Proceedings of the 10^{th} Brazilian Congress of Thermal Sciences and Engineering – ENCIT 2004
Braz. Soc. of Mechanical Sciences and Engineering – ABCM, Rio de Janeiro, Brazil, Nov. 29 – Dec. 03, 2004

Paper CIT04-0059

TRANSPORT PHENOMENA 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. *A simulation of the rarefied gas flows is very important in many engineering fields, e.g. microsystems, electronic, aeronautics, etc. Nowadays, the development of MEMS(Micro-Electro-Mechanical Systems) atracts many scientists and engineers because of its promising future. The size of a microsystem is already of the order to the molecular mean free path and, under this condition the equations of Continuum Mechanics are not valid and if one uses these equations his results will not agree with experimental data because the gas rarefaction is not considered. The Knudsen number, defined as the ratio between the mean free path and a characteristic scale of the gas flow, characterizes the gas rarefaction. For moderately small Knudsen numbers the gas rarefaction can be taken into account via the slip boundary conditions applied to the equations of the Continuum Mechanics. For systems of gaseous mixtures there are three kinds of slip at the surface: viscous, thermal and diffusion slip. The slip boundary condition are introduced via the slip coefficients, which are calculated applying the methods of Rarefied Gas Dynamics on the basis of the Boltzmann equation. In the present work we determine the slip coefficients for three mixtures of the noble gases (Neon-Argon, Helium-Argon and Helium-Xenon) and study the influence of the intermolecular interaction potential and the chemical composition of the mixture upon these coefficients. The knowledge of the slip coefficients allow us to avoid a numerical solution of the kinetic Boltzmann equation (which requires great computational efforts) to solve some problems of engineering and to apply the equations of Continuum Mechanics for moderately rarefied gases.*

keywords: *slip coefficients, Boltzmann equation, rarefied gas mixtures*

1. Introduction

The simulation of the rarefied gas flows is very important in many engineering fields, e.g. electronic, aeronautic, etc. Nowadays, the development of the Micro-Electro-Mechanical Systems (MEMS) atracts many scientists and engineers because its promising future and it is one of the most revolutionary areas of technology.

The Knudsen number Kn, defined as the ratio between the molecular mean free path and a characteristic scale of the gas flow, characterizes the gas rarefaction. When $Kn < 0.01$ the Navier-Stokes equation with the no-slip boundary condition for the gas velocity on a solid surface can be used to describe the gas flow because the gas rarefaction can be neglected.

However, when the Knudsen number is moderately small ($0.01 \leq Kn \leq 0.1$, slip regime) the gas rarefaction must be taken into account and in this case the Navier-Stokes equation with the no-slip boundary condition are not valid. One example of this situation ocurrs in a microsystem which nowadays already has the order to the molecular mean free path. So, to describe the transport phenomena that appear in a gas flowing through a microsystem we can apply the methods of the Rarefied Gas Dynamics which are valid for any value of the Knudsen number. The starting point of the rarefied gas theory is the famous Boltzmann equation and the solution of this equation is very difficult and requires a great computational effort. To avoid a solution of the Boltzmann equation in the range $0.01 \leq Kn \leq 0.1$ and take into account a gas rarefaction we can solve the Navier-Stokes equation with the slip boundary condition for the gas velocity on a solid surface. This boundary condition is written as a function of the slip coefficients and means that the gas velocity is not equal to zero on a solid boundary but its tangential component depends on the velocity profile, temperature and concentration (in the case of a gaseous mixture) near the surface. For a single gas there are two slip coefficients, called viscous and thermal slip coefficients, and for a gaseous mixture there are three slip coefficients which are called viscous, thermal and diffusion slip coefficients.

To use the Navier-Stokes equation with the slip boundary condition for the gas velocity on a solid surface we need to know the numerical values of the slip coefficients for the single gas or gaseous mixture considered in the problem. For a single gas an extensive list of the papers published up to 1998 about slip coefficients with a critical analysis and recommended data can be found in the review (Sharipov and Seleznev, 1998). Some new results can be found in the Refs. (Barichello et al., 2001; Siewert, 2001; Siewert and Sharipov, 2002). In practice one deals with mixtures more often than a single gas and there are very few works providing the slip coefficients for gaseous mixtures; see, for example, the Refs. (Ivchenko et al., 2002; Ivchenko et al., 1997; Lang and Loyalka, 1970).

In the present work we determine numerically the viscous, thermal and diffusion slip coefficients as a function of the molar concentration for some mixtures of the noble gases using the methods of Rarefied Gas Dynamics. A study of the influence of the intermolecular interaction potential and chemical composition upon these coefficients is realized.

