

# TRANSPORT PHENOMENA IN RAREFIED GASEOUS SYSTEMS

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**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) attracts many scientists and engineers because of its promising future. The size of a microsystem is already of the order of the molecular mean free path and, under this condition the equations of Continuum Mechanics are not valid and if one uses these equations its results will not agree with experimental data because the gas rarefaction is not considered. The Knudsen number characterizes the gas rarefaction and, for moderately small Knudsen numbers the gas rarefaction can be taken into account via velocity slip and temperature jump boundary conditions applied to the Navier-Stokes and Fourier equations. The aim of the present work is to calculate the velocity slip and temperature jump coefficients for gaseous mixtures because in practice one deals with mixtures more often than a single gas. These coefficients are calculated applying the methods of the Rarefied Gas Dynamics on the basis of the Boltzmann equation. The influence of the interaction potential and composition of the mixture upon these coefficients is also realized. The knowledge of these coefficients allow us to avoid a numerical solution of the Boltzmann equation (which requires great computational efforts) to solve some problems of engineering and to apply the equations of Continuum Mechanics.

**Keywords:** velocity slip, temperature jump, rarefied gas, Boltzmann equation

## 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) attracts 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 and the Fourier equation with the temperature continuity condition on the gas-surface boundary can be used to describe the gas flow because the gas rarefaction can be neglected.

However, when the Knudsen number is moderately small ( $0.01 \leq Kn \leq 0.1$ ) the gas rarefaction must be taken into account and in this case the Navier-Stokes and Fourier equations can not be solved with the boundary conditions cited earlier. One example of this situation occurs in a microsystem which nowadays 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 have two possibilities: (i) apply the methods of the Rarefied Gas Dynamics on the basis of the Boltzmann equation which are valid for any value of the Knudsen number but requires a great computational efforts; (ii) apply the velocity slip and temperature jump boundary conditions to solve the Navier-Stokes and Fourier equations. These boundary conditions are written as

$$u'_y(0) = \sigma_p \frac{\mu v_0}{P_0} \frac{\partial u'_y}{\partial x'} + \sigma_\tau \frac{\mu}{\varrho} \frac{\partial \ln T}{\partial y'} + \sigma_c \frac{\mu}{\varrho} \frac{\partial \ln C}{\partial y'}, \quad v_0 = \left( \frac{2kT_0}{m} \right)^{1/2}, \quad \varrho = \varrho_{01} + \varrho_{02}, \quad (1)$$

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

where  $u'_y$  is the longitudinal component of the hydrodynamic velocity of the mixture,  $T_g$  is the temperature of the gas mixture at wall,  $x'$  is the coordinate normal to the surface and  $y'$  is the coordinate longitudinal to the surface.  $\mu$  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 quantities  $\sigma_p$ ,  $\sigma_\tau$  and  $\sigma_c$  are the viscous, thermal and diffusion slip coefficients and  $\zeta_\tau$  is the temperature jump coefficient.

To use the velocity slip and temperature jump boundary conditions we need to know the numerical values of the slip and jump 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 and jump 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 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 and jump coefficients for gaseous mixtures; see, for example, Refs. [Ivchenko et al., 2002, Ivchenko et al., 1997, Lang and Loyalka, 1970].

In the present work we determine numerically the slip and jump coefficients as a function of the molar concentration for some mixtures of the noble gases. A study of the influence of the intermolecular interaction potential and chemical composition upon these coefficients is realized.

## 2. Methodology to calculate the velocity slip and temperature jump coefficients

To calculate the slip and jump coefficients we need to solve the Boltzmann equation and apply the methods of Rarefied Gas Dynamics. As is known, the Boltzmann equation is an integro-differential equation very complex to be solved. Until today there are few works in which the exact Boltzmann equation is solved and the models equations continue to be good tools for practical calculations. The idea of the models equations is to substitute the exact expression to the collision operator by a simple expression satisfying the main properties of the former (conservation of mass, momentum and energy, etc). Many models were proposed for a gaseous mixtures and we choose the McCormack model [McCormack, 1973] because this model provides the correct expressions for all transport coefficients (viscosity, thermal conductivity, diffusion and thermal diffusion).

