Numerical Study of Comprehensive Kinetic Model in Plane Shock Wave Problem

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Abstract. The comprehensive kinetic model equation for unsteady one-dimensional flow is numerically solved to obtain a converging solution for a plane shock structure problem. This model equation is proposed by Oguchi (1998) on the basis of the Grad’s 13-moment approximation, and its collision term is expressed in an explicit function of the peculiar velocities. The problem is selected as a typical problem for surveying the applicability of the present model to gas dynamic problems. The numerical calculations are performed for some selected monatomic molecules with inverse power law potentials: Maxwell molecules, hard sphere molecules and helium gas molecules. The free-stream Mach number range is from 1.05 to 2.0. The resultant shock wave profiles of the number density exhibit reasonable forms with monotonic change, and the resultant shock thickness values agrees well with the corresponding Navier-Stokes values. The present results suggest us to open a way for the applicability of the present kinetic model to various gas dynamic problems in weakly rarefied conditions.

INTRODUCTION

The Boltzmann equation is a basic equation for rarefied gas dynamics, but its exact solution has been limited in a few cases mainly due to complexity of its integral term of molecular collisions, in spite of many intense research activities in these decades. Instead, several kinds of model equations and computational methods have been developed by many researchers to solve various problems on rarefied gas flows. Historically, the moment method was developed at an initial stage to avoid the difficulty directly approaching the complex integral term, introducing the moment equations for macroscopic physical properties as number density, flow velocity, temperature, stress tensor and heat flux vector. There are the Chapmann-Enskog method, the Grad’s 13-moment method [1] and so on for the moment method. Next, the kinetic model equation was introduced to approach directly the collision term by simplifying it, and to make it possible to obtain the distribution function in velocity space. There are the BGK [2] model, the Shakov [3] model and so on in this category. Furthermore, according to the recent development of computer technology, various computational methods have been developed for directly simulating the molecular motion [4] and for solving the Boltzmann equation [5,6].

The present paper is concerned with numerical study of a kinetic model, which is named as ‘comprehensive kinetic model’ by Oguchi [7]. This model equation is analytically derived under the assumption that the velocity distribution function in the collision term allows an expression based upon the thirteen-moment approximation proposed by Grad [1]. Then the full collision term is expressed as an analytic function of the peculiar velocities. The benefit of this model is its applicability to molecular gases obeying a wide range of the inverse power law potentials. The main purpose of the present study is to survey the applicability of this model equation to the rarefied gas dynamic problems in computational means. The plane shock wave problem is selected as a typical problem for testing this kinetic model equation. The model equation for unsteady one-dimensional flow is solved in velocity space by a time-marching numerical procedure to obtain a converging solution for a plane shock structure problem in steady one-dimensional flow. The numerical calculations are performed for some selected monatomic molecules with inverse power law potentials: Maxwell molecules, hard sphere molecules and helium gas molecules. The free-stream Mach number range is from 1.05 to 2.0.
In the comprehensive kinetic model equation, the velocity distribution functions involved in the collision term of the Boltzmann equation are assumed to take the form of the thirteen-moment approximation, proposed by Grad [1].

\[
F(V_m) = F_0(V) \left\{ 1 + \frac{p_{mn}V_m V_n}{2pRT} + \frac{q_m V_n}{pRT} \left( 5 - \frac{V^2}{RT} \right) \right\},
\]

where \( V_m \) is the peculiar velocity vector of molecules and \( F_0 \) is the local equilibrium distribution function given by

\[
F_0(V) = \frac{n}{(2\pi)^{3/2}} \exp \left( -\frac{V^2}{2RT} \right).
\]

In Eqs. (1) and (2), \( n \) denotes the number density, \( T \) the temperature, \( p \) the pressure, \( p_{mn} \) the stress tensor, \( q_m \) the heat flux vector, and \( R \) the gas constant. The subscript \( m \) or \( n \) denotes an axis among the Cartesian coordinates \( (x, y, z) \) adopted in the physical coordinates concerned. The summation is carried out over the repeated subscripts; i.e.

\[
V^2 = V_x V_x + V_y V_y + V_z V_z, \quad q_m V_n = q_x V_x + q_y V_y + q_z V_z.
\]

and \( p_{mn} V_m V_n = p_{xx} V_x^2 + p_{yy} V_y^2 + \ldots + p_{zz} V_z^2 \).

