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An accelerated discrete velocity method for flows of rarefied ternary gas mixtures in long rectangular channels

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ABSTRACT

An accelerated discrete velocity method is presented for rarefied three-component gas mixtures flowing through long rectangular ducts. The scheme is developed on the basis of the McCormack linearized kinetic model. Diffusion equations are derived for the velocity and the heat flow vector. The kinetic and diffusion equations are solved in a coupled iteration. Simulations are carried out for He–Ar–Xe mixture to test the computational performance of the scheme for pressure driven flow. It is shown that the accelerated method requires a fewer number of iterations and smaller computational time in a large part of the gas rarefaction from the transition region to the hydrodynamic limit than the non-accelerated one. These quantities are studied as a function of the convergence parameter also. The flow rates as a function of the rarefaction parameter and representative velocity profiles are shown. A good agreement is found between the total flow rate and the corresponding slip flow value at large rarefaction parameters. The present approach can be useful for fast computation of flows of ternary gas mixtures in long rectangular channels.

1. Introduction

Over the last few years, the numerical solution of kinetic equations has received significant attention in fluid and gas dynamic communities. Such an interest has mainly been stimulated by the emergence of micro-scale gas flows [1] and newer applications in vacuum technology [2].

Kinetic equations are integro-differential, and except a few cases where analytical results are available, they can be solved numerically. The techniques used in their solution can be classified as probabilistic or deterministic. Among the probabilistic approaches, the direct simulation Monte Carlo is most popular [3]. The deterministic techniques are typically based on the discretization of the spatial (temporal) and molecular velocity spaces [4]. Such approaches are generally referred as the discrete velocity methods. Flows of single gases through various long channels with circular [5], rectangular [6], annular [7], triangular [8,9], trapezoidal [9] or double-trapezoidal [10] cross sections have been solved by the discrete velocity method using kinetic iteration. Other discrete velocity calculations on the basis of implicit time marching schemes have also been performed [11–13]. These later techniques can be applied on unstructured grids and typically use parallel computation. Flows of binary gas mixtures in long channels have also been solved [14–17]. Recently, pressure and mole-fraction driven flows of three-component gas mixtures in the whole range of the gas rarefaction have been determined by using this technique [18]. However, it is known that the discrete velocity method slowly converges to the steady state result at higher values of the rarefaction parameter. In order to overcome this difficulty, the so-called synthetic accelerated discrete velocity methods can be used [19–24]. The derivation of these methods is challenging and non-trivial. So far such accelerated discrete velocity methods have been developed for single gases and binary gas mixtures. Therefore, it is useful to further develop these methods for flows of three-component gas mixtures also.

In this paper, an accelerated discrete velocity method is presented for isothermal flows of rarefied ternary gas mixtures driven by the local pressure and density gradients in long rectangular channels. The method is based on the McCormack linearized kinetic model [25]. Two diffusion equations are derived for the macroscopic velocity and the heat flow vector. These equations are used in the kinetic iteration of the discrete velocity method to accelerate the solution procedure. Simulations of flows of He–Ar–Xe mixture are performed in order to test the method. The computational performance in terms of the required number of iterations and the computational time is analyzed as a function of the rarefaction parameter. These quantities are studied in terms of the iteration criterion also. Representative velocity profiles are also

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shown. The remaining part of the paper is organized as follows: Section 2 defines the flow problem, Section 3 describes the McCormack model, Sections 4 and 5 present the moment equations and the numerical method, Section 6 contains the results and Section 7 concludes the paper.

2. Definition of the problem

The isothermal flow of ternary gas mixture is considered through a long rectangular duct. The axis of the channel lies in the z' coordinate direction, and its cross section is in the (x', y') coordinate sheet. The height, the width and the length of the duct are denoted by H, W and L. It is supposed that $H \leq W$ and the length is much larger than the width. The coordinates of the cross section are in the range of $x' \in [0, H]$ and $y' \in [0, W]$. The components of the mixture are denoted by $\alpha = 1, 2, 3$. The mole-fraction of the species is defined by $C_\alpha = n_\alpha / n$, where n_α is the component density and $n = \sum_\alpha n_\alpha$ is the total density.