2. Statement of the problem

To calculate the slip coefficients we consider a stationary flow of binary gaseous mixture in the semi-infinite space $x' \geq 0$ over an infinite solid surface fixed at $x' = 0$. The pressure P of the mixture is assumed to be constant over the whole space and equal to its equilibrium value P_0. The temperature T and molar concentration C of the mixture have longitudinal small gradients ξ_T and ξ_C, respectively. The slip boundary condition at the surface ($x' = 0$) is written as

$$u'_y = \sigma_\mathrm{P} \frac{\mu v_0}{P_0} \frac{\partial u'_y}{\partial x'} + \sigma_\mathrm{T} \frac{\mu}{\varrho} \frac{\partial \ln T}{\partial y'} + \sigma_\mathrm{C} \frac{\mu}{\varrho} \frac{\partial \ln C}{\partial y'}, \qquad v_0 = \left(\frac{2kT_0}{m} \right)^{1/2}, \qquad \varrho = \varrho_{01} + \varrho_{02}, \tag{1}$$

where u'_y is the longitudinal component of the hydrodynamic velocity of the mixture, μ is the stress viscosity of the mixture, k is the Boltzmann constant, $\varrho_{0\alpha} = n_{0\alpha} m_\alpha$ ($\alpha = 1, 2$) is the mass density of species α, m_α is the molecular mass and $n_{0\alpha}$ is the number density of species α. The dimensionless quantities σ_P, σ_T and σ_C are the viscous, thermal and diffusion slip coefficients, respectively.

The temperature and concentration of the mixture linearly depends on the y-coordinate

$$T(y) = T_0(1 + y\xi_\mathrm{T}), \qquad \xi_\mathrm{T} \ll 1, \tag{2}$$

$$C(y) = C_0(1 + y\xi_\mathrm{C}), \qquad \xi_\mathrm{C} \ll 1, \tag{3}$$

where $y = y'/\ell_0$ is the dimensionless longitudinal coordinate and ℓ_0 is the molecular mean free path defined as

$$\ell_0 = \frac{\mu v_0}{P_0}, \tag{4}$$

and T_0 and C_0 are the temperature and concentration of the mixture in the equilibrium state. The molar concentration C_0 of the mixture is defined as

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

For further derivations we introduced the following dimensionless quantities:

$$x = \frac{x'}{\ell_0}, \qquad \mathbf{c}_\alpha = \left(\frac{m_\alpha}{2kT_0} \right)^{1/2} \mathbf{v}_\alpha, \qquad u_y = \frac{u'_y}{v_0}, \tag{6}$$

where v_0 is a characteristic velocity defined in Eq. (1), $\mathbf{v}_\alpha$ is the molecular velocity of species α.

We assume that the hydrodynamic velocity $u_y(x)$ linearly depends on the x-coordinate far from the surface, i.e.

$$\lim_{x \to \infty} \frac{u_y(x)}{x} = \xi_\mathrm{u}, \tag{7}$$

where ξ_u is a constant velocity gradient assumed to be small ($\xi_\mathrm{u} \ll 1$). The Eq. (7) is valid out of the Knudsen layer because $x \to \infty$ means that the normal distance from the surface is larger than the molecular mean free path ℓ_0. So, from the equations (1) and (7) we will have the following velocity profile far from the surface:

$$\lim_{x \to \infty} u_y(x) = (\sigma_\mathrm{P} + x)\xi_\mathrm{u} + 2\sigma_\mathrm{T}\xi_\mathrm{T} + 2\sigma_\mathrm{C}\xi_\mathrm{C}. \tag{8}$$

In this work we calculated the velocity profile $u_y(x)$ using the methods of the Rarefied Gas Dynamics and this profile gave us the slip coefficients σ_P, σ_T and σ_C.

3. Methodology

As we mencioned earlier, the starting point to solve problems in Rarefied Gas Dynamics is the famous Boltzmann equation. The first step to solve this equation is to linearize the distribution function. In the present work we assumed the gradients of velocity ξ_{u}, temperature ξ_{T} and concentration ξ_{C} to be small, i.e. the gas is weakly disturbed, and consequently the distribution function of each species can be linearized as

$$f_\alpha(\mathbf{r},\mathbf{c}) = f_\alpha^M(y,\mathbf{c})[1 + h_\alpha(x,\mathbf{c})], \qquad h_\alpha \ll 1, \qquad \alpha = 1,2, \tag{9}$$

where

$$f_\alpha^M(y,\mathbf{c}) = n_\alpha(y)\left[\frac{m_\alpha}{2\pi k T(y)}\right]^{3/2} \exp\left\{-\frac{c_{\alpha x}^2 + [c_{\alpha y} - (m_\alpha/m)^{1/2} x \xi_{\mathrm{u}}]^2 + c_{\alpha z}^2}{T(y)/T_0}\right\}, \tag{10}$$

is the local Maxwellian corresponding to the state of the mixture far from the surface. The perturbation functions h_α obey the two coupled Boltmann equations (Ferziger and Kaper, 1972), which for the problem in question read

