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Viscous velocity, diffusion and thermal slip coefficients for ternary gas mixtures

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ABSTRACT

An approach is presented to determine the viscous velocity, diffusion and thermal slip coefficients for three-component gaseous mixtures. The gas is described by the McCormack linearized kinetic model. It is shown that two diffusion slip coefficients exist for a ternary mixture. The boundary problem is solved by the discrete velocity method. The slip coefficients are calculated and tabulated for He–Ar–Xe mixture at various values of the mole fractions for the hard-sphere and experimental potentials. It has been found that the diffusion and thermal slip coefficients are more sensitive to the interaction potential than the viscous one. Representative velocity profiles of the Knudsen layer are also shown. Furthermore, a test calculation is presented for pressure and mole fraction driven flows in a tube. The flow rates obtained by the slip solution are compared to the kinetic results. It is revealed that the slip flow approximation provides a relatively good estimation of the flow rates at higher rarefaction parameters. The present methodology and the tabulated data can be useful to determine the gaseous flow in the slip region for the ternary mixture.

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1. Introduction

Over the last years, significant effort has been made to study rarefied gas flows. This renewing interest has mainly been stimulated by the appearance of gaseous flows at the micro- and nano-scale [1] and new applications in vacuum science [2]. Gaseous flows can be characterized by the Knudsen number, the ratio of the molecular mean free path and the characteristic length scale of the flow. In the whole range of the rarefaction, the description should be based on the kinetic level [3]; however, if the flow is in the near continuum region, fluid dynamic equations can still be used with appropriate slip (or jump) boundary conditions for the macroscopic quantities.

The slip boundary condition is based on the viscous velocity, diffusion and thermal slip coefficients. The diffusion coefficient appears only for gaseous mixtures, of which species tend to acquire different speeds due to the finite rarefaction. At the kinetic level, the flow can be represented by the original Boltzmann or model kinetic equations. The viscous and thermal slip coefficients have been deduced for single gases by using direct numerical simulations [4–7] or variational approaches [8–10]. The viscous velocity, diffusion and thermal slip coefficients have been calculated for

binary mixtures [11–15]. The slip coefficients have been determined by experimental measurements for both single gases [16,17] and binary gas mixtures [18,19]. For a comprehensive overview on the subject and additional references, the reader may consult with the following review articles [20,21].

Recently, the McCormack kinetic model has been solved for pressure and mole-fraction driven three-component (ternary) gas mixture in long tubes [22]. It is interesting to determine the slip coefficients for flows of ternary mixtures. As it will be shown here, for multi-component gases, the diffusion phenomenon is more complex than for two-component mixtures.

The scope of this paper is to determine the viscous velocity, diffusion and thermal slip coefficients for ternary gas mixtures and to present a methodology for that purpose. The calculation is based on the McCormack linearized kinetic model. The boundary problem is solved by the discrete velocity method. As an example, the coefficients are calculated for He–Ar–Xe mixture at various values of the mole fraction and by using the hard-sphere or experimental potentials. Representative velocity profiles in the boundary layer are also shown. Finally, the coefficients are applied to pressure and mole fraction driven flows through a tube. The flow rates are deduced by using the slip flow assumption and compared to the corresponding kinetic results at higher values of the rarefaction parameter.

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2. Definition of the problems

The ternary gas mixture has three components, $\alpha = 1, 2$ and 3. The molecular masses and the densities of the species are denoted by m_α and n_α. The total density is $n = \sum_\alpha n_\alpha$. The partial mole fractions of the components are defined by $C_\alpha = n_\alpha/n$. The mean free path of the mixture is introduced such that

$$l_0 = \frac{\mu v_0}{P}, \tag{1}$$

where μ is the viscosity, $v_0 = \sqrt{2k_B T_0/m}$ is the characteristic molecular speed and P is the static pressure. Here, k_B, T_0 denote the Boltzmann constant and the reference temperature, and $m = \sum_\alpha C_\alpha m_\alpha$ is the average mass.

The flow configuration is described in Cartesian coordinate system (x', y', z'). The gas is bounded by a solid plate located at $x' = 0$, having its normal vector pointing toward direction x'. A steady gas flow is assumed along direction z'. The velocity has only z-component $\boldsymbol{u}' = (0, 0, u'_z)$. The boundary condition at the plate is diffuse reflection. In the following, the specific problems for the viscous, diffusion and thermal slip coefficients are discussed separately.

2.1. Viscous slip flow

For the viscous slip problem, there is a shear flow of the gas along the plate. The velocity far from the surface is given by

$$\lim_{x' \to \infty} u'_z(x') = v_0 \left(\sigma_P + \frac{x'}{l_0} \right) \epsilon, \tag{2}$$

where σ_P is the viscous slip coefficient and ϵ is the dimensionless gradient of the velocity. It is assumed that ϵ is small (i.e. $\epsilon \ll 1$); hence, the gas is slightly perturbed around equilibrium.