The present kinetic model equation is obtained by substituting Eq. (1) into the collision term of the Boltzmann equation and neglecting the higher-order cross product terms of \( V_m \) under the assumption of weakly rarefied gases. The resultant formula for the collision term is derived after performing the double integrals regarding the azimuth and the deflection angle between colliding molecules over the whole angles, and is expressed for arbitrary inverse-power law potentials as follows:

\[
\frac{DF(t, x_m, v_m)}{dt} = -vF_0(C) \left\{ \frac{p_{mn}C_m C_n}{p} P_1 + \frac{q_m C_m}{p\sqrt{RT}} Q_1 \right\},
\]

where \( v_m \) is the molecular velocity and the normalized peculiar velocities \( C_m \) and \( C \) are defined by \( C_m = V_m(RT)^{1/2} \) and \( C^2 = C_n C_m \). The functions \( P_1 \) and \( Q_1 \) are given as functions of \( C \) through the functions \( P \) and \( Q \) by

\[
P_1(C) = \sqrt{\frac{2}{\pi}} \frac{3(2)^{(r-5)/(r-1)}\exp\left(-\frac{C^2}{2}\right)}{\frac{5}{2}} \left( P(C) - \frac{C}{2} \right) Q(C),
\]

\[
Q_1(C) = \sqrt{\frac{2}{\pi}} \frac{8(2)^{(r-5)/(r-1)}\exp\left(-\frac{C^2}{2}\right)}{5} \left( P(C) - \frac{C}{2} \right) Q(C),
\]

\[
P(C) = \int_0^{2\pi} e^{-2x^2} \left( \frac{x^2}{C} + \frac{3r}{2C^2} + \frac{3}{4C^3} \right) \exp(2Cr) \left( \frac{x^2}{C} - \frac{3r}{2C^2} + \frac{3}{4C^3} \right) \exp(-2Cr) dr,
\]

\[
Q(C) = \int_0^{2\pi} e^{-2x^2} \left( \frac{x^2}{C} - \frac{r}{2C^2} \right) \exp(2Cr) + \left( \frac{r}{2C} + \frac{r}{2C^2} \right) \exp(-2Cr) dr,
\]

where \( r \) is a half of the relative velocity of colliding molecules, normalized by \((RT)^{1/2}\), and \( s^{-1} \) is the inverse power of the molecular potential: \( s = 5 \) for Maxwell molecules, \( s = \infty \) for hard sphere molecules, and \( s = 14.6 \) for helium gas molecules. Analytical formulae of \( P_1 \) and \( Q_1 \) are given as \( P_1 = 3/8 \) and \( Q_1 = (C^2-5)/10 \) for Maxwell molecules, and as

\[
P_1 = \frac{3}{4(2\pi)^{1/2}} \left( 1 + \frac{2}{C^2} + \frac{3}{C^3} \right) \exp\left(-\frac{C^2}{2}\right) + K \left( \frac{C}{2C^2} + \frac{3}{C^3} \right) \exp\left(-\frac{C^2}{2}\right),
\]

\[
Q_1 = \frac{1}{5(2\pi)^{1/2}} \left( C^2 - 4 + \frac{9}{C} \right) \exp\left(-\frac{C^2}{2}\right) + \frac{1}{10} \left( C^3 - 3C - \frac{15}{C} + \frac{9}{C^2} \right) \exp\left(-\frac{C^2}{2}\right),
\]

for hard sphere molecules. The collision frequency \( \nu \) is given by

\[
\nu = \frac{5\sqrt{\pi}}{\Gamma\left\{4 - 2/(s - 1)\right\}} \frac{p}{\mu},
\]

where \( \Gamma(x) \) is the gamma function and \( \mu \) is the gas viscosity: \( \nu = (4/3)(p/\mu) \) for Maxwell molecules, and \( \nu = (5 \pi^{1/2} / 24)(p/\mu) \) for hard sphere molecules. Eq. (3) is the kinetic model equation which contains the thirteen moments \( n, u_m, T, p, p_{mn}, q_m \) of the velocity distribution function, together with the law of state; \( p = knT \), and with the
relations among the normal and shearing stresses; \( p_{mn} = 0 \) and \( p_{ms} = p_{mn} \). The macroscopic flow velocity is denoted by \( u_m \), and \( k \) is the Boltzmann constant.

