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Numerical simulation of heat transfer flows by a direct solution of generalized kinetic models

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ABSTRACT

The heat conduction between two infinite parallel plates is numerically simulated based on a kinetic relaxation model for one-dimensional flows. For this purpose, two distribution functions which depend only on longitudinal velocity are introduced to avoid the multiplicity of integrals. The kinetic model equations in terms of newly defined functions are used to investigate one-dimensional heat transfer between two walls of constant temperature ratio. Generalization of the kinetic models allows the correct estimation of the heat flux for arbitrary Prandtl numbers. The steady solutions are compared with the results of the exact Boltzmann equation to validate the possibility of applying the present kinetic models. The temperature jumps near the solid surface are naturally achieved by the difference of the particle distributions from a local equilibrium state. It is shown that the relative temperature jumps at both plate surfaces increases as the Knudsen number of the flow increases. The temperature profiles by means of the generalized kinetic models agree well with those of the exact Boltzmann equation for various Knudsen numbers.

1. Introduction

The Boltzmann kinetic equation, which describes the nonlinear evolution in a gas flow, has been solved for numerous applications. Since the equation can provide temporal microscopic distributions of gas particles, the direct methods for solving this equation are the most natural and definite way of studying the time evolution process for rarefied gases. However, this kinetic equation is extremely difficult to handle in complex processes because of its intractable nature of binary collision operator. Both the mathematical difficulty in evaluating the collision integrals and the problem of multi-dimensionality have been challenging issues for applying the numerical solution of the Boltzmann equation into engineering problems.

The direct simulation Monte Carlo (DSMC) method, which was initiated by Bird [1–4], is one of the most popular approaches for solving the Boltzmann kinetic equation in an indirect manner. The direct Monte Carlo simulation is characterized by the random estimation of velocity grids to describe the nonequilibrium parts of the distribution function. Owing to its simplicity, the Monte Carlo method has been successfully used for the simulations in which experiment cannot be easily conducted [5–10]. However, the DSMC method requires many spatial grid points to obtain reliable results for simulating high-density flows. Different from this statistical approach, the method based on direct integration has recently been revealed that it is possible to provide uniform accuracy for computing a wide range of Knudsen numbers without very detailed meshes [11].

The direct numerical approach of solving the Boltzmann kinetic equation was firstly proposed by Nordsieck and Hicks [12] in the 1960s. The methodology utilizes the Monte Carlo evaluation of the integral over a finite region of velocity space, but treatment of the collisions between unlike species was not included in the study. Aristov and Tcheremissine elaborated the conservative method for solving the Boltzmann equation [13–15], in which the number of particles, momentum, and energy of gas are automatically conserved at every time step. Rykov [16] proposed a method of averaging of the Boltzmann kinetic equation over the transverse velocities for the simulation of one-dimensional flows. Rykov and Shil'tsov [17] then adopted the conservative scheme to the averaged kinetic equations for conserving the macroscopic fluxes of molecules. Since 1970s, some improvement to this conservative method has been made in solving the Boltzmann kinetic equation, and this approach has been successfully applied to simulate simple three-dimensional gas flows and recondensation of a multi-component mixture [11,18,19].

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For practical purposes, it is convenient to replace the collision integral by a relaxation term with the aid of a mean free path treatment. This relaxation model equation [20] expresses that collisions among particles tend to relax the distribution function to a local equilibrium state with a damping frequency. Since this relaxation approximation of the integral terms was proposed based on a simple physical assumption, it is hard to guarantee that the kinetic model is valid to describe the important features of the kinetic processes. Recently, there have been some theoretical attempts to develop a method of solving the kinetic relaxation model by preserving the main features of the exact equation [21–23]. The methodology of solving the generalized version of the kinetic model, which was constructed by Shakov [24–26], not only ensures the conservation properties, but also includes the Prandtl number correction of the heat fluxes.

In the present study, the steady process of the one-dimensional heat transfer flows between two infinite parallel plates was investigated based on the solution of the relaxation models. The heat conduction between two solid surfaces of fixed temperatures has already been studied by various kinetic methods, such as the DSMC method [2], the direct numerical method based on the exact equation [27,28], and the four moment method [29]. Here, the method of directly solving the generalized kinetic models was applied to describe the evolution of monatomic gas in a rarefied gas flow. Two distribution functions in terms of only longitudinal velocity were newly defined to reduce the computational cost in the evaluation of multiple integrals. The relationship between the temperature jump and the Knudsen number of the flow was numerically analyzed by the direct solution of the boundary-value problem. The predicted results were compared with those of other kinetic approaches, and the possibility of applying the generalized kinetic models was verified.

2. Numerical methods

The distribution function $f(t, x, \boldsymbol{\xi})$ of a monatomic gas is assumed to evolve according to the generalized Krook model (S-model) [24]. This model kinetic equation is obtained from the approximation to the collision term in the Boltzmann transport equation as follows

$$\frac{\partial f}{\partial t} + \xi_x \frac{\partial f}{\partial x} = \nu\left(f^+ - f\left(t, x, \boldsymbol{\xi}\right)\right). \tag{1}$$

Here, ξ_x is the particle velocity of gas in the x-direction, ν is the collision frequency, and the local equilibrium state f^+ is determined from the moments of the distribution function for the velocity phase space [23].

$$f^+ = f_M\left[1 + \frac{4}{5}(1-\mathrm{Pr})\frac{2q_x\xi_x'}{nT^2}\left(\frac{\xi_x'^2+\xi_y^2+\xi_z^2}{T} - \frac{5}{2}\right)\right],$$
$$f_M = \frac{n}{(\pi T)^{3/2}}\exp\left(-\frac{\xi_x'^2+\xi_y^2+\xi_z^2}{T}\right), \quad \xi_x' \equiv \xi_x - U. \tag{2}$$

Here, f_M is the locally Maxwellian distribution, n is the number density of gas, U is the longitudinal velocity, T is the temperature, q_x is the heat flux, and Pr is the Prandtl number.