$$c_{\alpha x}\frac{\partial h_\alpha}{\partial x} = \ell_0\left(\frac{m_\alpha}{2kT_0}\right)^{1/2}\sum_{\beta=1}^{2}\hat{L}_{\alpha\beta}h_\alpha - c_{\alpha y}\left[2\left(\frac{m_\alpha}{m}\right)^{1/2} c_{\alpha x}\xi_{\mathrm{u}} + \left(c_\alpha^2 - \frac{5}{2}\right)\xi_{\mathrm{T}} + \eta_\alpha \xi_{\mathrm{C}}\right], \tag{11}$$

where

$$\eta_1 = 1, \qquad \eta_2 = -\frac{C_0}{(1 - C_0)}. \tag{12}$$

$\hat{L}_{\alpha\beta}$ is the linearized collision operator between species α and β, which in quite general form reads

$$\hat{L}_{\alpha\beta} = \int f_0^M w(\mathbf{v}_\alpha,\mathbf{v}_\beta;\mathbf{v}'_\alpha,\mathbf{v}'_\beta)[h'_\alpha + h'_\beta - h_\alpha - h_\beta]\mathrm{d}\mathbf{v}_\beta \mathrm{d}\mathbf{v}'_\beta \mathrm{d}\mathbf{v}'_\alpha, \tag{13}$$

where $w(\mathbf{v}_\alpha,\mathbf{v}_\beta;\mathbf{v}'_\alpha,\mathbf{v}'_\beta)$ is the probability density that two molecules of species α and β having the velocities $\mathbf{v}'_\alpha$ and $\mathbf{v}'_\beta$ will have sthe velocities $\mathbf{v}_\alpha$ and $\mathbf{v}_\beta$, respectively, after a collision between them. The function $w(\mathbf{v}_\alpha,\mathbf{v}_\beta;\mathbf{v}'_\alpha,\mathbf{v}'_\beta)$ depends on the intermolecular interaction potential. The difficulty to solve the Boltzmann equation is in the calculation of the collision operator and until today there are few works in which the exact Boltzmann equation is solved. The model equations continue to be good tools for practical calculations because they allow us to reduce essentially the computational efforts. The idea of the model equation is to substitute the exact expression of the collision operator by a simple expression satisfying the main properties of the former (conservation of mass, momentum and energy and H-theorem). Many models were proposed for a gaseous mixture; see, e.g. Refs. (Sirovich, 1962; Morse, 1964; Hamel, 1965; McCormack, 1973; Marin and Garzó, 1997).

In the present work we apply the McCormack model which provides the correct expressions of all transport coefficients (viscosity, thermal conductivity, diffusion and thermal diffusion) for a mixture. According to Ref. (McCormack, 1973), the collision operator can be written as

$$\begin{aligned}\hat{L}_{\alpha\beta}h_\alpha = {} & -\gamma_{\alpha\beta}h_\alpha + 2\left(\frac{m_\alpha}{m}\right)^{1/2}\left[\gamma_{\alpha\beta}u_\alpha - \nu_{\alpha\beta}^{(1)}(u_\alpha - u_\beta) - \frac{1}{2}\nu_{\alpha\beta}^{(2)}\left(q_\alpha - \frac{m_\alpha}{m_\beta}q_\beta\right)\right]c_{\alpha y} \\ & +4[(\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(3)})\Pi_\alpha + \nu_{\alpha\beta}^{(4)}\Pi_\beta]c_{\alpha x}c_{\alpha y} + \frac{4}{5}\left(\frac{m_\alpha}{m}\right)^{1/2}\left[(\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(5)})q_\alpha + \nu_{\alpha\beta}^{(6)}\right. \\ & \left.\times\left(\frac{m_\beta}{m_\alpha}\right)^{1/2} q_\beta - \frac{5}{4}\nu_{\alpha\beta}^{(2)}(u_\alpha - u_\beta)\right]c_{\alpha y}\left(c_\alpha^2 - \frac{5}{2}\right)\end{aligned} \tag{14}$$

where

$$u_\alpha(x) = \frac{1}{\pi^{3/2}}\left(\frac{m}{m_\alpha}\right)^{1/2}\int \exp{(-c_\alpha^2)}h_\alpha(x,\mathbf{c}_\alpha)c_{\alpha y}\mathrm{d}\mathbf{c}_\alpha, \tag{15}$$

is the longitudinal component of the hydrodynamic velocity of the specie α,

$$q_\alpha(x) = \frac{1}{\pi^{3/2}}\left(\frac{m}{m_\alpha}\right)^{1/2}\int \exp{(-c_\alpha^2)}h_\alpha(x,\mathbf{c}_\alpha)c_{\alpha y}\left(c_\alpha^2 - \frac{5}{2}\right)\mathrm{d}\mathbf{c}_\alpha, \tag{16}$$

