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Accelerated discrete velocity method for axial-symmetric flows of gaseous mixtures as defined by the McCormack kinetic model

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ABSTRACT

An accelerated discrete velocity method is presented to calculate the steady axial-symmetric flows of gaseous mixtures defined by the McCormack kinetic model. The scheme is formulated in cylindrical coordinates. Diffusion equations for the macroscopic velocity and the heat-flow are derived on the basis of the projected McCormack equations. The solutions of the kinetic equations are carried out iteratively by using the discrete velocity method. The diffusion equations are also solved in each stage of the iteration in order to accelerate the scheme. Pressure driven flows of He/Xe and Ne/Ar mixtures through a cylindrical tube are simulated in order to study the computational performance of the approach. It is shown that the required number of iterations and the computational times are significantly reduced at intermediate and large values of the rarefaction parameter by using the accelerated method. In the hydrodynamic limit, the flow rates of the components converge to the corresponding slip flow results. Flows driven by mole fraction gradient are also successfully simulated. Typical velocity and heat-flow profiles for pressure driven flow of He/Xe mixture are shown and commented on.

1. Introduction

The numerical solution of the Boltzmann or other kinetic equations has received much attention in the scientific community over the last years due to the increasing interest in new technologies at the micro- and nano-scale, i.e. gaseous micro- and nano-fluidics [1,2], and more traditional applications in rarefied gas dynamics, such as vacuum science [3].

One of the most accurate treatments for solving kinetic equations is the discrete velocity method (DVM), where the microscopic velocity and spatial spaces are discretized, the differential operators and the integrals are approximated by finite differences and quadratures and the resulting discrete equations are solved computationally. The method has extensively been used for the solution of linearized kinetic equations describing the flows of rarefied single gases through various channels [4,5]. For gaseous mixtures, the McCormack kinetic model has also been solved by the DVM for several flow configurations [6,7]. However, it is well-known that the original DVM has some drawbacks near the hydrodynamic limit: the iteration slowly converges and the results are biased by the accumulated rounding errors. To overcome this difficulty, the synthetic type acceleration can be used successfully [8,9]. The accelerated DVM has been developed for rectangular and triangular geometries [10–12], which can be described in Cartesian coordinates. Recently, it has been applied for axial-symmetric flows of single gases [13]. It is straightforward to extend the method for the more complicated case of axial-symmetric flows of gaseous mixtures. Since the development for mixtures is more complex and contains several non-trivial derivations, it is useful to present the case of gaseous mixtures in a separate communication.

In this paper, an accelerated discrete velocity method is developed for calculating the steady axial-symmetric flows of gaseous mixtures on the basis of the McCormack kinetic model. The method is formulated in cylindrical coordinates. Two diffusion equations for the macroscopic velocity and the heat-flow are derived on the basis of the moments of the reduced McCormack equations. The solution of the kinetic problem is carried out in an iterative manner by using the discrete velocity method. The two diffusion equations are used to accelerate the iteration performance. They are solved in a coupled iteration with the original kinetic equations by the finite-difference method. Pressure driven flows of He/Xe and Ne/Ar mixtures are simulated in order to analyze the standard and accelerated schemes. The number of iterations and the computational times are studied. Mole fraction driven flows are also calculated for validation purposes. Typical velocity and heat-flow profiles of pressure driven flow of He/Xe mixture at various rarefaction parameters are shown.

2. Definition of the problem

The steady flow of a binary gas mixture through a cylindrical tube with radius R and length L is considered. The tube is assumed to be long, $R \ll L$. The axis of the tube lies along the z' coordinate

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direction, while its cross section is located in the (x', y') coordinate sheet. Dimensionless coordinates are introduced according to $x = x'/R$, $y = y'/R$ and $z = z'/R$. On the cross section, (r, ϕ) polar coordinates are also introduced such that $x = r\cos(\phi)$ and $y = r\sin(\phi)$.

The densities and the molecular masses of species $\alpha = 1, 2$ are denoted by $n_\alpha(z)$ and m_α. The mole fraction of the first component is defined by $C = n_1/n$, where $n = n_1 + n_2$ is the total density. The flow is characterized by the rarefaction parameter

$$\delta = \frac{PR}{\mu v_0}, \tag{1}$$

where P is the pressure, μ is the viscosity and $v_0 = \sqrt{2k_BT/m}$ is the characteristic molecular speed. Here, k_B is the Boltzmann constant, T is the temperature and $m = Cm_1 + (1-C)m_2$ is the average mass.

