

A self-diffusion problem in a dilute gas in steady Couette flow is analyzed. The results are obtained from a kinetic model proposed for a multicomponent gas. This model is constructed by replacing the Boltzmann collision operator by a relaxation-time term, in the same spirit as in the BGK equation for a single gas. Using a Chapman-Enskog-like expansion around the steady Couette flow, a self-diffusion tensor is obtained, that is a highly nonlinear function of the velocity gradient. Finally, the velocity distribution function of tagged particles is given explicitly.

1. INTRODUCTION

The kinetic theory of dilute gases is based on the Boltzmann equation (BE). However, due to the complex structure of the Boltzmann collision integral, it is a very hard task to find explicit results. This problem has given rise to the search of mathematically simpler kinetic equations that retain the main physical properties, namely the conservation of mass, momentum and energy. For a single gas, perhaps the most used kinetic model is the one proposed by Bhatnagar, Gross, and Krook (BGK). In this model, the Boltzmann collision integral is approximated by a relaxation term with a characteristic time that is modeled according to the interaction potential^{1,4} considered. In the case of multicomponent systems, several models^{5,6} have been suggested within the same spirit. Like the Boltzmann collision operator, these models conserve mass, momentum and energy. However, and in contrast to the set of Boltzmann equations, none of them is compatible with a closed kinetic equation for the total distribution function in the particular case of mechanically identical components (self-diffusion case). Anyway, it must be noticed that these models are usually applied to the study of transport phenomena in disparate-mass binary gases, and, in this limit the above consistency property is not necessary.

Recently, we have constructed a kinetic model for a multicomponent gas that recovers the BGK equation in the self-diffusion case. In the same manner as in previous models, it conserves mass, momentum and energy. Although the model is not restricted to any range of mass ratios, it is specially appropriate to study systems constituted by like particles. In the model, the self- and cross-collision terms take other than the local state of the system seen as a whole. On the other hand, the model may be useful to study general transport properties, because the proposed collision term is valid beyond the linear regime (Navier-Stokes hydrodynamic order). For the sake of simplicity the model is restricted to Maxwell interaction, although the generalization to other interaction potentials can also be made. The aim of this paper is to use the above model to analyze the self-diffusion transport coefficient of a dilute gas in steady planar Couette flow. For this state the normal component of the BGK equation is arbitrarily far from equilibrium, known^{7,8} in order to evaluate the self-diffusion coefficient we use a Chapman-Enskog-like expansion around the above solution. Therefore, we get a transport coefficient tensor that is a highly nonlinear function of the velocity gradient. Although our results are restricted to first order in

concentration gradient, it would not be difficult to proceed beyond that order.

The plan of the paper is as follows. In Section 2, the model is introduced. It is shown that it is compatible with the BGK equation for a single gas and the parameters that define the BGK reference distribution function are explicitly given. In Section 3, self-diffusion in steady Couette flow is considered. The knowledge of the solution to the BGK equation in the above state allows us to find a generalized Fick's law. Due to that anisotropy of the system, a self-diffusion tensor, rather than a scalar, appears. Finally, some concluding remarks are made in Section 4.

2. KINETIC MODEL

We consider an N-component mixture. Let us suppose that the time evolution of the system is described by the following set of coupled equations

$$\frac{\partial f_i}{\partial t} + \vec{\nabla} \cdot \vec{v} f_i = - \sum_{j=1}^N \zeta_{ij} (f_i^R - f_{ij}^R) \tag{1}$$

$$= \sum_{j=1}^N K_{ij}$$

where $f_i(\vec{r}, \vec{v}; t)$ is the one-particle distribution function of species i . ζ_{ij} is an effective collision frequency of a particle of species i with a particle of species j . It has the general property $n_i \zeta_{ij} = n_j \zeta_{ji}$. Also, f_i^R is a reference distribution function whose functional dependence on hydrodynamic fields will be determined by requiring K_{ij} to be compatible with the BGK equation for a single gas when a system of mechanically identical particles is considered. For this reason, we propose for f_{ij} the form

$$f_{ij}^R = n_i \left(\frac{m_i}{2\pi k_B T} \right)^{3/2} \exp \left(- \frac{m_i}{2k_B T} v^2 \right) [1 + A_{ij} \vec{E}_{ij} \cdot \vec{v} + C_{ij} v^2] \tag{2}$$