The rarefaction of the mixture is described by the local rarefaction parameter

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

where P is the pressure, μ is the viscosity and $v_0 = \sqrt{2k_B T/m}$ is the characteristic speed of the gas. Here, k_B, T denote the Boltzmann constant and the temperature, respectively, and $m = \sum_\alpha C_\alpha m_\alpha$ is the average mass of the mixture.

It is supposed that the flow is driven by the local density gradients

$$X_\alpha = \frac{dn_\alpha}{dz'}\frac{H}{n_\alpha}, \tag{2}$$

which are considered arbitrary but small $|X_\alpha| \ll 1$. Such a situation corresponds to pressure and/or mole-fraction driven flows in the long channel. Since the channel is long, a linearized description can be used. It is convenient to reformulate the density gradients as $X_\alpha = \epsilon E_\alpha$, where $\epsilon \ll 1$ is a small parameter and $E_\alpha \sim O(1)$.

One of the most important quantities is the local flow rate defined by

$$G'_\alpha = \iint_A n_\alpha u'_{\alpha z} dx' dy' \tag{3}$$

with u'_α and A denoting the axial velocity of species α and the area of the cross section. Due to the linearization, this quantity can be written by

$$G'_\alpha = -\frac{n_\alpha HW v_0}{2} G_\alpha, \tag{4}$$

where G_α is the dimensionless flow rate.

3. Kinetic description

The gas is described by the velocity distribution function, $f_\alpha(\boldsymbol{v}, x', y', z')$, which is linearized according to

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

where

$$f_\alpha^{(0)}(\boldsymbol{v}, z') = n_\alpha(z')\pi^{-3/2} v_{0\alpha}^{-3} \exp\left(-\frac{v^2}{v_{0\alpha}^2}\right) \tag{6}$$

is the local equilibrium distribution, and $h_\alpha(\boldsymbol{v}, x', y')$ is the perturbation function. In this description, $\boldsymbol{v}$ denotes the molecular velocity and $v_{0\alpha} = v_0\sqrt{m/m_\alpha}$.

It is convenient to introduce dimensionless coordinates and velocity variables $x = x'/H$, $y = y'/H$, $z = z'/H$ and $\boldsymbol{c}_\alpha = \boldsymbol{v}_\alpha / v_{0\alpha}$. The distribution function obeys the McCormack kinetic model [25], which in the new coordinates reads such that

$$c_{\alpha x}\frac{\partial h_\alpha}{\partial x} + c_{\alpha y}\frac{\partial h_\alpha}{\partial y} = \omega_\alpha \sum_\beta Q_{\alpha\beta} - E_\alpha c_{\alpha z}, \tag{7}$$

where the collision term $Q_{\alpha\beta}$ is defined by

$$\begin{aligned} Q_{\alpha\beta} = &-\gamma_{\alpha\beta} h_\alpha + 2\left(\frac{m_\alpha}{m}\right)^{1/2} A_{\alpha\beta} c_{\alpha z} + 4B_{\alpha\beta x} c_{\alpha x} c_{\alpha z} + 4B_{\alpha\beta y} c_{\alpha y} c_{\alpha z} \\ &+ \frac{4}{5}\left(\frac{m_\alpha}{m}\right)^{1/2} D_{\alpha\beta} c_{\alpha z}\left(c_\alpha^2 - \frac{5}{2}\right). \end{aligned} \tag{8}$$

Here, the unknown coefficients are given as

$$\begin{aligned} A_{\alpha\beta} &= \gamma_{\alpha\beta} u_{\alpha z} - \nu_{\alpha\beta}^{(1)}(u_{\alpha z} - u_{\beta z}) - \frac{1}{2}\nu_{\alpha\beta}^{(2)}\left(q_{\alpha z} - \frac{m_\alpha}{m_\beta} q_{\beta z}\right), \\ B_{\alpha\beta i} &= (\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(3)}) p_{\alpha i z} + \nu_{\alpha\beta}^{(4)} p_{\beta i z}, \\ D_{\alpha\beta} &= (\gamma_{\alpha\beta} - \nu_{\alpha\beta}^{(5)}) q_{\alpha z} + \nu_{\alpha\beta}^{(6)}\left(\frac{m_\beta}{m_\alpha}\right)^{1/2} q_{\beta z} - \frac{5}{4}\nu_{\alpha\beta}^{(2)}(u_{\alpha z} - u_{\beta z}), \end{aligned} \tag{9}$$