In the present paper, Eq. (3) is expressed in a normalized form for unsteady, one-dimensional flows as

\[
\frac{\partial \bar{F}}{\partial t} + v_x \frac{\partial \bar{F}}{\partial x} = -v_x \bar{F}_0 \left( C \right) \left[ \frac{p_{ss}}{p} \left( C^2 - \frac{C_x^2 + C_y^2}{2} \right) \right] p + \frac{q_x C}{p} \underbrace{\left( \frac{2}{T} \right)}_{Q},
\]

(9)

with \( F_0 \left( C \right) = n(\pi T)^{-3/2} \exp(-C^2/2) \), where both of \( p_{ss} \) and \( p_{xy} \) are replaced by \( -p_{xy}/2 \) from the relation of \( p_{mn} = 0 \). The state variables \( n, T \) and \( p \) are normalized by the upstream equilibrium values \( n_1, T_1 \) and \( p_1 \), respectively, ahead of the shock wave. The velocities \( u (= u_x) \), \( v_y \) and \( V_m \) are normalized by \( (2RT_1)^{1/2} \), and then we have \( C_m = V_m/(T/2)^{1/2} \). The stress \( p_{ss} \) and the heat flux \( q_x \) are normalized, respectively, by \( p_1 \) and \( p_1(2RT_1)^{1/2} \). The distribution function \( F \) is normalized by \( n(2RT_1)^{-3/2} \). The mean free path \( \lambda_x \) for hard sphere molecules in the upstream equilibrium flow is used as a reference length, and is given by \( \lambda_x = 16 \mu_1/(5n,m(2\pi RT_1)^{1/2}) \). The reference time \( t_1 \) is given by \( t_1 = \lambda_x/(2RT_1)^{1/2} \), and is also used for obtaining the normalized collision frequency \( \nu \), which is given by \( \nu = \left( 2^{(3\nu-1)} \Gamma \left\{ (4-2(s-1)) \right\} n \right)T^{(s-1)/2} \). \( \nu = 32n/(15 \pi)^{1/2} \) for Maxwell molecules and \( \nu = (1/3)nT^{1/2} \) for hard sphere molecules. The five moments \( n, u, T \) and \( p, q_x \) are obtained in normalized forms as follows

\[
\begin{align*}
\frac{n}{\nu} & = \int F^2 \nu, & \frac{p}{\nu} & = \int \frac{1}{3} V^2 \nu, & \frac{q}{\nu} & = \int \frac{1}{3} V^2 \nu.
\end{align*}
\]

(10)

For one-dimensional flow analyses, we may introduce the reduced distribution functions \( G \) and \( H \), whose definitions and resultant formulae are described in the Appendix, and the calculations are actually performed for some cases of the present problem. In the present paper, however, the numerical solutions of Eq. (9) for the distribution function \( F \) is exhibited in order to look into the general feature of the model equation, considering future extensions to multi-dimensional flows.

The flow situation is assumed to be a steady supersonic flow crossing a normal shock wave with positive velocity. The initial conditions are given by upstream and downstream equilibrium distribution functions \( F_{01} \) and \( F_{02} \) in a discontinuous form at \( x = 0 \). The boundary conditions for \( F \) are given at \( x = \pm \infty \) by these equilibrium distribution functions. The model equation (9) is numerically solved with the initial and boundary conditions described above for each grid point in velocity space \( (v_x, v_y, v_z) \) by using the Beam-Warming scheme, which is given in the present problem as follows [8,9],

\[
\frac{1 + \Delta t v_x}{\Delta x} \frac{\partial}{\partial x} \Delta F^{n+1} = -\Delta t \left( v_x \frac{\partial F^n}{\partial x} - F^n \right) - \left( \Delta t \right)^4 \omega \Delta t \frac{\partial^4 F^n}{\partial x^4},
\]

\[
\Delta F^{n+1} = F^{n+1} - F^n, \quad \frac{\partial F^n}{\partial x} = \frac{F^n_{i+1} - F^n_{i-1}}{2\Delta x},
\]