The flow is described by the velocity distribution function of the molecules $f_\alpha(\boldsymbol{v}, r, \phi, z)$, where $\boldsymbol{v}$ denotes the molecular speed. Since the tube is long, the speed of the gas is small compared to the characteristic molecular speed and the distribution function can be linearized as $f_\alpha(\boldsymbol{v}, r, \phi, z) = f_\alpha^{(0)}(\boldsymbol{v}, z)[1 + h_\alpha(\boldsymbol{v}, r, \phi)]$, where

$$f_\alpha^{(0)}(\boldsymbol{v}, z) = n_\alpha(z)\left(\frac{m_\alpha}{2\pi k_BT}\right)^{3/2}\exp\left(-\frac{m_\alpha v^2}{2k_BT}\right) \tag{2}$$

is the local equilibrium and $h_\alpha(\boldsymbol{v}, r, \phi)$ denotes the perturbation function. For later purposes, dimensionless molecular velocities and their representations in Descartes and cylindrical coordinates are introduced according to $\boldsymbol{c}_\alpha = (\boldsymbol{v}/v_0)\sqrt{m_\alpha/m}$ and $c_{\alpha x} = c_{\alpha T}\cos(\varphi)$, $c_{\alpha y} = c_{\alpha T}\sin(\varphi)$, $c_{\alpha z}$. Here, $c_{\alpha T} = \sqrt{c_{\alpha x}^2 + c_{\alpha y}^2}$. The absolute value of $\boldsymbol{c}_\alpha$ is denoted as c_α. The Descartes and cylindrical representations are used interchangeably in the following.

The present method is designed for isothermal flows driven by arbitrary gradients of the component densities along the axis of the tube. In this way, two types of flow, namely flows driven by pressure (P) or mole fraction (C) gradients are considered. The dimensionless gradients of the relevant local macroscopic quantities for these two types of flow are defined by $X_P = (1/n)\partial n/\partial z$, $X_C = (1/C)\partial C/\partial z$, respectively. The method can easily be modified to simulate temperature gradient driven flows as well. The modified method for temperature driven flows has been checked by the author, and it works well. However, these results are not considered in this paper. The author may report the results elsewhere.

The flow of the mixture is described by the McCormack kinetic equation [14] along the radial coordinate ($\phi = 0$) such that

$$\begin{aligned} c_{\alpha x}\frac{\partial h_\alpha}{\partial r} - \frac{c_{\alpha y}}{r}\frac{\partial h_\alpha}{\partial \varphi} &= -\gamma_\alpha\omega_\alpha h_\alpha + \omega_\alpha\sqrt{\frac{m_\alpha}{m}}\left[2A_\alpha c_{\alpha z}\right. \\ &\quad \left. + 4B_\alpha c_{\alpha x}c_{\alpha z} + \frac{4}{5}C_\alpha c_{\alpha z}\left(c_\alpha^2 - \frac{5}{2}\right)\right] \\ &\quad - [X_P + \eta_\alpha X_C]\,c_{\alpha z}, \end{aligned} \tag{3}$$

where

$$A_\alpha = \gamma_\alpha u_\alpha - \nu_{\alpha\beta}^{(1)}(u_\alpha - u_\beta) - \frac{1}{2}\nu_{\alpha\beta}^{(2)}\left(q_\alpha - \frac{m_\alpha}{m_\beta}q_\beta\right), \tag{4}$$

$$B_\alpha = \kappa_\alpha\sqrt{\frac{m}{m_\alpha}}p_\alpha + \nu_{\alpha\beta}^{(4)}\sqrt{\frac{m}{m_\alpha}}p_\beta, \tag{5}$$

$$C_\alpha = \lambda_\alpha q_\alpha + \nu_{\alpha\beta}^{(6)}\sqrt{\frac{m_\beta}{m_\alpha}}q_\beta - \frac{5}{4}\nu_{\alpha\beta}^{(2)}(u_\alpha - u_\beta) \tag{6}$$

and

$$\omega_\alpha = \sqrt{\frac{m_\alpha}{m}}\left[\frac{C}{\gamma_1} + \frac{1-C}{\gamma_2}\right]\delta. \tag{7}$$

In these expressions, $\alpha, \beta = 1, 2$ and $\beta \neq \alpha$. The quantities γ_α, $\nu_{\alpha\beta}^{(k)}$, λ_α and κ_α are collision frequencies, which can be deduced for a particular interaction model and can be found in Ref. [15] for the hard-sphere interaction. It is noted that λ_α and κ_α are the linear combinations of $\nu_{\alpha\beta}^{(k)}$. The collision frequencies, γ_α and $\nu_{\alpha\beta}^{(k)}$, for hard-sphere molecules can also be found in Refs. [6,7,10,12]. In addition, $\eta_1 = 1$ and $\eta_2 = -C/(1-C)$ for the mole fraction driven flow.