is the longitudinal component of the heat flux vector of the specie α,

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

is the xy-component of the stress tensor of the specie α, and

$$\nu_{\alpha\beta}^{(1)} = \frac{16}{3} \frac{m_{\alpha\beta}}{m_\alpha} n_\beta \Omega_{\alpha\beta}^{(11)}, \tag{18}$$

$$\nu_{\alpha\beta}^{(2)} = \frac{64}{15} \left(\frac{m_{\alpha\beta}}{m_\alpha}\right)^2 n_\beta \left(\Omega_{\alpha\beta}^{(12)} - \frac{5}{2}\Omega_{\alpha\beta}^{(11)}\right), \tag{19}$$

$$\nu_{\alpha\beta}^{(3)} = \frac{16}{5} \frac{m_{\alpha\beta}^2}{m_\alpha m_\beta} n_\beta \left(\frac{10}{3}\Omega_{\alpha\beta}^{(11)} + \frac{m_\beta}{m_\alpha}\Omega_{\alpha\beta}^{(22)}\right), \tag{20}$$

$$\nu_{\alpha\beta}^{(4)} = \frac{16}{5} \frac{m_{\alpha\beta}^2}{m_\alpha m_\beta} n_\beta \left(\frac{10}{3}\Omega_{\alpha\beta}^{(11)} - \Omega_{\alpha\beta}^{(22)}\right), \tag{21}$$

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

$$\nu_{\alpha\beta}^{(6)} = \frac{64}{15} \left(\frac{m_{\alpha\beta}}{m_\alpha}\right)^3 \left(\frac{m_\alpha}{m_\beta}\right)^{3/2} n_\beta \left[-\Omega_{\alpha\beta}^{(22)} + \frac{55}{8}\Omega_{\alpha\beta}^{(11)} - \frac{5}{2}\Omega_{\alpha\beta}^{(12)} + \frac{1}{2}\Omega_{\alpha\beta}^{(13)})\right]. \tag{23}$$

The quantity $m_{\alpha\beta}$ is the reduced mass and $\Omega_{\alpha\beta}^{(ij)}$ are the Chapman-Cowling integrals given in Ref. (Ferziger and Kaper, 1972) which depend on the intermolecular interaction potential. For the rigid-spheres model the expressions for the Omega integrals are given in Ref. (Ferziger and Kaper, 1972) and for a realistic potential see the Ref. (Kestin et al., 1984).

The parameter $\gamma_{\alpha\beta}$ is proportional to the collision frequency between species α and β and it is presented in Ref. (Sharipov and Kalempa, 2002).

The equation (11) is solved assuming the diffuse scattering of gaseous molecules at the solid surface, i.e.

$$h_\alpha(x, \mathbf{c}_\alpha) = 0 \quad \text{for} \quad c_{\alpha x} \geq 0 \quad \text{at} \quad x = 0. \tag{24}$$

Since the Eq. (11) is linear, its solution can be split into three independent parts as

$$h_\alpha = h_\alpha^{(u)}\xi_{\mathrm{u}} + h_\alpha^{(\mathrm{T})}\xi_{\mathrm{T}} + h_\alpha^{(\mathrm{C})}\xi_{\mathrm{C}}. \tag{25}$$

The bulk velocity of the mixture u_y is related to the hydrodynamic velocities of the species as

$$u_y = \left[\frac{1}{\varrho}(\varrho_1 u_1 + \varrho_2 u_2) + x\right]\xi_{\mathrm{u}}, \tag{26}$$

and, as consequence of the Eq. (25), the bulk velocity also can be split into three independent parts as

$$u_y = [u_y^{(u)} + x]\xi_{\mathrm{u}} + u_y^{(\mathrm{T})}\xi_{\mathrm{T}} + u_y^{(\mathrm{C})}\xi_{\mathrm{C}}. \tag{27}$$

When we use the Eq. (8) and (27) we obtain the slip coefficients via the assymptotic behavior of the bulk velocities $u_y^{(i)}$ $(i = u, T, C)$ far from the surface, i.e.

$$\sigma_{\mathrm{P}} = \lim_{x\to\infty} u_y^{(u)}(x), \qquad \sigma_{\mathrm{T}} = 2\lim_{x\to\infty} u_y^{(\mathrm{T})}(x), \qquad \sigma_{\mathrm{C}} = 2\lim_{x\to\infty} u_y^{(\mathrm{C})}(x). \tag{28}$$

So, every coefficient is calculated separately by solving the Eq. (11). These equations were solved by the discret velocity method given in Ref. (Sharipov and Subbotin, 1993) with the relative numerical error less than 0.1%. The numerical accuracy was estimated by comparing the results for different grid parameters.

4. Numerical results and discussion

The numerical results presented here are for the following mixtures of the noble gases: Neon-Argon, Helium-Argon and Helium-Xenon. Such combinations represent mixtures of gases having quite different mass ratios and allow us to investigate the dependence of the slip coefficients on this parameter.

