still applied but the gas rarefaction must be taken into account via the temperature jump boundary condition. This condition is introduced via the temperature jump coefficient. The knowledge of this coefficient is very important in many engineering fields such as aerothermodynamics of space vehicles, vacuum systems, mechanical and electrical microsystems (MEMS) and in many other situations where the Knudsen number is not so small to neglect the gas rarefaction. The aim of the present work is to calculate the temperature jump coefficient for gaseous mixtures because in practice one deals with mixtures more often than a single gas. A study of the influence of the intermolecular interaction potential and chemical composition upon this coefficient is also presented. This work also show us how to avoid a numerical solving of the kinetic Boltzmann equation for a specific problem and, at the same time, take into account a gas rarefaction.*

keywords: *temperature jump, Boltzmann equation, rarefied gas mixtures, Fourier equation*

1. Introduction

Usually, to calculate the 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 Kn, defined as the ratio between the molecular mean free path and a characteristic scale of the gas flow, is so small, say $Kn < 0.01$, that the gas rarefaction can be neglected. If the Knudsen number is in the range $0.01 \leq Kn \leq 0.1$ the gas rarefaction can not be neglected and the Fourier equation with the temperature continuity condition can not be applied because there is a temperature jump on the gas-surface boundary. In this range of the Knudsen number the Boltzmann equation must be solved but its solution is very difficult and requires much computational efforts. To avoid the solution of the Boltzmann equation and to consider the gas rarefaction we can solve que Fourier equation with the temperature jump boundary condition, which reads

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

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 mixture, P is the local pressure of the mixture, m is the mean molecular mass of the mixture and k is the Boltzmann constant. The dimensionless quantity ζ_{T} is the temperature jump coefficient, which must be calculated applying the Boltzmann equation. When ζ_{T} is known the Fourier equation with the temperature jump condition (1) can be solved.

A knowledge of the temperature jump coefficient is very important in many engineering fields such as aerothermodynamics of space vehicles, vaccum systems, mechanical and electrical microsystems (MEMS) and in many other situations where the gas rarefaction can not be neglected.

Nowadays there are many works devoted to numerical calculation of the temperature jump coefficient for a single gas, see e.g. Refs. (Loyalka, 1989; Sone et al., 1989; Barichello and Siewert, 2000; Siewert, 2003) in the open literature. In practice one deals with gaseous mixtures more often than with a single gas and there are very few work about this topic, see e.g. Refs. (Loyalka, 1974; Onishi, 1997).

The aim of the present work is to calculate the temperature jump coefficient $\zeta_{\rm T}$ 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 (Sharipov and Subbotin, 1993) applied to the McCormack model equation (McCormack, 1973). A study fo the influence of the intermolecular interaction potential and chemical composition upon this coefficient is presented.

2. Methodology

To calculate the temperature jump coefficient we consider a binary gaseous mixture occupying a semi-infinite space $x' \geq 0$ over an infinite solid surface fixed at $x' = 0$ and having a temperature $T_w = T_0$. The mixture has a small temperature gradient $\xi_{\rm T}$ normal to the surface, which is constant far from the surface, i.e.,

$$T(x') = T_0 \left[1 + \left(\zeta_{\rm T} + \frac{x'}{\ell_0} \right) \xi_{\rm T} \right], \quad \text{at} \quad x' \to \infty, \tag{2}$$

where

$$\ell_0 = \frac{\mu v_0}{P_0}, \qquad v_0 = \left(\frac{2kT_0}{m} \right)^{1/2}, \tag{3}$$

is the mean free path. The quantity v_0 is a characteristic molecular velocity and

$$m = C_0 m_1 + (1 - C_0) m_2 \tag{4}$$

is the mean molecular mass of the mixture. The quantity m_α ($\alpha = 1, 2$) is the molecular mass of specie α and C_0 is the equilibrium concentration defined as

$$C_0 = \frac{n_{01}}{n_{01} + n_{02}}, \tag{5}$$

where $n_{0\alpha}$ is the equilibrium number density of specie α.