where $\vec{v} = \vec{v} - \vec{u}$ is the peculiar velocity, n_i is the mass of a particle of species i , n_i is the number density of species i , \vec{u} is the local velocity of the mixture and T is the local temperature of the mixture. The parameters A_{ij} , \vec{E}_{ij} and C_{ij} will be obtained later. The expression (2) resembles some kind of linearization around a local equilibrium characterized by the hydrodynamic fields of the system seen as a whole. The collision operator K_{ij} depends on species i and j as well as on the state of the mixture. The physical picture of the model is that the main global effect of the collisions on particles of species i is to produce a tendency toward the local equilibrium state of the mixture. The details of the collisions with species j are taken into account through the parameters A_{ij} , \vec{E}_{ij} , and C_{ij} . In this way, the model seems to be more adequate to study systems in which masses are of the same order.

In order to specify the parameters A_{ij} , \vec{E}_{ij} and C_{ij} the following conditions are required:

- (i) The kinetic model must preserve conservation of mass, momentum and energy of the total mixture; and conservation of mass for each

separate component:

$$\int d\vec{v} K_{ij} = 0 \tag{3}$$

$$\int d\vec{v} m_i \vec{v} K_{ij} + \int d\vec{v} m_j \vec{v} K_{ji} = 0$$

$$\int d\vec{v} m_i v^2 K_{ij} + \int d\vec{v} m_j v^2 K_{ji} = 0$$

These conditions are sufficient to guarantee that our model reduces to the BGK equation when mechanically equivalent particles are considered. For that, it is necessary that the collision frequency ζ_{ij} appearing in Eq. (1) has the property,

$$\zeta = \sum_j \zeta_{ij} \tag{4}$$

for any species i . This property is verified by the exact collision frequency given by the BE, and it holds for any interaction potential. Obviously, relation (4) defines the collision frequency of the system ζ . Therefore, Eq. (4) leads to that either ζ_{ij} does not depend on the temperature (Maxwell molecules) or that it depends only on the mixture temperature T . Here, we restrict ourselves to Maxwell molecules. The model can be extended to other potentials if one assumes that ζ_{ij} only depends on T .

(ii) The collisional transfer of momentum and energy must be the same as that of the Boltzmann equation for Maxwell molecules. This condition, along with Eqs. (3), (4) give the following expressions for the parameters defining the model:

$$A_{ij} = -3 \frac{k_B T}{m_i} C_{ij} \tag{5}$$

$$\vec{E}_{ij} = \frac{m_i}{k_B T} (\vec{u}_{ij} - \vec{u}) \tag{6}$$

$$C_{ij} = \frac{m_i}{2k_B T} \left[\frac{T_j - T}{T} + 3 \frac{m_j}{k_B T} (\vec{u}_{ij} - \vec{u})^2 \right] \tag{7}$$

where we have introduced the quantities

$$\vec{u}_{ij} = (m_i \vec{u}_i + m_j \vec{u}_j) / (m_i + m_j) \tag{8}$$

$$T_{ij} = T_i + 2 \left[\frac{m_i m_j}{m_i + m_j} \right]^2 \left[\frac{m_i}{6k_B} (\vec{u}_i - \vec{u}_j) \right] \tag{9}$$

Here, \vec{u}_i is the local velocity of species i and T_i is the local temperature of species i .

3. SELF-DIFFUSION IN STEADY COUETTE FLOW

We consider a dilute gas in a stationary state with temperature and velocity gradients (steady Couette flow). The physical situation

considered is the steady state of a gas between two parallel plates kept at different temperatures and in relative motion. An exact normal solution to the BGK equation describing heat and momentum transport in that state has been constructed. Our aim here is to study the self-diffusion coefficient when the system seen as a whole is in this steady Couette flow. This will be done with the kinetic model described in the previous section for Maxwell molecules.