### 2.1 Slip coefficients

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  $\xi_T$  and  $\xi_c$ , respectively. The slip boundary condition at the surface ( $x' = 0$ ) is given in Eq. (1). The temperature and concentration of the mixture linearly depends on the  $y$ -coordinate

$$T(y) = T_0(1 + y\xi_T), \quad \xi_T \ll 1, \quad (3)$$

$$C(y) = C_0(1 + y\xi_c), \quad \xi_c \ll 1, \quad (4)$$

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

$$\ell_0 = \frac{\mu v_0}{P_0}, \quad (5)$$

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

$$C_0 = \frac{n_{01}}{n_{01} + n_{02}}, \quad (6)$$

where  $n_{01}$  and  $n_{02}$  are the equilibrium number densities of each gas species.

For further derivations we introduced the following dimensionless quantities:

$$x = \frac{x'}{\ell_0}, \quad \mathbf{c}_\alpha = \left( \frac{m_\alpha}{2kT_0} \right)^{1/2} \mathbf{v}_\alpha, \quad u_y = \frac{u'_y}{v_0}, \quad (7)$$

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

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

$$\lim_{x \rightarrow \infty} \frac{u_y(x)}{x} = \xi_u, \quad (8)$$

where  $\xi_u$  is a constant velocity gradient assumed to be small ( $\xi_u \ll 1$ ). The Eq. (8) is valid out of the Knudsen layer because  $x \rightarrow \infty$  means that the normal distance from the surface is larger than the molecular mean free path  $\ell_0$ . So, from the equations (1) and (8) we will have the following velocity profile far from the surface:

$$\lim_{x \rightarrow \infty} u_y(x) = (\sigma_p + x)\xi_u + 2\sigma_T\xi_T + 2\sigma_c\xi_c. \quad (9)$$

So, the slip coefficients are calculated via velocity profile of the mixture. To calculate the velocity profile of the mixture, first of all we need to linearize the McCormack equation. As we assumed the gradients of velocity  $\xi_u$ , temperature  $\xi_T$  and concentration  $\xi_c$  to be small, i.e. the gas is weakly disturbed, the distribution function of each species can be linearized as

$$f_\alpha(\mathbf{r}, \mathbf{c}) = f_\alpha^M(y, \mathbf{c})[1 + h_\alpha(x, \mathbf{c})], \quad h_\alpha \ll 1, \quad \alpha = 1, 2, \quad (10)$$

where

$$f_\alpha^M(y, \mathbf{c}) = n_\alpha(y) \left[ \frac{m_\alpha}{2\pi kT(y)} \right]^{3/2} \exp \left\{ -\frac{c_{\alpha x}^2 + [c_{\alpha y} - (m_\alpha/m)^{1/2}x\xi_u]^2 + c_{\alpha z}^2}{T(y)/T_0} \right\}, \quad (11)$$

is the local Maxwellian corresponding to the state of the mixture far from the surface. The perturbation functions  $h_\alpha$  obey the two coupled Boltzmann equations [Ferziger and Kaper, 1972], which for the problem in question read

$$c_{\alpha x} \frac{\partial h_\alpha}{\partial x} = \ell_0 \left( \frac{m_\alpha}{2kT_0} \right)^{1/2} \sum_{\beta=1}^2 \hat{L}_{\alpha\beta} h_\alpha - c_{\alpha y} \left[ 2 \left( \frac{m_\alpha}{m} \right)^{1/2} c_{\alpha x} \xi_u + \left( c_\alpha^2 - \frac{5}{2} \right) \xi_T + \eta_\alpha \xi_C \right], \quad (12)$$

where

$$\eta_1 = 1, \quad \eta_2 = -\frac{C_0}{(1 - C_0)}. \quad (13)$$

$\hat{L}_{\alpha\beta}$  is the linearized collision operator given in [McCormack, 1973]. The equation (12) is solved assuming the diffuse scattering of gaseous molecules at the solid surface, i.e.

$$h_\alpha(x, \mathbf{c}_\alpha) = 0 \quad \text{for} \quad c_{\alpha x} \geq 0 \quad \text{at} \quad x = 0. \quad (14)$$