The concentration of the mixture is not constant and we have to take into account a concentration gradient $\xi_{\rm C}$ established due to the temperature gradient. So, the asymptotic behavior of the concentration has the form

$$\lim_{x' \to \infty} \frac{dC}{dx'} = \frac{C_0}{\ell_0} \xi_{\rm C} = const. \tag{6}$$

The 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 $\xi_{\rm C}$ and the temperature gradient $\xi_{\rm T}$ is the following

$$\xi_{\rm C} = -(1 - C_0) a_{\rm T} \xi_{\rm T}, \tag{7}$$

where $a_{\rm T}$ is the thermal diffusion factor.

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

$$q_x = -\kappa \frac{T_0}{\ell_0} \xi_{\rm T}, \tag{8}$$

where κ is the thermal conductivity coefficient of the mixture which includes both the heat flux through a mixture with an uniform concentration and the heat flux due to a concentration gradient. Because of the heat conservation law the heat flux q_x does not vary in the whole space.

To calculate the temperature jump coefficient $\zeta_{\rm T}$ we solved the McCormakc kinetic equation (McCormack, 1973). The first step to solve this equation consist of linearize the distribution function. Since we assumed the temperature gradient $\xi_{\rm T}$ to be small ($\xi_{\rm T} \ll 1$), the distribution function of each species can be linearized as

$$f_\alpha(\mathbf{r}, \mathbf{c}) = f_\alpha^M(x, \mathbf{c})[1 + h_\alpha(x, \mathbf{c}) \xi_{\rm T}], \qquad h_\alpha \ll 1, \tag{9}$$

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

$$f_\alpha^M(x, \mathbf{c}) = n_{\alpha\infty}(x) \left[\frac{m_\alpha}{2\pi k T_\infty(x)} \right]^{3/2} \exp \left[-\frac{c_\alpha^2}{T_\infty(x)/T_0} \right], \tag{10}$$

$$T_\infty(x) = T_0[1 + x\xi_{\mathrm{T}}], \tag{11}$$

$$n_{\alpha\infty} = n_{\alpha 0}[1 - x\xi_{\mathrm{T}}(1 + \eta_\alpha)], \tag{12}$$

$$\eta_1 = (1 - C_0)a_{\mathrm{T}}, \qquad \eta_2 = -C_0 a_{\mathrm{T}}. \tag{13}$$

Note that the following dimensionless quantities were introduced:

$$x = \frac{x'}{\ell_0}, \qquad \mathbf{c}_\alpha = \left(\frac{m_\alpha}{2kT}\right)^{1/2} \mathbf{v}_\alpha, \tag{14}$$

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

The perturbation function h_α obey the two coupled Boltzmann equations which for the problem in question read

$$c_{\alpha x}\frac{\partial h_\alpha}{\partial x} = \ell_0 \left(\frac{m_\alpha}{2kT_0}\right)^{1/2} \sum_{\beta=1}^{2} \hat{L}_{\alpha\beta} h_\alpha - c_{\alpha x}\left(c_\alpha^2 - \frac{5}{2} - \eta_\alpha\right), \qquad \alpha = 1, 2. \tag{15}$$

$\hat{L}_{\alpha\beta} h_\alpha$ is the linearized collision operator between species α and β. Here we used the McCormack model (McCormack, 1973) to write this operator as

$$\begin{aligned}\hat{L}_{\alpha\beta} h_\alpha = {} & -\gamma_{\alpha\beta} h_\alpha + \gamma_{\alpha\beta}\nu_\alpha - \left(\frac{m_\alpha}{m}\right)^{1/2} \nu_{\alpha\beta}^{(2)} \left(q_\alpha - \frac{m_\alpha}{m_\beta} q_\beta\right) c_{\alpha x} + \left[\gamma_{\alpha\beta}\tau_\alpha - 2\frac{m_{\alpha\beta}}{m_\beta}(\tau_\alpha - \tau_\beta)\nu_{\alpha\beta}^{(1)}\right]\left(c_\alpha^2 - \frac{3}{2}\right) \\ & + 2[(\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(3)})\Pi_{\alpha xx} + \nu_{\alpha\beta}^{(4)}\Pi_{\beta xx}]\left[c_{\alpha x}^2 - \frac{1}{2}(c_{\alpha y}^2 + c_{\alpha z}^2)\right] + \frac{8}{10}\left(\frac{m_\alpha}{m}\right)^{1/2} \left[(\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(5)})q_\alpha + \nu_{\alpha\beta}^{(6)} \right. \\ & \left. \times \left(\frac{m_\beta}{m_\alpha}\right)^{1/2} q_\beta\right] c_{\alpha x}\left(c_\alpha^2 - \frac{5}{2}\right),\end{aligned} \tag{16}$$