where $i = x, y$ and $\gamma_{\alpha\beta}$, $\nu_{\alpha\beta}^{(n)}$ are collision frequencies. The quantity $\gamma_{\alpha\beta}$ appears only in the combination $\gamma_\alpha = \gamma_{\alpha\alpha} + \gamma_{\alpha\beta} + \gamma_{\alpha\zeta}$, where $\alpha \neq \beta \neq \zeta$ and $\alpha \neq \zeta$. γ_α and $\nu_{\alpha\beta}^{(n)}$ can be determined on the basis of Ref. [17] for example. The quantity ω_α is connected to the rarefaction parameter, and its expression can be found in Ref. [18].

The relevant dimensionless macroscopic quantities, the axial component of the velocity, the shear stress and the axial heat flow can be obtained as the moments of the distribution function

$$u_{\alpha z} = \pi^{-3/2}\left(\frac{m}{m_\alpha}\right)^{1/2} \int c_{\alpha z} h_\alpha e^{-c_\alpha^2} d\boldsymbol{c}_\alpha, \tag{10}$$

$$p_{\alpha i z} = \pi^{-3/2} \int c_{\alpha i} c_{\alpha z} h_\alpha e^{-c_\alpha^2} d\boldsymbol{c}_\alpha, \tag{11}$$

$$q_{\alpha z} = \pi^{-3/2}\left(\frac{m}{m_\alpha}\right)^{1/2} \int c_{\alpha z}\left(c_\alpha^2 - \frac{5}{2}\right) h_\alpha e^{-c_\alpha^2} d\boldsymbol{c}_\alpha. \tag{12}$$

On the wall of the channel, a diffuse reflection boundary condition is assumed for the distribution function: $h_\alpha(\boldsymbol{c}_\alpha^i, x_b, y_b) = 0$, where $\boldsymbol{c}_\alpha^i$ denotes the incoming velocity directions and x_b, y_b are the boundary coordinates.

The above description can be simplified by introducing the following reduced distribution function

$$\Phi_\alpha^{(k)} = \pi^{-1/2}\left(\frac{m}{m_\alpha}\right)^{1/2} \int_{-\infty}^{+\infty} \phi^{(k)}(c_{\alpha z}) h_\alpha e^{-c_{\alpha z}^2} dc_{\alpha z}, \tag{13}$$

where $k = 1, 2$ and $\phi^{(1)} = c_{\alpha z}$, $\phi^{(2)} = c_{\alpha z}(c_{\alpha z}^2 - 3/2)$. In terms of these functions, the kinetic equation is written by

$$c_{\alpha x}\frac{\partial \Phi_\alpha^{(k)}}{\partial x} + c_{\alpha y}\frac{\partial \Phi_\alpha^{(k)}}{\partial y} = \omega_\alpha \sum_{\beta=1}^{3} Q_{\alpha\beta}^{(k)} - E_\alpha \eta^{(k)}\left(\frac{m}{m_\alpha}\right)^{1/2}, \tag{14}$$

where

$$\begin{aligned} Q_{\alpha\beta}^{(1)} = &-\gamma_{\alpha\beta}\Phi_\alpha^{(1)} + A_{\alpha\beta} + 2\left(\frac{m}{m_\alpha}\right)^{1/2} B_{\alpha\beta x} c_{\alpha x} \\ &+ 2\left(\frac{m}{m_\alpha}\right)^{1/2} B_{\alpha\beta y} c_{\alpha y} + \frac{2}{5} D_{\alpha\beta}(c_{\alpha x}^2 + c_{\alpha y}^2 - 1), \end{aligned} \tag{15}$$

$$Q_{\alpha\beta}^{(2)} = -\gamma_{\alpha\beta}\Phi_\alpha^{(2)} + \frac{3}{5} D_{\alpha\beta} \tag{16}$$

and $\eta^{(1)} = 1/2$, $\eta^{(2)} = 0$.