To study the influence of the intermolecular interaction potencial upon the slip coefficients we used the rigid-spheres model and a realistic potential. In our numerical code we need the diameters of every specie and in the case of the rigid-spheres they were calculated via the experimental data on the viscosities of the single gases Helium, Neon, Argon and Xenon at temperature $T = 300K$ given in Ref. (Kestin et al., 1984). For the realistic potential the diameters of each specie are given in Ref. (Kestin et al., 1984).

4.1. Viscous slip coefficient

The Fig. (1) presents the viscous slip coefficient σ_P as a function of the molar concentration C_0.

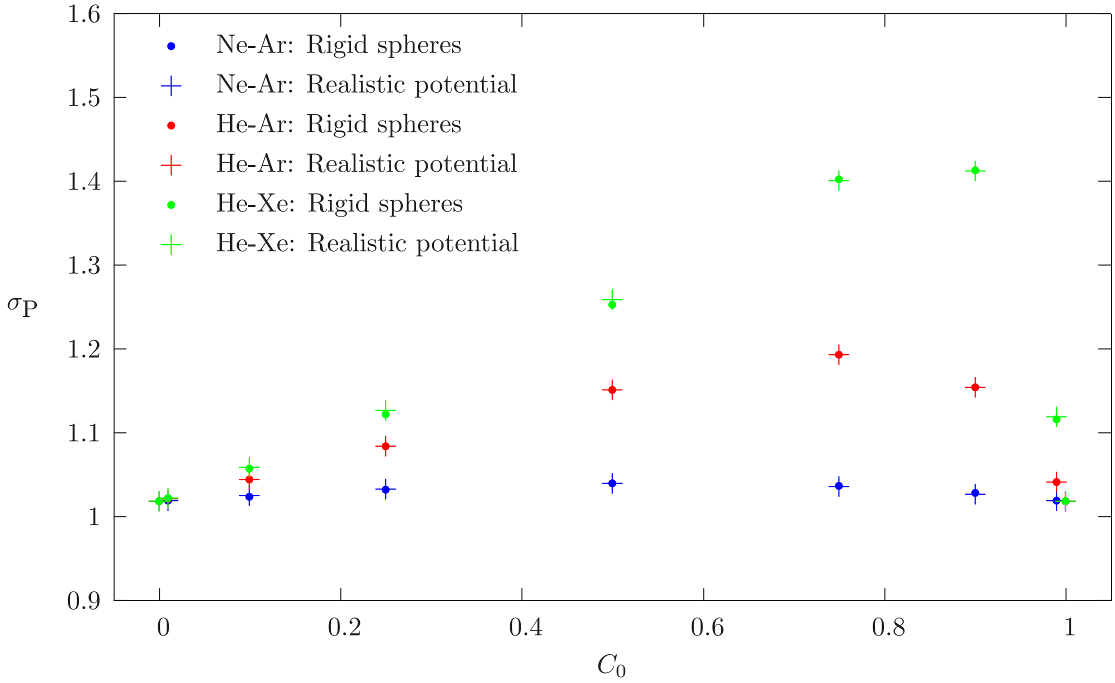

Figure 1: Viscous slip coefficient σ_P vs molar concentration C_0

From these data we may conclude:

(i) At the limits corresponding to a single gas ($C_0 = 0$ and $C_0 = 1$) the viscous slip coefficient is exactly the same as that obtained for a single gas in Refs. (Siewert and Sharipov, 2002,Sharipov, 2003).

(ii) We can say that the viscous slip coefficient is not sensitive to the intermolecular interaction potential because the difference between the results of σ_P for rigid-spheres and realistic potential is within 0.4% for all mixtures considered in the present work.

(iii) If the mass ratio is large, a small concentration of the heavy species changes the viscous slip coefficient significantly. For the mixture He-Xe with $C_0 = 0.99$ (1% of Xe) the viscous slip coefficient changes about 10% its relative value for a single gas.

(iv) The value of the viscous slip coefficient increases by increasing the mass ratio. For the mixture He-Xe (mass ratio equal to 32.804) the viscous slip coefficient reaches the value 1.414. So, for the mixtures considered here we can say that the viscous slip coefficient varies in the interval from 1.018 to 1.414.

4.2. Thermal slip coefficient

The numerical data on the thermal slip coefficient σ_T obtained in the present work are given in Fig. (2). From these data we may conclude the following:

(i) Like the viscous slip coefficient, at the limits corresponding to a single gas ($C_0 = 0$ and $C_0 = 1$) the thermal slip coefficient is exactly the same as that obtained in Refs. (Sharipov, 2003;Siewert and Sharipov, 2002) for a single gas.

(ii) In contrast to the viscous slip coefficient, the thermal slip coefficient is very sensitive to the intermolecular interaction potential. The difference between the results for the rigid-spheres and that for the realistic potential reaches 4%, 18% and 42% for the mixtures Ne-Ar, He-Ar and He-Xe, respectivaly, i.e., the difference increases by increasing the mass ratio.