where $m_{\alpha\beta}$ is the reduced mass of the mixture, the dimensionless moments of the distribution function are given as

$$\nu_\alpha(x) = \frac{1}{\pi^{3/2}} \int \exp(-c_\alpha^2) h_\alpha(x, \mathbf{c}_\alpha)\, \mathrm{d}\mathbf{c}_\alpha, \tag{17}$$

$$\tau_\alpha(x) = \frac{1}{\pi^{3/2}} \int \exp(-c_\alpha^2) h_\alpha(x, \mathbf{c}_\alpha) \left(\frac{2}{3}c_\alpha^2 - 1\right) \mathrm{d}\mathbf{c}_\alpha, \tag{18}$$

$$\Pi_{\alpha xx}(x) = \frac{1}{\pi^{3/2}} \int \exp(-c_\alpha^2) h_\alpha(x, \mathbf{c}_\alpha) \left(c_{\alpha x}^2 - \frac{1}{3}c_\alpha^2\right) \mathrm{d}\mathbf{c}_\alpha, \tag{19}$$

$$q_\alpha(x) = \frac{1}{\pi^{3/2}} \left(\frac{m}{m_\alpha}\right)^{1/2} \int \exp(-c_\alpha^2) h_\alpha(x, \mathbf{c}_\alpha) c_{\alpha x} c_\alpha^2\, \mathrm{d}\mathbf{c}_\alpha. \tag{20}$$

The quantities $\nu_{\alpha\beta}^{(k)}$ are given in Ref. (Sharipov and Kalempa, 2002) and the parameters $\gamma_{\alpha\beta}$ are proportional to the collision frequency between species α and β and appear only in the combinations

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

We defined γ_1 and γ_2 as:

$$\gamma_\alpha = \frac{P_{0\alpha}}{\mu_\alpha}, \tag{22}$$

where $P_{0\alpha}$ is the equilibrium partial pressure and μ_α is the partial viscosity given in Ref. (Sharipov and Kalempa, 2002).

With the help of Eq. (8) we may reduce the number of unknown moments in the collision operator (16) using the following relation

$$C_0 q_1(x) + (1 - C_0) q_2(x) = -\frac{m\kappa}{2k\mu}. \tag{23}$$

To solve the system of kinetic equations (15) we assumed the impermeability condition on the surface with the diffuse scattering of gaseous particles, i.e.

$$h_\alpha(0,\mathbf{c}_\alpha) = \frac{2}{\pi}\int_{c'_{\alpha x}<0} c'_{\alpha x} h_\alpha(0,c'_{\alpha x}) \exp\left(-c'^2_\alpha\right) \mathrm{d}\mathbf{c}'_\alpha, \qquad c_{\alpha x} \geq 0, \tag{24}$$

and used the discrete velocity method (Sharipov and Subbotin, 1993). Once the equation is solved and the temperature profile is known then the temperature jump coefficient ζ_T is calculated as

$$\zeta_\mathrm{T} = \lim_{x\to\infty} \tau(x), \tag{25}$$

where

$$\tau(x) = C_0\tau_1 + (1-C_0)\tau_2. \tag{26}$$

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

3. Numerical results and discussion

The numericall calculation were carried out for the mixtures Ne-Ar, He-Ar and He-Xe. These mixtures have quite different atomic mass ratios and allow us to study the dependence of the temperature jump coefficient on this parameter.

The influence of the intermolecular interaction potential upon the temperature jump coefficient also was studied using two intermolecular interactions potentials: the rigid spheres model and a realistic potential. To calculate the molecular diameter d_α of every species α the experimental data on the viscosities μ_α of the single gases He, Ne, Ar and Xe at the temperature $T = 300K$ given in Ref. (Kestin et al., 1984) were used. For the realistic potential the Omega integrals $\Omega^{(ij)}_{\alpha\beta}$ that appear in the expressions for the quantities $\nu^{(k)}_{\alpha\beta}$ were calculated using the empirical expressions given in Ref. (Kestin et al., 1984) assuming the temperature equal to 300K. These expressions reproduce all transport coefficients of the mixtures within the experimental error.