Since the Eq. (12) is linear, its solution can be split into three independent parts as

$$bqh_\alpha = h_\alpha^{(u)} \xi_u + h_\alpha^{(T)} \xi_T + h_\alpha^{(C)} \xi_C. \quad (15)$$

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

$$u_y = \left[ \frac{1}{\rho} (\rho_1 u_1 + \rho_2 u_2) + x \right] \xi_u, \quad (16)$$

and, as consequence of the Eq. (15), the bulk velocity also can be split into three independent parts as

$$u_y = [u_y^{(u)} + x] \xi_u + u_y^{(T)} \xi_T + u_y^{(C)} \xi_C. \quad (17)$$

When we use the Eq. (9) and (17) we obtain the slip coefficients via the asymptotic behavior of the bulk velocities  $u_y^{(i)}$  ( $i = u, T, C$ ) far from the surface, i.e.

$$\sigma_F = \lim_{x \rightarrow \infty} u_y^{(u)}(x), \quad \sigma_T = 2 \lim_{x \rightarrow \infty} u_y^{(T)}(x), \quad \sigma_C = 2 \lim_{x \rightarrow \infty} u_y^{(C)}(x). \quad (18)$$

So, every coefficient is calculated separately by solving the Eq. (12). These equations were solved by the discret velocity method given in (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.

## 2.2 Temperature jump coefficient

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  $\xi_T$  normal to the surface, which is constant far from the surface, i.e.,

$$T(x') = T_0 \left[ 1 + \left( \zeta_T + \frac{x'}{\ell_0} \right) \xi_T \right], \quad \text{at} \quad x' \rightarrow \infty, \quad (19)$$

where the mean free path  $\ell_0$  is given in Eq. (5) and the characteristic molecular velocity  $v_0$  is given in Eq. (1).

$$m = C_0 m_1 + (1 - C_0) m_2 \quad (20)$$

is the mean molecular mass of the mixture. The quantity  $m_\alpha$  ( $\alpha = 1, 2$ ) is the molecular mass of specie  $\alpha$  and  $C_0$  is the equilibrium concentration defined in Eq. (6).

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

$$\lim_{x' \rightarrow \infty} \frac{dC}{dx'} = \frac{C_0}{\ell_0} \xi_C = \text{const.} \quad (21)$$

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  $\xi_C$  and the temperature gradient  $\xi_T$  is the following

$$\xi_C = -(1 - C_0) a_T \xi_T, \quad (22)$$

where  $a_T$  is the thermal diffusion factor.

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

$$q_x = -\kappa \frac{T_0}{\ell_0} \xi_T, \quad (23)$$

where  $\kappa$  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  $\zeta_T$  we solved the McCormack kinetic equation (McCormack, 1973). The first step to solve this equation consist of linearize the distribution function. Since we assumed the temperature gradient  $\xi_T$  to be small ( $\xi_T \ll 1$ ), the distribution function of each species can be linearized as

$$f_\alpha(\mathbf{r}, \mathbf{c}) = f_\alpha^M(x, \mathbf{c})[1 + h_\alpha(x, \mathbf{c})\xi_T], \quad h_\alpha \ll 1, \quad (24)$$

where  $f_\alpha^M$  is the local Maxwellian corresponding to the state of the mixture at the infinity, i.e.

$$f_\alpha^M(x, \mathbf{c}) = n_{\alpha\infty}(x) \left[ \frac{m_\alpha}{2\pi k T_\infty(x)} \right]^{3/2} \exp \left[ -\frac{c_\alpha^2}{T_\infty(x)/T_0} \right], \quad (25)$$

$$T_\infty(x) = T_0[1 + x\xi_T], \quad (26)$$

$$n_{\alpha\infty} = n_{\alpha 0}[1 - x\xi_T(1 + \eta_\alpha)], \quad (27)$$

$$\eta_1 = (1 - C_0)a_T, \quad \eta_2 = -C_0a_T. \quad (28)$$

The perturbation function  $h_\alpha$  obey the two coupled Boltzmann equations which for the problem in question read

$$c_{\alpha x} \frac{\partial h_\alpha}{\partial x} = \ell_0 \left( \frac{m_\alpha}{2kT_0} \right)^{1/2} \sum_{\beta=1}^2 \hat{L}_{\alpha\beta} h_\alpha - c_{\alpha x} \left( c_\alpha^2 - \frac{5}{2} - \eta_\alpha \right), \quad \alpha = 1, 2. \quad (29)$$

$\hat{L}_{\alpha\beta} h_\alpha$  is the linearized collision operator between species  $\alpha$  and  $\beta$  given in (McCormack, 1973).