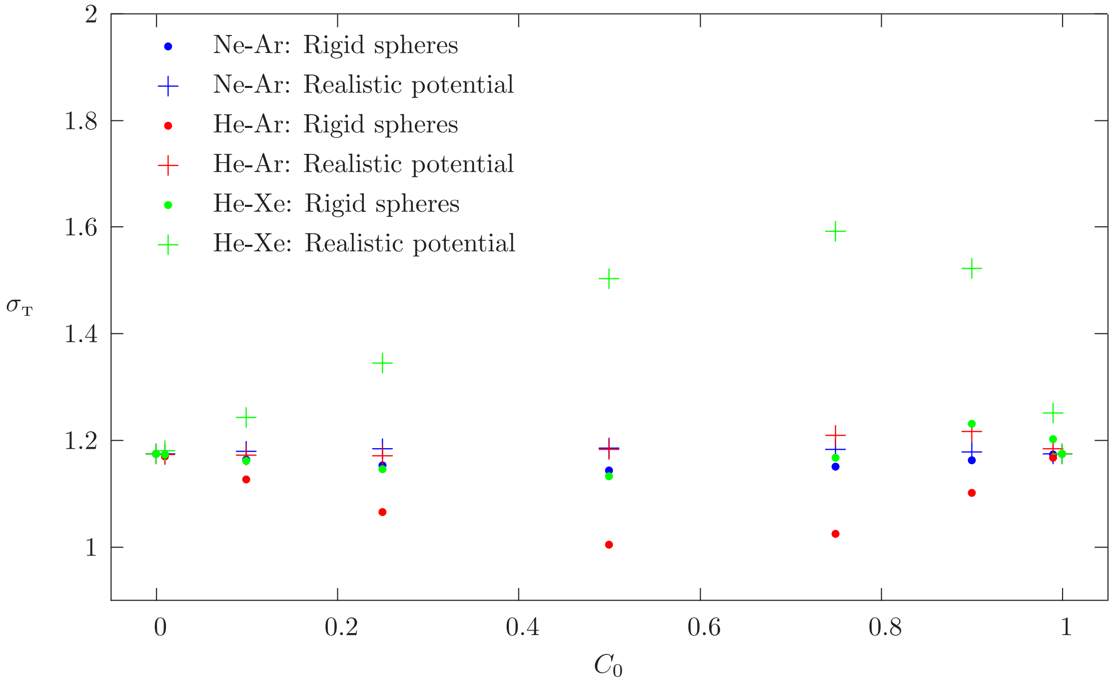

Figure 2: Thermal slip coefficient σ_T vs molar concentration C_0

(iii) For the rigid-spheres the thermal slip coefficient at $C_0 = 0.5$ is always smaller than that for a single gas, while for a realistic potencial it is almost larger than that of a single gas. The strong dependence of this coefficient on the intermolecular interaction potential was noted previously in Ref. (Loyalka, 1990). So, what results are more reliable? Since the diameters 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 realistc potential are more reliable than those based on the hard sphere model.

(iv) Considering that the values of the thermal slip coefficient based on the realistic potential are more reliable than those for the rigid sphere model we conclude that for a fixed value of the concentration C_0 this coefficient increases by increasing the mass ratio. For the mixtures considered in the present work the thermal slip coefficient varies in the range from 1.171 to 1.592.

(v) For the mixture with large mass ratio (He-Xe) a small concentration of the heavy specie changes significantly the thermal slip coefficient. In the mixture of He-Xe, 1% of Xe changes for 7% the thermal slip coefficient relatively its values for a single gas.

4.3. Diffusion slip coefficient

The Fig. (3) presents the results obtained for the diffusion slip coefficient vs molar concentration for the mixtures considered in this work.

From these data we may conclude:

(i) The diffusion slip coefficient is sensitive to the intermolecular interaction potential. The difference between this coefficient for the rigid-spheres and that for the realistic potential increases by increasing of the mass ratio of the mixture. For the mixture with the largest mass ratio (He-Xe) this difference reaches 30%. This sensibility to the intermolecular interaction potential was noted previously in the Ref. (Loyalka, 1975).

(ii) For all situations considered in this work the diffusion slip coefficient is positive. This physically means that the mixture flows from the region with a lower concentration to the region of the higher concentration of the light component.

(iii) The diffusion slip coefficient is a monotonic function of the molar concentration and reaches its maximum value for a given mixture at $C_0 = 1$. Note, the value of σ_C at $C_0 = 1$ must be considered as a limit value because the concentrationn $(1 - C_0)$ means that the first component of the mixture is single and the diffusion slip phenomenon does not exist. So, the values that appear in the Fig. (3) correspond to the concentration very close to unity but not equal to unity.