For a steady state with gradients along the y direction only, a "normal" solution to the BGK equation can be written in the form

$$f(y, \vec{v}) = [1 + \frac{y}{\zeta} \frac{\partial}{\partial y}]^{-1} f_0(y, \vec{v}) \tag{10}$$

$$= \sum_{k=0}^{\infty} (-1)^k [\frac{y}{\zeta} \frac{\partial}{\partial y}]^k f_0(y, \vec{v})$$

where $f_0(y, \vec{v})$ is the local equilibrium distribution function. Of course, this expression is only formal because the collision frequency ζ and the local distribution f_0 are both functionals of the distribution f . Besides, the functional form of ζ depends on the interaction potential considered. Nevertheless, the influence of the interaction on ζ can be scaled out by introducing an auxiliary variable ζ through the relation

$$d\zeta = \zeta(y) dy \tag{11}$$

Taking into account this relation, it can be shown that the BGK equation admits a normal solution characterized by the profiles

$$p = nk_B T = \text{const.}, \tag{12}$$

$$\frac{\partial u_x}{\partial \zeta} = \alpha = \text{const.}, \tag{13}$$

$$\frac{\partial^2 n}{\partial \zeta^2} = -\frac{2m}{k_B} \gamma = \text{const.}, \tag{14}$$

provided that the dimensionless parameters γ and α are related through the equation

$$\gamma \frac{d}{d\zeta} [2\gamma \frac{d}{d\zeta} (\gamma \zeta)] + (3\gamma - \alpha^2) \frac{d}{d\zeta} (\gamma \zeta) = 0, \tag{15}$$

where

$$F(\gamma) = \frac{2}{\gamma} \int_0^{\infty} du u \exp(-u^2/2) K_0(2\gamma^{-1/4} u^{1/2}), \tag{16}$$

being K_0 the zeroth-order modified Bessel function. From the solution (10) the fluxes can be calculated. The irreversible momentum and heat fluxes happen to be nonanalytic functions of the velocity gradient, the last flux being linear in the temperature gradient.

Suppose now that some particles of the system in steady Couette flow are tagged, but otherwise all the particles are mechanically equivalent. Let $h(y, \vec{v}; t)$ be the distribution function of the tagged particles, whose temporal evolution will be assumed to be governed by the kinetic model defined by Eqs. (5)-(9). In the particular case of

identical masses, the kinetic equation for $h(\vec{x}, \vec{v}, t)$ becomes

$$\frac{\partial h}{\partial t} + \vec{v} \cdot \nabla h = -\zeta (h - \phi), \tag{17}$$

where ϕ is a reference function given by

$$\phi = [\frac{n_1}{n} + \frac{m}{2D} \vec{v} \cdot \vec{v} + \frac{1}{2D} (\frac{m}{2k_B T} v^2 - \frac{3}{2}) (p_1 - n_1 k_B T)] f_0 \tag{18}$$

Here, n_1 is the number density of tagged particles, $p = nk_B T$ is the pressure,

$$\vec{v} = \int d\vec{v}' \vec{v}' h, \tag{19}$$

is the flux of tagged particles, and

$$p_1 = \frac{1}{3} \int d\vec{v}' m v'^2 h, \tag{20}$$

is a partial pressure of tagged particles. The method analogous to the Chapman-Enskog. Nevertheless, we take steady Couette flow, rather than local equilibrium, as the zeroth order reference state. In this way the transport coefficients obtained retain the full nonlinear dependence on the velocity and temperature gradients. Thus, we look for normal solutions to Eq. (17) by expanding

$$h = h^{(0)} + \epsilon h^{(1)} + \epsilon^2 h^{(2)} + \dots, \tag{21}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial t} + \epsilon^2 \frac{\partial}{\partial t} + \dots, \tag{22}$$

where ϵ is an auxiliary parameter measuring the nonuniformity of the concentration of tagged particles. The definition of $\epsilon_k/\partial t$ is taken from the usual kth approximation to the hydrodynamic balance equations. In our analysis, we shall restrict ourselves to first order in ϵ .

By introducing the expansions (21) and (22) into Eq. (17) and collecting terms of equal power in ϵ , one gets in the lowest order the equation

$$\vec{v} \cdot \nabla h^{(0)} = -\zeta (h^{(0)} - \phi^{(0)}), \tag{23}$$

whose solution is

$$h^{(0)}(y, \vec{v}; t) = \frac{n_1(y; t)}{n(y)} f(y, \vec{v}), \tag{24}$$

where $f(y, \vec{v})$ is the solution of Eq. (10). By substituting Eq. (24) into the first order Chapman-Enskog approximation, one obtains that