To solve the system of kinetic equations (29) we assumed the impermeability condition on the surface with the diffuse scattering of gaseous particles, i.e.

$$h_\alpha(0, \mathbf{c}_\alpha) = \frac{2}{\pi} \int_{c'_{\alpha x} < 0} c'_{\alpha x} h_\alpha(0, c'_{\alpha x}) \exp(-c'^2_\alpha) d\mathbf{c}'_\alpha, \quad c_{\alpha x} \geq 0, \quad (30)$$

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  $\zeta_T$  is calculated as

$$\zeta_T = \lim_{x \rightarrow \infty} \tau(x), \quad (31)$$

where

$$\tau(x) = C_0\tau_1 + (1 - C_0)\tau_2. \quad (32)$$

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 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).

### 3.1 Viscous slip coefficient

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

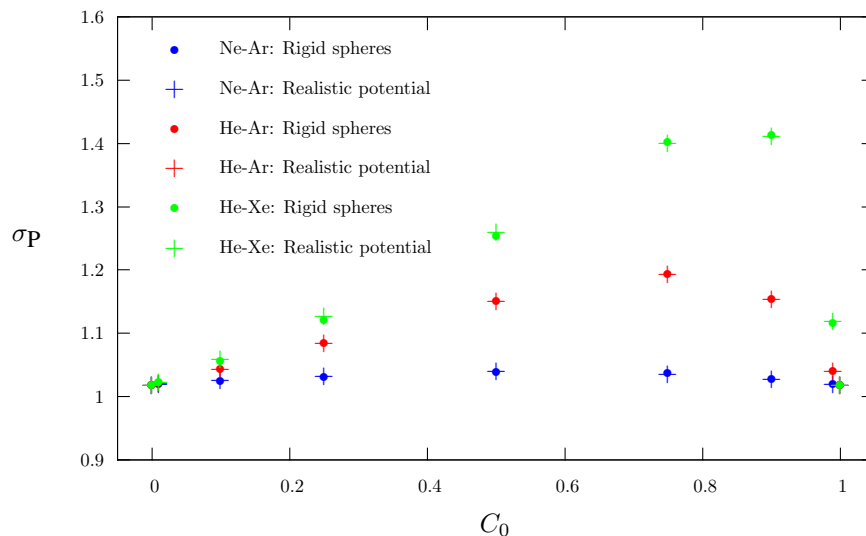


Figure 1. Viscous slip coefficient  $\sigma_p$  vs molar concentration  $C_0$

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  $\sigma_p$  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.

### 3.2 Thermal slip coefficient

The numerical data on the thermal slip coefficient  $\sigma_T$  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. [Siewert and Sharipov, 2002, Sharipov, 2003] 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, respectively, i.e., the difference increases by increasing the mass ratio.
- (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 potential 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. [Ivchenko et al., 1997]. 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 realistic 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.