The Figs. (1)-(3) show the results obtained in the present work for the temperature jump coefficient as a function of the concentration C_0 for both interaction potentials.

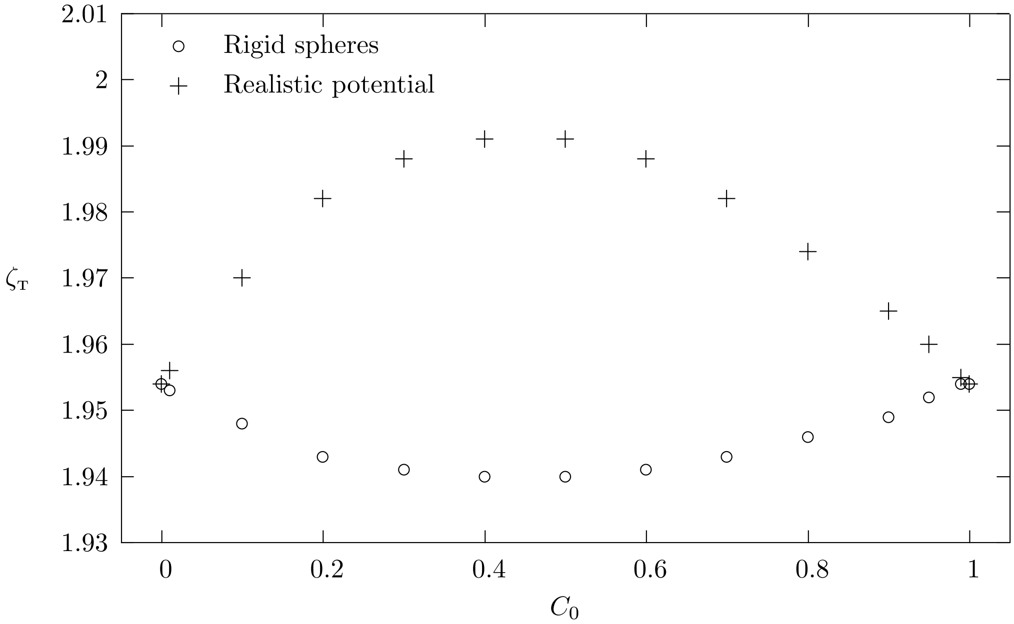

Figure 1: Mixture of Ne-Ar: temperature jump coefficient vs concentration

From these data we may conclude the following:

- At the limits corresponding to a single gas ($C_0 = 0$ and $C_0 = 1$) the temperature jump coefficient is exactly the same as that obtained from the Shakov model in Ref. (Sharipov, 2003). This is a natural result because the McCormack model is reduced to the Shakov model in the case of a single gas.

- This coefficient is very sensitive to the intermolecular interaction potential. The difference between $\zeta_{\rm T}$ 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 mass ratio m_2/m_1. For the rigid spheres $\zeta_{\rm T}$ has a non-monotone dependence on the concentration. It has a minimum near $C_0 = 0.5$ and a maximum near $C_0 = 0.99$. For the realistic potential $\zeta_{\rm T}$ is always larger than that of a single gas. Thus, the intermolecular interaction potential changes qualitatively the dependence of the temperature jump coefficient on the mixture concentration.

- As the temperature jump coefficient is very sensitive to the interaction potential so what results are more reliable? Since the diameters of each species for the rigid spheres were calculated from experimental data on the viscosity of the single gases they cannot provide a good agreement with experimental data on the other transport coefficients. At the same time, the realistic potential provides experimental values of all transport coefficients. Naturally, the results based on the realistic potential are more reliable than those based on the rigid spheres.