Due to the smallness of ϵ, the problem can be linearized. The velocity is decomposed as

$$\boldsymbol{u}' = (\boldsymbol{u}'^K + \boldsymbol{u}'^R)\epsilon, \tag{3}$$

where $\boldsymbol{u}'^K$ contains the kinetic boundary layer and $\boldsymbol{u}'^R = (0, 0, u'^R_z)$ is a reference velocity profile with $u'^R_z(x') = x'/l_0$. The viscous slip coefficient can be obtained such that

$$\sigma_P = \lim_{x' \to \infty} \frac{u'^K_z(x')}{v_0}. \tag{4}$$

The gas mixture is described at the kinetic level by the velocity distribution function of the molecules $f_\alpha(\boldsymbol{v}', x', y', z')$ with $\boldsymbol{v}'$ denoting the molecular velocity. This function is linearized as

$$f_\alpha = f_\alpha^{(0)}(\boldsymbol{v}', x')[1 + \epsilon h_\alpha(\boldsymbol{v}', x', y', z')], \tag{5}$$

where h_α is the perturbation function and

$$f_\alpha^{(0)}(\boldsymbol{v}', x') = \pi^{-3/2} n_{0\alpha} v_{0\alpha}^{-3} \exp \left[(\boldsymbol{v}' - \boldsymbol{u}'^R \epsilon)^2 / v_{0\alpha}^2 \right] \tag{6}$$

is the Maxwell equilibrium function. Here, $v_{0\alpha} = v_0 \sqrt{m_\alpha/m}$ and $n_{0\alpha}$ is an assumed equilibrium for the densities.

2.2. Diffusion slip flow

In the case of the diffusion flow, the flow is generated by non-zero gradients of the densities of the species along the plate with the constraint that the static pressure is constant. This means that the flow is induced by the gradients of the mole-fractions along the tangential direction, but there is no pressure gradient. The diffusion flow can appear in engineering applications when the mole-fraction is non-uniform. It is a rarefaction phenomenon, like the viscous velocity slip, and does not appear in the hydrodynamic

limit. The mole-fraction gradients cause a constant bulk velocity of the mixture as a whole far from the surface.

The dimensionless gradients of the densities are defined by

$$X_\alpha = \frac{\partial n_\alpha}{\partial z'} \frac{l_0}{n_{0\alpha}}. \tag{7}$$

The constraint of the constant pressure can be written as

$$\sum_{\alpha=1}^{3} C_\alpha X_\alpha = 0. \tag{8}$$

It is assumed that the density gradients are small ($X_\alpha \ll 1$). Hence, the flow is slightly perturbed around equilibrium, and a linearized description can be applied. In the case of a binary mixture, Eq. (8) indicates that one of the driving terms can be chosen freely, while the another one is determined by the constraint. Hence, for binary mixtures, there is only one mole-fraction gradient which can be defined freely for the diffusion problem (see e.g. Ref. [13]). However, for ternary gas mixtures, it follows from Eq. (8) that two of the three X_α can be chosen freely. This means that due to the linearization, the overall problem can be decomposed of two sub-problems. In this work, two different flows with

$$X_1 = C_2\eta, \qquad X_2 = -C_1\eta, \qquad X_3 = 0 \tag{9}$$

or

$$X_1 = C_3\eta, \qquad X_2 = 0, \qquad X_3 = -C_1\eta \tag{10}$$

are considered. Here, η is a small parameter ($\eta \ll 1$), which plays the same role as ϵ in the case of the viscous problem. It follows from the above discussion that two diffusion slip coefficients exist for a ternary gas mixtures. In fact, Eq. (8) indicates that $N - 1$ diffusion slip coefficients exist if the gas has N number of components.

For flows defined by Eq. (9) or (10), the velocity of the mixture far from the surface is constant

$$\lim_{x' \to \infty} \frac{u'_z(x')}{v_0} = \sigma_C^{(k)}\eta, \tag{11}$$

where $\sigma_C^{(j)}$ is defined as the diffusion slip coefficient having two components. Here, superscript $j = 1, 2$ is introduced in order to denote the two different flows defined by either Eq. (9) or (10), respectively.

The meaning of the two diffusion slip coefficients is that they provide the bulk velocity of the mixture far from the surface for the above defined two sub-problems, Eqs. (9)–(10). Due to the linearization, for arbitrary small density gradients obeying the constraint of Eq. (8), the bulk velocity can be determined by using the density gradients and the two diffusion slip coefficients by superposition.

Let us consider an example. Suppose that the mole-fractions of the components vary along the plate, but the pressure is constant; hence, Eq. (8) holds. By using the definition of the sub-problems, Eqs. (9)–(10), and the diffusion slip coefficients, Eq. (11), the bulk velocity far from the surface can be obtained by

$$\lim_{x' \to \infty} \frac{u'_z(x')}{v_0} = -\sigma_C^{(1)} \frac{X_2}{C_1} - \sigma_C^{(2)} \frac{X_3}{C_1}. \tag{12}$$

Therefore, if the mole-fractions C_α and the density gradients X_α of the components are given, the bulk velocity far from the surface can be calculated by using Eq. (12) for the diffusion flow problem. Here, it is useful to emphasize that the dimensionless density gradients are proportional to the mean free path, Eq. (7). Hence, if the mean free path is doubled for example, the velocity slip is also doubled. This indicates that the diffusion slip velocity is proportional to the Knudsen number, which is defined as $Kn \propto l_0/L_C$, where L_C denotes the characteristic macroscopic size of the