(11)

where the superscript \( n \) denotes the time step, the subscript \( i \) denotes the mesh point address of \( x \), and \( F_{C} \) is the collision term of Eq.(9). The fourth derivative term is the damping term for numerical errors in the central difference scheme, and \( \omega \) is the damping constant below 1/8. Eq. (11) is a simultaneous equation system for \( \Delta F \), and is solved at each time step by using an elimination method for the equation system with tri-diagonal matrix. The solution of the next time step is obtained from \( F^{n+1} = F^n + \Delta F^{n+1} \). The initial and boundary conditions are given as \( \Delta F = 0 \) and \( F = F_{01} \) or \( F_{02} \) for Eq. (11). The convergence to a steady flow solution is decided by evaluating the converging behaviors of the macroscopic quantities. The present computational scheme is based on the existing implicit schemes [8,9], which were used for solving the BGK [2] and Shakov [3] model equations.

The functions \( P_1 \) and \( Q_1 \) in the collision term are calculated in every four-dimensional grid points \( (x, v_x, v_y, v_z) \) at each time step. The integration for the functions \( P \) and \( Q \) in Eqs.(6) and (7) is also numerically carried out over a limited range of \( r \). In Fig. 1, the integrand \( P^n = \int P^n \cdot dr \) is plotted against \( r \) for several values of \( C \) in case of Maxwell molecules, since it is useful for actual calculation to understand its functional nature. The functions \( P_1 \) and \( Q_1 \) are calculated by numerical integration of \( P \) and \( Q \) for the mesh width \( \Delta r = 0.5 \), and are plotted against \( C \) for Maxwell, hard sphere and helium gas molecules in Fig. 2. The resultant curves coincide with analytical ones within enough accuracy for Maxwell and hard sphere molecules.

The calculations are performed for the upstream Mach number range 1.05 - 2.0 in cases of Maxwell, hard sphere and helium gas molecules. The computational range in velocity space is given by the condition \(-4(T_2)^{1/2} \leq V_m \leq +4(T_2)^{1/2}\) or \(-4(2T_2)^{1/2} \leq C_m \leq +4(2T_2)^{1/2}\), where the subscript 2 denotes the downstream equilibrium state. The mesh size in each direction is \( \Delta v_x = 8(T_2)^{1/2}/28 \) or \( \Delta v_y = \Delta v_z = 8(T_2)^{1/2}/18 \). The positions of mesh points are slightly
shifted from the original dividing points in such a way that the point \( \nu_{m} = 0 \) becomes a central point between \( \nu_{m} = -D \nu_{m}/2 \) and \( +D \nu_{m}/2 \), in order to minimize the singular behavior at \( \nu_{x} = 0 \). This singularity appears as the solution approaches to the steady state solution, since the collision term \( F_{C}^{\nu} \) does not always vanish at \( \nu_{x} = 0 \) for arbitrary \( p_{ex} \) and \( q_{c} \). The \( \nu \)-coordinate is transformed to the \( \xi \)-coordinate through the relation \( \nu = \nu \tan(\xi) \), where \( A \) and \( B \) are constants for adjusting the \( \nu \)-range for calculation and the mesh size in the range of \( (-\pi/2 \leq \xi \leq \pi/2) \), in order to convert the infinite range of \( \nu \) to a finite range of \( \xi \). The mesh size is selected as \( \Delta \xi = \pi/(500B) \) and the time step is selected as \( \Delta t = 5(\Delta x)_{\text{num}}/[(\nu_{m})_{\text{max}} + (5T_{2}/6)^{1/2}] \). The upstream and downstream boundary conditions are imposed on the mesh points close to the outer boundaries of \( \nu_{x} = \pm \pi/2 \).

FIGURE 1. Integrand \( P_1' \) as a function of \( r \) for \( C = 0.5, 1, 2 \) and \( 4 \) (Maxwell molecules).