It is convenient to introduce two different distribution functions which are independent of the magnitude of the transverse velocities.

$$\varphi(t, x, \xi_x) = \int f d\xi_y d\xi_z, \quad \psi(t, x, \xi_x) = \int \left(\xi_y^2 + \xi_z^2\right) f d\xi_y d\xi_z. \tag{3}$$

These distribution functions are calculated with the integration of f over all possible values of ξ_y and ξ_z, so that the system of kinetic equations can be obtained in terms of the functions φ and ψ.

$$\frac{\partial \varphi}{\partial t} + \xi_x \frac{\partial \varphi}{\partial x} = \nu\left(\varphi^+ - \varphi(t, x, \xi_x)\right), \quad \frac{\partial \psi}{\partial t} + \xi_x \frac{\partial \psi}{\partial x} = \nu\left(\psi^+ - \psi(t, x, \xi_x)\right),$$
$$\varphi^+ = \frac{n}{(\pi T)^{3/2}}\exp\left(-\frac{\xi_x'^2}{T}\right)\left[1 + \frac{4}{5}(1-\mathrm{Pr})\frac{2q_x\xi_x'}{nT^2}\left(\frac{\xi_x'^2+\xi_y^2+\xi_z^2}{T} - \frac{3}{2}\right)\right],$$
$$\psi^+ = \frac{n}{(\pi T)^{3/2}}\exp\left(-\frac{\xi_x'^2}{T}\right)\left[1 + \frac{4}{5}(1-\mathrm{Pr})\frac{2q_x\xi_x'}{nT^2}\left(\frac{\xi_x'^2+\xi_y^2+\xi_z^2}{T} - \frac{1}{2}\right)\right], \tag{4}$$

For boundary-value problem, the steady solution of the kinetic model equations can be achieved by the following iterative processes.

$$\xi_x \frac{\partial \varphi^k}{\partial x} = \nu\left(\left(\varphi^+\right)^k - \varphi^{k+1}\right), \quad \xi_x \frac{\partial \psi^k}{\partial x} = \nu\left(\left(\psi^+\right)^k - \psi^{k+1}\right). \tag{5}$$

The different finite-difference method is applied according to the sign of the $\xi_{x\beta}$, which represents the particle velocity at the β-th segment of velocity space.

$$\varphi_{i,\beta}^{k+1} = \left(\varphi^+\right)_{i,\beta}^k - \frac{\xi_{x\beta}}{\nu\Delta x} \times\left[\frac{\varphi_{i+1,\beta}^k - \varphi_{i-1,\beta}^k}{2} - \mathrm{sign}\left(\xi_{x\beta}\right)\frac{\varphi_{i+1,\beta}^k - 2\varphi_{i,\beta}^k + \varphi_{i-1,\beta}^k}{2}\right] \tag{6}$$

The solution of differential equation in terms of ψ is obtained by the same finite-difference method for both collisionless flow and relaxation stage.

The moment relations [16] between the macroscopic flow properties with the functions φ and ψ are expressed as follows

$$n = \int \varphi d\xi_x, \quad U = \frac{1}{n}\int \xi_x \varphi d\xi_x,$$
$$T = \frac{2}{3}\frac{1}{n}\int\left[(\xi_x - U)^2\varphi + \psi\right]d\xi_x,$$
$$q_x = \int (\xi_x - U)\left[(\xi_x - U)^2\varphi + \psi\right]d\xi_x. \tag{7}$$

3. Results and discussions

This section deals with the heat transfer in a rarefied gas between two parallel plates of a constant temperature ratio, which is one of the classical kinetic problems. The steady solution of the one-dimensional heat transfers was numerically investigated by means of the direct solution for the generalized kinetic models. The computational domain for the one-dimensional boundary-value problem is considered as a finite segment of length L. The space between the two plates is assumed to be filled with monatomic gas, so that it is not necessary to consider the vibrational frequency in the kinetic model equations. Since monatomic gas is only considered, the Prandtl number corresponding to the generalized kinetic models was set to 2/3. The correlation between the collision frequency ν and the Knudsen number of the flow, which is a ratio of the mean free path to the characteristic length L, is in the following form [23]

$$\nu = \frac{8}{5\sqrt{\pi}}\frac{1}{Kn}\frac{nT}{\mu}. \tag{8}$$

Here, μ is the dynamic viscosity, which is assumed to be a function of temperature only and is proportional to $T^{0.5}$ for monatomic hard sphere gas.

The solid surfaces at x=0 and x=L have fixed temperatures T_0 and T_L, respectively, and the temperature ratio between the cold wall and the hot wall is also assumed to be given during the solution of the equations. The boundary conditions for the functions

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