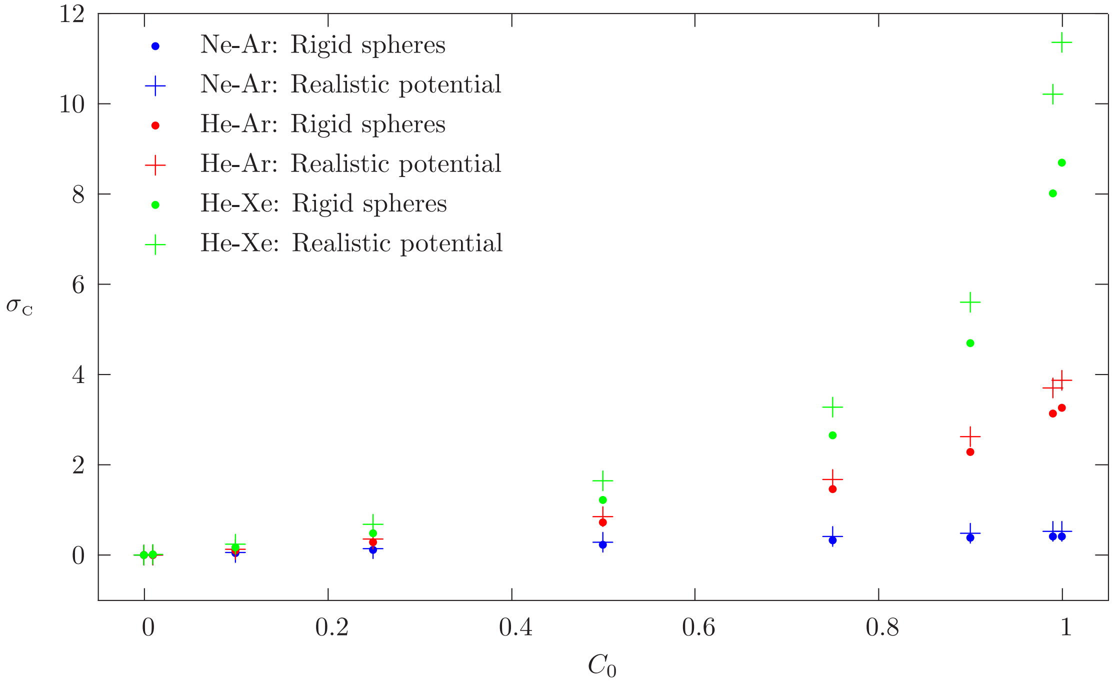

Figure 3: Diffusion slip coefficient σ_{C} vs molar concentration C_0

5. Application of the slip coefficients to a classical problem

In this section we presented an example of application of the viscous slip coefficient to a classical problem. Let us consider a flow of gaseous mixture through a long tube caused by a longitudinal pressure gradient. Assuming the slip boundary condition (1) the velocity profile is obtained from the Navier-Stokes equation as

$$u'_y(r) = -\frac{1}{4\mu}\frac{dP}{dy'}(a^2 - r^2 + 2\sigma_{\mathrm{P}} a \ell_0), \tag{29}$$

where a is the tube radius, r is the radial coordinate and the y' coordinate is directed along the tube axis. If we introduce the reduced flow rate as

$$G = -\frac{4P_0}{a^3 v_0}\left(\frac{dP}{dy'}\right)^{-1}\int_0^a u'_y(r) r \mathrm{d}r, \tag{30}$$

and then use the Eq. (29) into (30) we obtain

$$G = \frac{\delta}{4} + \sigma_{\mathrm{P}}, \qquad \delta = \frac{a}{\ell_0}, \tag{31}$$

where δ is the rarefaction parameter inversely proportional to the Knudsen number. In Ref. (Sharipov and Kalempa, 2002) the flow rate G of mixture through a tube was calculated numerically over the wide range of the gas rarefaction δ on the basis of the kinetic equation. In terms of the kinetic coefficients Λ_{PP} e Λ_{PC} tabulated in Ref. (Sharipov and Kalempa, 2002), the quantity G reads

$$G = \Lambda_{\mathrm{PP}} - \frac{m_2 - m_1}{m}(1 - C_0)\Lambda_{\mathrm{PC}}. \tag{32}$$

In Table 1 the values of G for the mixture He-Ar at $C_0 = 0.5$ calculated with $\sigma_{\mathrm{P}} = 1.151$ by Eq. (31) are compared with the numerical solution of the kinetic equation for the same mixture expressed by Eq. (32).

From this table one can see that the use of correct value for σ_{P} allow us to calculate the flow rate G with a good accuracy in the sufficiently large range of the gas rarefaction δ. So, one really extends the range of applicability of the hydrodynamic equations if one uses the slip boundary condition with the correct value of σ_{P}.