The relevant macroscopic quantities, the axial velocity, the rz component of the shear stress and the axial heat-flow, are the moments of the perturbation function

$$u_\alpha = \pi^{-3/2}\sqrt{\frac{m}{m_\alpha}}\int d\boldsymbol{c}_\alpha h_\alpha c_{\alpha z}\exp(-c_\alpha^2), \tag{8}$$

$$p_\alpha = \pi^{-3/2}\int d\boldsymbol{c}_\alpha h_\alpha c_{\alpha x}c_{\alpha z}\exp(-c_\alpha^2), \tag{9}$$

$$q_\alpha = \pi^{-3/2}\sqrt{\frac{m}{m_\alpha}}\int d\boldsymbol{c}_\alpha h_\alpha c_{\alpha z}\left(c_\alpha^2 - \frac{5}{2}\right)\exp(-c_\alpha^2). \tag{10}$$

The kinetic equation, Eq. (3), is supplemented with the boundary condition at the wall of the tube. In the present work, the diffuse reflection boundary condition is assumed. The condition for perturbation function can be written by $h_\alpha(\boldsymbol{c}_\alpha, 1) = 0$ for the incoming velocity directions $c_{\alpha x} < 0$.

One of the interests of the paper is in the dimensionless component flow rates defined by

$$G_\alpha = 4\int_0^1 dru_\alpha(r)r. \tag{11}$$

2.1. Projected formalism

The above formulation can be simplified by introducing the new variables

$$\Phi_\alpha^{(1)} = \pi^{-1/2}\sqrt{\frac{m}{m_\alpha}}\int_{-\infty}^{+\infty} dc_{\alpha z}h_\alpha c_{\alpha z}\exp(-c_{\alpha z}^2), \tag{12}$$

$$\Phi_\alpha^{(2)} = \pi^{-1/2}\sqrt{\frac{m}{m_\alpha}}\int_{-\infty}^{+\infty} dc_{\alpha z}h_\alpha c_{\alpha z}\left(c_{\alpha z}^2 - \frac{3}{2}\right)\exp(-c_{\alpha z}^2). \tag{13}$$

In terms of these two quantities, the kinetic equation can be written by

$$\begin{aligned} &c_{\alpha x}\frac{\partial \Phi_\alpha^{(1)}}{\partial r} - \frac{c_{\alpha y}}{r}\frac{\partial \Phi_\alpha^{(1)}}{\partial \varphi} \\ &\quad = -\gamma_\alpha\omega_\alpha\Phi_\alpha^{(1)} + \omega_\alpha\left[A_\alpha + 2B_\alpha c_{\alpha x} + \frac{2}{5}C_\alpha\left(c_{\alpha T}^2 - 1\right)\right] \\ &\qquad - \frac{1}{2}\sqrt{\frac{m}{m_\alpha}}[X_P + \eta_\alpha X_C], \end{aligned} \tag{14}$$

$$c_{\alpha x}\frac{\partial \Phi_\alpha^{(2)}}{\partial r} - \frac{c_{\alpha y}}{r}\frac{\partial \Phi_\alpha^{(2)}}{\partial \varphi} = -\gamma_\alpha\omega_\alpha\Phi_\alpha^{(2)} + \omega_\alpha\frac{3}{5}C_\alpha. \tag{15}$$

The macroscopic quantities are given by

$$u_\alpha = \pi^{-1}\int_{-\infty}^{+\infty} dc_{\alpha x}\int_{-\infty}^{+\infty} dc_{\alpha y}\Phi_\alpha^{(1)}\exp(-c_{\alpha T}^2), \tag{16}$$

$$p_\alpha = \pi^{-1}\sqrt{\frac{m_\alpha}{m}}\int_{-\infty}^{+\infty} dc_{\alpha x}\int_{-\infty}^{+\infty} dc_{\alpha y}\Phi_\alpha^{(1)}c_{\alpha x}\exp(-c_{\alpha T}^2), \tag{17}$$

$$\begin{aligned} q_\alpha &= \pi^{-1}\int_{-\infty}^{+\infty} dc_{\alpha x} \\ &\quad \times \int_{-\infty}^{+\infty} dc_{\alpha y}[\Phi_\alpha^{(1)}(c_{\alpha T}^2 - 1) + \Phi_\alpha^{(2)}]\exp(-c_{\alpha T}^2). \end{aligned} \tag{18}$$