



## *Ab initio* simulation of heat transfer through a mixture of rarefied gases



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### ABSTRACT

The heat flux problem for a binary gaseous mixture confined between two parallel plates with different temperatures is studied on the basis of the direct simulation Monte Carlo method with an implementation of *ab initio* potential. The calculations were carried for a wide range of the gas rarefaction, for several values of the mole fraction and for two values of the temperature difference. The smaller value of the difference corresponds to the limit when the nonlinear terms are negligible, while the larger value describes a nonlinear heat transfer. The heat flux, temperature, and mole fraction distributions are presented. To study the influence of the intermolecular potential, the same simulations are carried out for the hard sphere molecular model. A relative deviation of the results based on this model from those based on the *ab initio* potential is analyzed. It is pointed out that the difference between the heat flux of the two potentials is about 8% and 5% for the small and large temperature differences, respectively. The temperature distribution between plates is weakly affected by the molecular potential, while the chemical composition variation is the most sensitive quantity for the considered problem. The reported results can be used as benchmark data to test model kinetic equations for gaseous mixtures.

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### 1. Introduction

In our previous paper [1], we showed that any intermolecular potential can be implemented into the direct simulation Monte Carlo (DSMC) method [2] with the same computational effort as that for the hard sphere (HS) molecular model. Since reliable information about intermolecular potentials of many gases can be found in literature, see e.g. Refs. [3,4], it is not necessary to use the potentials like variable hard spheres [2], variable soft spheres [5] and generalized hard spheres [6] elaborated specifically for the DSMC method. Recently, the *ab initio* (AI) potentials were calculated for practically all noble gases and their mixtures, see e.g. Refs. [7–14]. An implementation of this potential into the DSMC [15] made this method completely free from tuned parameters usually extracted from experiments. Such an approach allows us to obtain benchmark data which can be used to test kinetic models and approximate methods in order to solve many practical problems of heat and mass transfer with modest computational effort, but without losing reliability.

Our recent paper [16] reports benchmark data for the Couette flow of helium–argon mixture over the whole range of the gas rarefaction based on the AI intermolecular potential. A comparison of the results obtained for the AI potential with those for the HS potential showed that the Couette flow is weakly sensitive to the

potential. In the present paper, we continue to study the influence of the intermolecular potential on various types of mixture flows. More specifically, a heat transfer through a mixture confined between two plates is calculated applying the DSMC technique. The calculations are carried out over a wide range of the gas rarefaction for both AI and HS potentials.

The flow to be considered here is a classical problem of fluid mechanics. Many researchers studied this problem in case of a single rarefied gas, see e.g. Refs. [17–26]. On our knowledge, there are very few papers [27–31] on heat transfer through a mixture of rarefied gases. The works [27,30,31] provide results based on the Boltzmann equation with the HS potential. The paper [28] reports results on the heat flux based on the linearized McCormack (MC) model [32] of the Boltzmann equation. The paper [29] is also based on the MC model, but two potentials were used, viz., HS and the so-called realistic potential (RP). A comparison of results based on these two potentials showed that the heat transfer is strongly sensitive to the potential. As was shown in Refs. [33–38], many other phenomena in gaseous mixtures are very sensitive to the potential of the intermolecular interaction. Thus, it is important to obtain benchmark results based on the *ab initio* calculations for a large number of phenomena.

The aim of the present paper is to calculate the heat flux through a binary mixture of rarefied gases confined between two parallel plates based on the AI potential implemented into the DSMC method. To study the influence of the potential on heat flux, temperature and chemical composition distributions, the same problem will be solved for the HS molecular model too.

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## 2. Statement of the problem

Consider a binary gaseous mixture confined between two parallel plates fixed at  $x = \pm H/2$  and having different temperatures  $T_0 \pm \Delta T/2$ , respectively. Thus,  $H$  is the distance between the plates and  $\Delta T$  is the temperature difference. We are going to calculate the heat flux  $q'_x$ , temperature  $T(x)$  profile and mole fraction  $C(x)$  distribution between the plates.

Besides the relative temperature difference  $\Delta T/T_0$ , the solution of the problem is determined by two more parameters. The first one is the mole fraction defined as

$$C = n_1/(n_1 + n_2), \quad (1)$$

where  $n_1$  and  $n_2$  are the number density of species. Because of thermodiffusion phenomenon, the mole fraction varies between the plates so that we will distinguish the equilibrium value  $C_0$ , i.e. its value at  $\Delta T = 0$ , and the local mole fraction  $C(x)$  which is a function of the coordinate  $x$  when  $\Delta T \neq 0$ .

The other parameter determining the solution is the rarefaction parameter defined as

$$\delta = H/\ell, \quad \ell = \mu_0 v_0/p_0, \quad (2)$$

where  $\ell$  is the equivalent mean-free-path,  $\mu_0$  is the viscosity of mixture at the equilibrium temperature  $T_0$ ,  $p_0$  is the equilibrium pressure, and  $v_0$  is the characteristic molecular speed of the mixture given as

$$v_0 = \sqrt{2k_B T_0/m}, \quad (3)$$

$k_B$  is the Boltzmann constant,  $m$  is the mean molecular mass of mixture given as

$$m = C_0 m_1 + (1 - C_0) m_2, \quad (4)$$

$m_1$  and  $m_2$  being the molecular masses of species.