Table 1: Reduced flow rate G through a tube vs the rarefaction parameter δ, mixture of He-Ar at $C_0 = 0.5$

δ	(Sharipov and Kalempa, 2002)	Eq. (31)
2	1.701	1.651
4	2.195	2.151
10	3.676	3.651
20	6.162	6.151
40	11.15	11.15

6. Conclusion

The viscous, thermal and diffusion slip coefficients were calculated as a function of the concentration of the mixtures Ne-Ar, He-Ar and He-Xe. For the mixture with a high ratio of the molecular mass, i.e. He-Xe, the slip coefficients differs significantly from that for a single gas. The viscous slip coefficient has a weakly dependence on the intermolecular interaction potential while the thermal and diffusion slip coefficients depend on the interaction potential. The range of the slip coefficients variation increases by increasing the mass ratio of the species of the mixture. An example of application of the slip boundary condition to the Navier-Stokes equation showed that the use the correctly calculated viscous slip coefficient extends significantly the range of the gas rarefaction where the hydrodynamic equations can be applied.

7. Acknowledgements

The authors acknowledge the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq, Brazil) and also the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES, Brazil) for the support of their research.

8. References

Barichello, L. B., Camargo, M., Rodrigues, P., and Siewert, C. E., 2001, Unified solution to classical flow problem based on the BGK model, “Z. Angew. Math. Phys. (ZAMP)”, Vol. 52, No. 3, pp. 517–534.

Ferziger, J. H. and Kaper, H. G., 1972, “Mathematical Theory of Transport Processes in Gases”, North-Holland Publishing Company, Amsterdam.

Hamel, B. B., 1965, Kinetic model for binary gas mixture, “Phys. Fluids”, Vol. 8, No. 3, pp. 418–425.

Ivchenko, I. N., Loyalka, S. K., and Tompson, R. V., 1997, Slip coefficients for binary gas mixture, “J. Vac. Sci. Technol. A”, Vol. 15, No. 4, pp. 2375–2381.

Ivchenko, I. N., Loyalka, S. K., and Tompson, R. V., 2002, Boundary slip phenomena in a binary gas mixture, “Z. Angew. Math. Phys. (ZAMP)”, Vol. 53, No. 1, pp. 58–72.

Kestin, J., Knierim, K., Mason, E. A., Najafi, B., Ro, S. T., and Waldman, M., 1984, Equilibrium and transport properties of the noble gases and their mixture at low densities, “J. Phys. Chem. Ref. Data”, Vol. 13, No. 1, pp. 229–303.

Lang, H. and Loyalka, S., 1970, An Exact Expression for the Diffusion Slip Velocity in a Binary Gas Mixture, “Phys. Fluids”, Vol. 13, No. 7, pp. 1871–1873.

Loyalka, S., 1975, The Q and F integrals for the BGK Model, “J.Transp.Theory Statistical Phys.”, Vol. 4, pp. 55.

Loyalka, S. K., 1990, Slip and jump coefficients for rarefied gas flows: variational results for Lennard-Jones and $n(r)$-6 potencial, “Physica A”, Vol. 163, pp. 813–821.

Marin, C. and Garzó, V., 1997, Kinetic model for momentum transport in a binary mixture, Shen, C., editor, “Rarefied Gas Dynamics”, pp. 91–96, Beijing. 20st Int. Symp., China, 1996, Pekin University Press.

McCormack, F. J., 1973, Construction of linearized kinetic models for gaseous mixture and molecular gases., “Phys. Fluids”, Vol. 16, pp. 2095–2105.

Morse, T. F., 1964, Kinetic Model Equations for a gas mixture, “Phys. Fluids”, Vol. 7, No. 12, pp. 2012–2013.

Sharipov, F., 2003, Application of the Cercignani-Lampis scattering kernel to calculations of rarefied gas flows. II. Slip and jump coefficients, “Eur. J. Mech. B / Fluids”, Vol. 22, pp. 133–143.

Sharipov, F. and Kalempa, D., 2002, Gaseous mixture flow through a long tube at arbitrary Knudsen number, “J. Vac. Sci. Technol. A”, Vol. 20, No. 3, pp. 814–822.

Sharipov, F. and Seleznev, V., 1998, Data on internal rarefied gas flows, “J. Phys. Chem. Ref. Data”, Vol. 27, No. 3, pp. 657–706.

Sharipov, F. M. and Subbotin, E. A., 1993, On optimization of the discrete velocity method used in rarefied gas dynamics, “Z. Angew. Math. Phys. (ZAMP)”, Vol. 44, pp. 572–577.

Siewert, C. E., 2001, Kramers’ problem for a variable collision frequency model, “Eur. J. Appl. Math.”, Vol. 12, pp. 179–191.

Siewert, C. E. and Sharipov, F., 2002, Model equations in rarefied gas dynamics: Viscous-slip and thermal-slip coefficients, “Phys. Fluids”, Vol. 14, No. 12, pp. 4123–4129.

Sirovich, L., 1962, Kinetic modeling of gas mixture, “Phys. Fluids”, Vol. 5, No. 8, pp. 908–918.