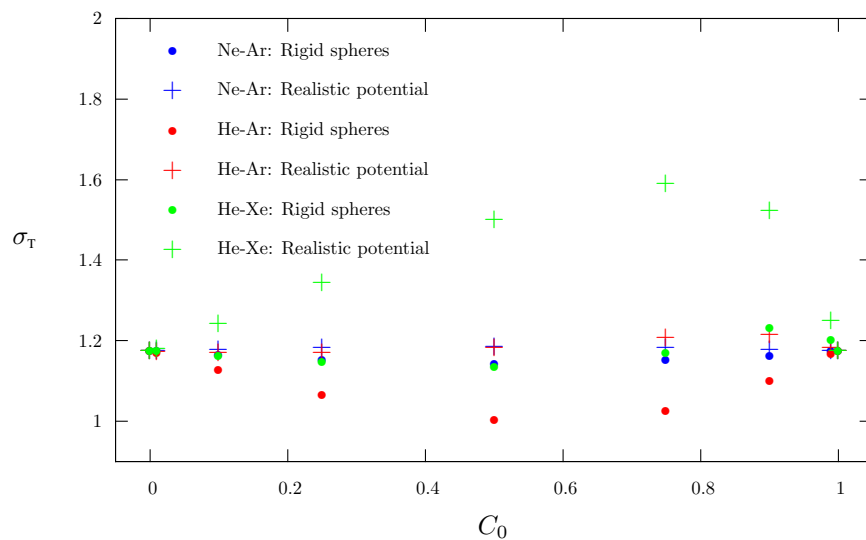


Figure 2. Thermal slip coefficient  $\sigma_T$  vs molar concentration  $C_0$

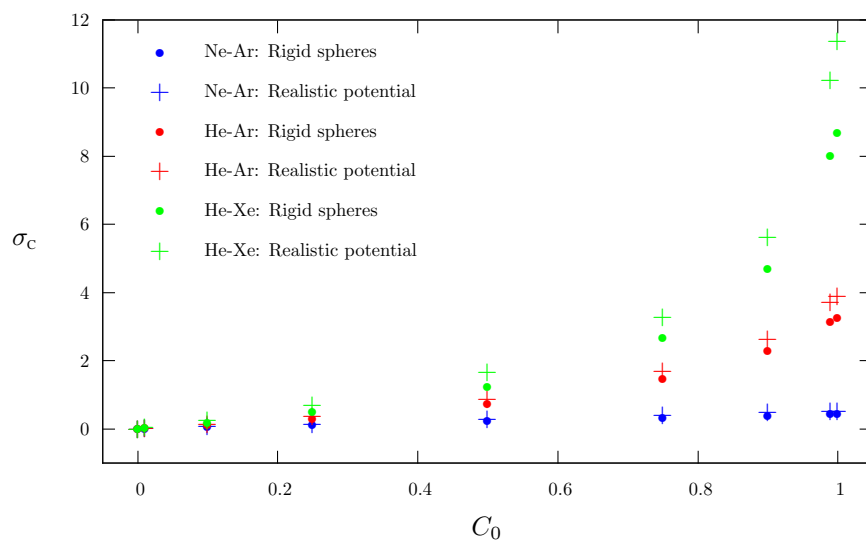


Figure 3. Diffusion slip coefficient  $\sigma_c$  vs molar concentration  $C_0$

(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.

### 3.3 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. [Ivchenko et al., 1997].

(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  $\sigma_c$  at  $C_0 = 1$  must be considered as a limit value because the

concentration  $(1 - C_0)$  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.

### 3.4 Temperature jump coefficient

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.