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

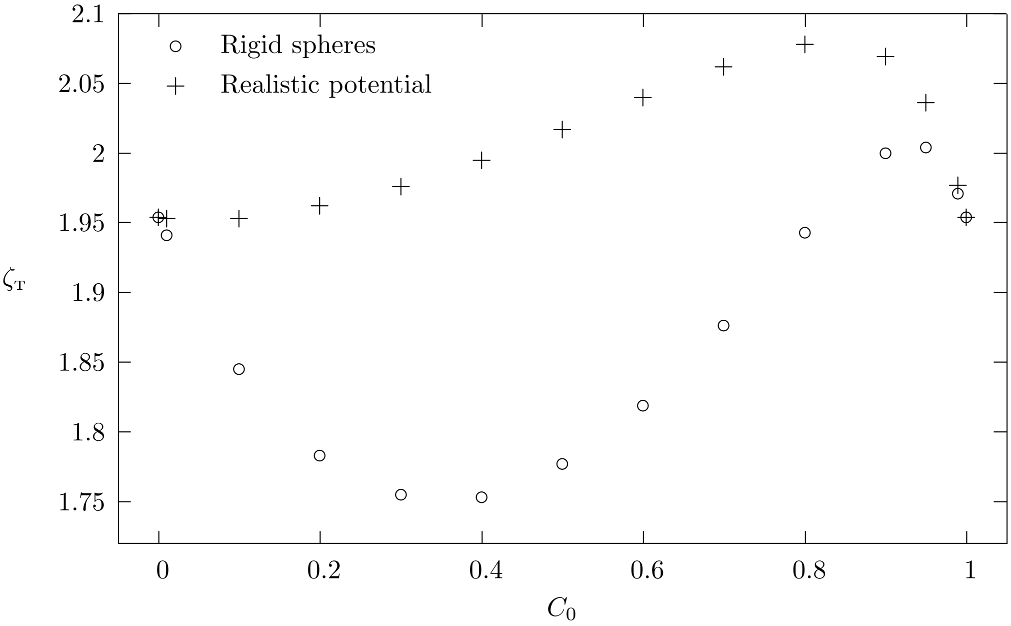

Figure 2: Mixture of He-Ar: temperature jump coefficient vs concentration

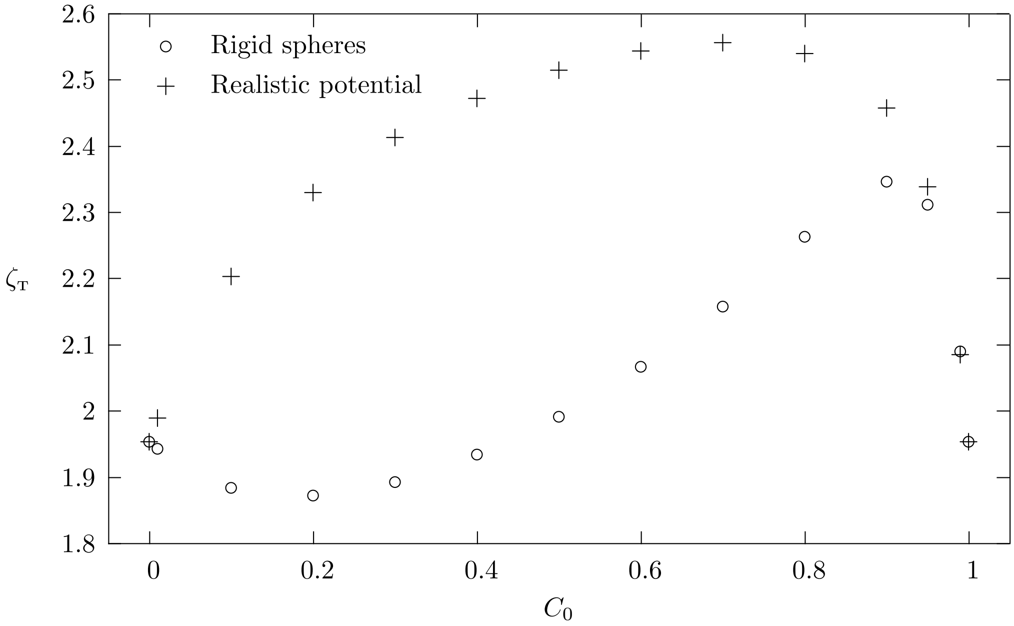

Figure 3: Mixture of He-Xe: temperature jump coefficient vs concentration

- The value of the temperature jump coefficient increases by increasing the mass ratio m_2/m_1. So, the mixture He-Xe has the larger values for the temperature jump coefficient.

4. Conclusion

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

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