$$h^{(1)} = -\frac{1}{\zeta} \nabla \cdot \nabla \left(\frac{n_1}{n} \right) \mathbf{e} + \left[\frac{m}{2\beta} \nabla \cdot \mathbf{J}^{(1)} + \frac{1}{2\beta} \left(-\frac{mV^2}{2k_B} - \frac{3}{2} \right) p_1^{(1)} \right] \mathbf{e}_0, \quad (25)$$

where $\mathbf{J}^{(1)}$ and $p_1^{(1)}$ are defined from the distribution $h^{(1)}$. Taking velocity moments in Eq. (25) one gets

$$J_1^{(1)} = -\frac{2}{m} \frac{\beta}{\zeta} D_{1k} \frac{\partial}{\partial x_k} \left(\frac{n_1}{n} \right), \quad (26)$$

$$p_1^{(1)} = -\frac{2}{3} \frac{\beta k_B}{m} \frac{\alpha^2}{\zeta^2} \frac{\partial^2}{\partial y^2} F(\gamma) \frac{\partial}{\partial y} \frac{\partial}{\partial y} \left(-\frac{n_1}{n} \right). \quad (27)$$

Equation (26) corresponds to a generalization of Fick's law, where D_{ik} is the dimensionless self-diffusion tensor, whose nonzero components are given by

$$D_{xx} = 1 - 2\gamma \left(1 - \frac{\alpha^2}{\gamma} \right) \left(1 + \gamma \frac{d}{d\gamma} \right) F(\gamma), \quad (28)$$

$$D_{zz} = 1 - 2\gamma \left(1 + \gamma \frac{d}{d\gamma} \right) F(\gamma), \quad (29)$$

$$D_{yy} = 3 - (D_{xx} + D_{zz}), \quad (30)$$

$$D_{xy} = D_{yx} = -\alpha F(\gamma) \quad (31)$$

Equations (28)-(31) have been derived keeping the first order in the gradient of concentration of tagged particles, but all the orders in the velocity and temperature gradients are included. Both gradients induce cross effects in the self-diffusion of particles. Thus, a gradient of concentration along the direction of the velocity flow (x -axis) creates a transport of tagged particles parallel to the velocity and temperature gradients (y -axis). In contrast to what happens in the uniform shear flow problem¹¹, the self-diffusion tensor is symmetric and its trace is a constant.

In addition to the fluxes, the knowledge of the explicit form of the distribution of the whole system $f(\mathbf{v}, \mathbf{v}')$ allows us to obtain the first-order velocity distribution function of tagged particles $h^{(1)}(\mathbf{r}, \mathbf{v}; t)$. Thus, by substituting Eqs. (26) and (27) into Eq. (25) and after some algebra, $h^{(1)}$ can be written in the form

$$h^{(1)}(\mathbf{r}, \mathbf{v}; t) = -\frac{1}{\zeta} \mathbf{e}_0 \left[\frac{\beta}{m} V_k + V_{1k} D_{1k} - \frac{1}{3} \frac{\alpha^2}{\gamma} \left(\frac{mV^2}{2k_B} - \frac{3}{2} \right) \right] \times \frac{k_B}{m} \frac{\partial}{\partial y} \frac{\partial}{\partial y} \delta_{ky} \left] \frac{\partial}{\partial x_k} \left(\frac{n_1}{n} \right) \quad (32)$$

IV. FINAL REMARKS

We have proposed a kinetic model for a multicomponent gas mixture. The model can be seen as an extension of the BGK equation for a single gas. According to the proposed collision terms, the model is expected to be suitable for systems like particles. Besides, the model is not restricted to near-equilibrium states, and then it may be useful

to study general transport phenomena. As an application of this model, we have analyzed the self-diffusion problem when the system seen as a whole is in steady Couette flow far from equilibrium. In this situation, an explicit solution to the BGK equation is known. Using a Chapman-Enskog-like expansion around the Couette flow state, the flux of tagged particles to first order has been obtained. A self-diffusion tensor can be identified, which is a highly nonlinear function of the velocity gradient. Due to the explicit knowledge of the Couette flow distribution, the velocity distribution function of the tagged particles $h^{(1)}(\mathbf{r}, \mathbf{v}; t)$ can be given explicitly. Work now is in progress to study the dependence of $h^{(1)}(\mathbf{r}, \mathbf{v}; t)$ on the imposed gradients.

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