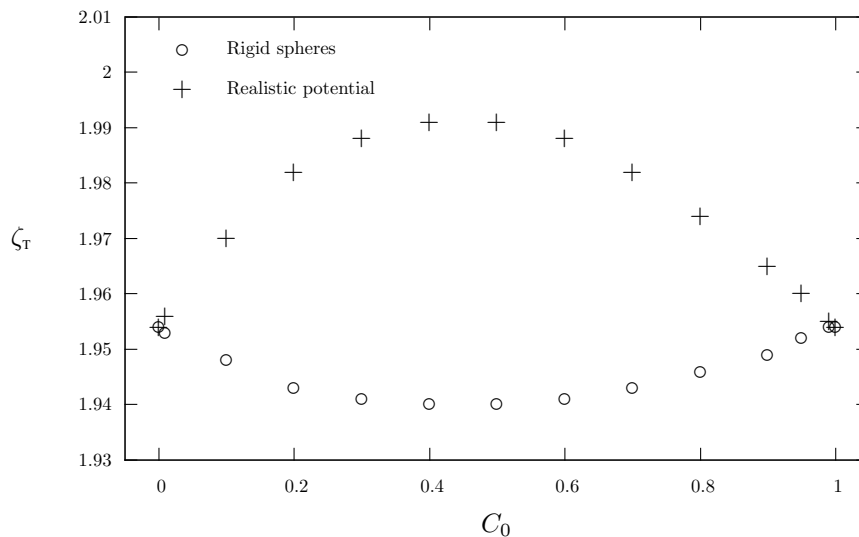


Figure 4. Mixture of Ne-Ar: temperature jump coefficient vs concentration

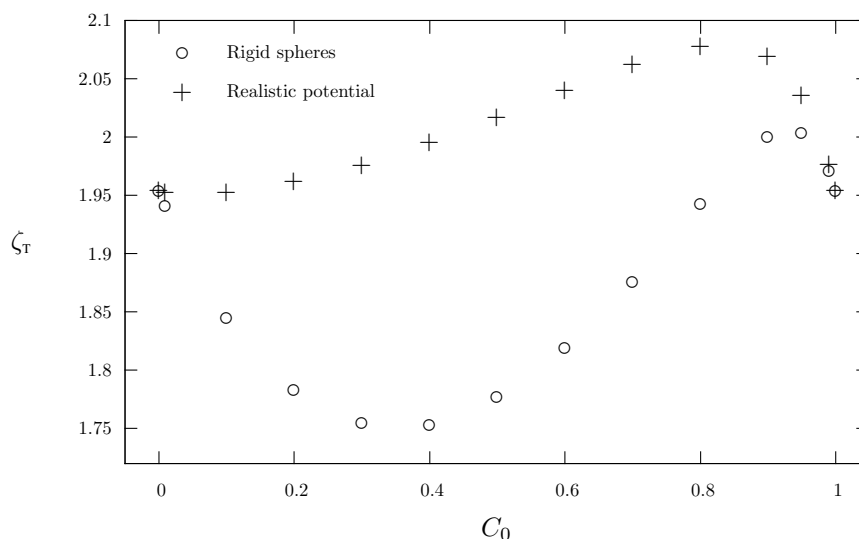


Figure 5. Mixture of He-Ar: temperature jump coefficient vs concentration

From these data we may conclude the following:

(i) 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.

ii) This coefficient is very sensitive to the intermolecular interaction potential. The difference between  $\zeta_T$  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  $\zeta_T$  has a non-monotone dependence on the concentration. It has a minimum near  $C_0 = 0.5$  and a maximum near  $C_0 = 0.99$ .

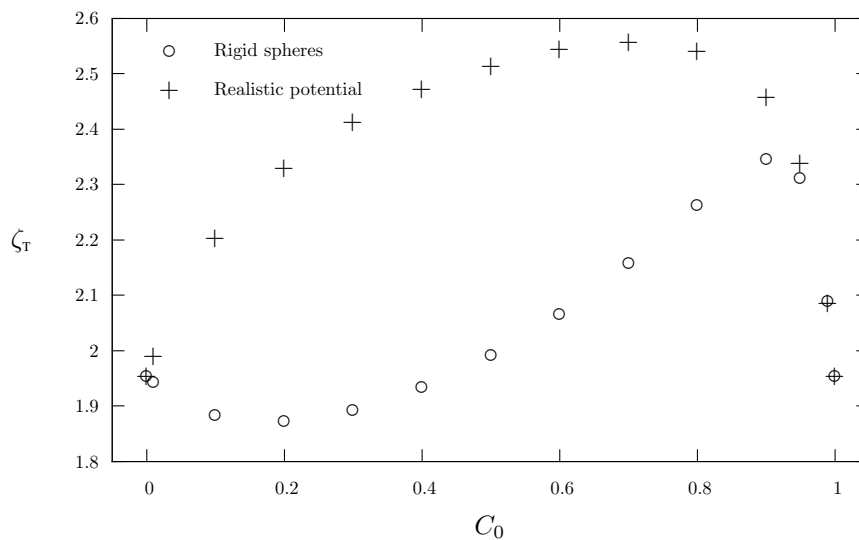


Figure 6. Mixture of He-Xe: temperature jump coefficient vs concentration

For the realistic potential  $\zeta_T$  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.

(iii) 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.

(iv) 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%.

(v) 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.

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