The solution of the problem is also determined by the gas-surface interaction law, but in the present work we are not interested in the influence of this interaction on the heat transfer. Therefore, the diffuse scattering of gaseous particles of both species on the plates is assumed.

The results will be given in terms of the dimensionless heat flux  $q$  defined by

$$q = -q'_x T_0 / (p_0 v_0 \Delta T), \quad (5)$$

which is always positive. Since the reduced heat flux  $q$  weakly depends on relative temperature drop  $\Delta T/T_0$ , the knowledge of this quantity allows us to use data obtained for a specific value of  $\Delta T/T_0$  over a wide range of this ratio.

We are going to calculate  $q$  as a function of the parameters  $\Delta T/T_0$ ,  $C_0$ , and  $\delta$  for both HS and AI potentials with the numerical error less than 0.5%. Moreover, the temperature and mole fraction profiles will be reported. A comparison of the results based on these two different potentials will allow us to study their influence on the heat transfer through a mixture.

## 3. Free-molecular regime

In the free-molecular regime ( $\delta \rightarrow 0$ ) the problem is easily solved for the diffuse scattering of gaseous particles on the walls, see e.g. Refs. [2,29]. In this case, the heat flux reads

$$q'_x = -\frac{4p_0 v_0}{\sqrt{\pi}} \left[ C_0 \sqrt{\frac{m}{m_1}} + (1 - C_0) \sqrt{\frac{m}{m_2}} \right] \frac{\theta \sqrt{1 - \theta^2}}{\sqrt{1 + \theta} + \sqrt{1 - \theta}}, \quad (6)$$

where

$$\theta = \Delta T / 2T_0. \quad (7)$$

The dimensionless heat flux (5) takes the form

$$q = \frac{2}{\sqrt{\pi}} \left[ C_0 \sqrt{\frac{m}{m_1}} + (1 - C_0) \sqrt{\frac{m}{m_2}} \right] \frac{\sqrt{1 - \theta^2}}{\sqrt{1 + \theta} + \sqrt{1 - \theta}}. \quad (8)$$

The temperature of the mixture is given as the geometric average of the surface temperatures, i.e.

$$T = T_0 \sqrt{1 - \theta^2}. \quad (9)$$

The mole fraction in this regime is equal to its equilibrium values  $C_0$ .

In order to estimate the deviation of the non-linear solution (8) from the linearized one, the expansion with respect to the temperature difference  $\Delta T/T_0$  is obtained as

$$q = \frac{1}{\sqrt{\pi}} \left[ C_0 \sqrt{\frac{m}{m_1}} + (1 - C_0) \sqrt{\frac{m}{m_2}} \right] \left[ 1 - \frac{3}{32} \left( \frac{\Delta T}{T_0} \right)^2 + O \left( \left( \frac{\Delta T}{T_0} \right)^4 \right) \right], \quad (10)$$

$$\frac{T}{T_0} = 1 - \frac{1}{8} \left( \frac{\Delta T}{T_0} \right)^2 + O \left( \left( \frac{\Delta T}{T_0} \right)^4 \right). \quad (11)$$

## 4. Hydrodynamic regime

In the hydrodynamic regime ( $\delta \gg 1$ ), the solution is based on the Fourier equation

$$q'_x = -\kappa (dT/dx), \quad (12)$$

where  $\kappa$  is the heat conductivity of mixture. Substituting the Fourier Eq. (12) into the energy conservation law, the equation for the temperature distribution is obtained as

$$\frac{d}{dx} \left( \kappa \frac{dT}{dx} \right) = 0. \quad (13)$$

The main difficulty to solve this equation is that the coefficient  $\kappa$  is a function of both temperature  $T$  and chemical composition  $C$  of mixture. The fact is that, in a non-isothermal mixture being at rest, a mole fraction gradient is established which is related to the temperature gradient as

$$dC/dx = -(k_T/T)(dT/dx), \quad (14)$$

where  $k_T$  is the thermal diffusion ratio which is also a function of local temperature and mole fraction. Thus, the mole fraction distribution is not known *a priori* that makes a rigorous analytical solution of Eq. (13) for mixture not possible.

The contribution of non-linear terms into the heat flux and temperature distribution can be estimated for a single gas. Like in the previous work [16], here we will restrict ourselves by the approximation assuming the following dependence of the thermal conductivity  $\kappa$  on temperature

$$\kappa(T) = \kappa_0 (T/T_0)^\omega, \quad (15)$$

where  $\kappa_0 = \kappa(T_0)$ . Then, Eq. (13) is easily solved as

$$T/T_0 = (A + Bx)^{1/(\omega+1)}. \quad (16)$$

Combining Eqs. (12) and (16), the heat flux is obtained as

$$q'_x = -\kappa_0 B. \quad (17)$$

The unknown constant  $A$  and  $B$  are found under the temperature continuity condition, i.e.

$$T = T_0 \pm \Delta T/2, \quad \text{at } x = \pm H/2, \quad (18)$$

so that

$$A = \left[ (1 + \theta)^{\omega+1} + (1 - \theta)^{\omega+1} \right] / 2, \quad (19)$$

$$B = \left[ (1 + \theta)^{\omega+1} - (1 - \theta)^{\omega+1} \right] / H, \quad (20)$$

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