FIGURE 2. Functions \( P_1 \) and \( Q_1 \) as functions of \( C \) for Maxwell, helium gas and hard sphere molecules.

RESULTS AND DISCUSSION

In Fig. 3, a convergence parameter \( \sigma = [\Delta n/(n \Delta t)]_{\text{max}} \) is plotted against the time step for the upstream Mach number \( M_{1} = 1.2 \) in both cases of Maxwell and hard sphere molecules, where \( \Delta n \) is the increment of the number density in the time step \( \Delta t \). The parameter means the maximum increasing rate of the number density per time step or the maximum increasing rate of the overall summation of the distribution function \( F \) per time step, since we have the relation \( \Delta n/n = (\Sigma \Delta F)/((\Sigma F)) \). A good convergence is obtained for both cases of Maxwell and hard sphere molecules. The similar converging behaviors of the parameter \( \sigma \) are also obtained for the other cases of \( M_{1} \) and for helium gas molecules. That is, the steady flow solutions are obtained within a good numerical accuracy as solutions of the present kinetic model equation for a plane shock structure problem. The solutions at 2,000 time steps are adopted as converging solutions. An example of the resultant distribution function is exhibited in Fig. 4, where the product of \( \nu_{x} \) and \( F \) on the \( \nu_{x} = \nu_{y} \) plane is illustrated in a bird-view style. The product \( \nu_{x}F \) is obtained as a smooth
function of $v_x$ and $v_y$ (or $v_z$) in a converging solution, since we have a converging behavior of $[\partial v_x F / \partial x - F_x^*] \to 0$ in Eq. (11) irrespective of the singular nature at $v_x = 0$.

**FIGURE 3.** Convergence history of the parameter $\sigma$: Maxwell and hard sphere molecules, $M_1 = 1.2$.

**FIGURE 4.** An example of the distribution function $F(x = 0; v_x, v_y)$ exhibited by $v_x F$: Maxwell molecules, $M_1 = 1.2$.

In Figs. 5 and 6, the number density profiles $n(x)$ (solid lines) are shown in comparison with the corresponding profiles obtained from Navier-Stokes solutions (dotted lines). Fig. 5 shows four number density profiles for $M_1 = 1.05, 1.2, 1.5$ and $2.0$ in a case of Maxwell molecules. The horizontal length scale of each curve is adjusted to fit the shock thickness. The length scale is exhibited by a multiple of the mean free path $\lambda_1$ at the foot of each curve. Fig. 6 shows three number density profiles for $M_1 = 1.2$ in cases of Maxwell, helium gas and hard sphere molecules. The resultant profiles exhibit a close similarity to the Navier-Stokes ones, though there are some slight discrepancies among the corresponding profiles in the downstream side of shock structure. Reasonable solutions are obtained for a Mach number range of 1.05 to 2.0, which is beyond a theoretical limit of the Mach number for the moment solution [1]. Fig. 7 shows the normalized inverse shock thickness $1/\delta$ plotted against $M_1 - 1$ for Maxwell molecules in comparison with the Navier-Stokes and DSMC solutions [10]. The normalized shock thickness $\delta$ is defined by the maximum slope of the number density as $\delta = (n_2 - n_1)(dn/dx)_{\max}$. The evaluated values of the shock thickness closely coincide with the Navier-Stokes values from $M_1 = 1.05$ to 2.0.
In Fig. 8, the normal stress $p_{xx}$ and the heat flux $q_x$ are plotted against $x$ with the Navier-Stokes solutions for $M_1 = 1.2$ in a case of Maxwell molecules. The recent solutions [5,6] of the Boltzmann equation for hard sphere molecules are also plotted for comparison. The resultant profiles of $p_{xx}$ and $q_x$ (solid lines) exhibit mostly reasonable ones. We can conclude from Figs. 5 to 8 that some reasonable solutions are obtained by using the present kinetic model equation under the assumption of weakly rarefied gases, even for such a highly rarefied situation as shock structure problem.

**FIGURE 5.** Comparison between the number density profiles $n(x)$ for the present model and Navier-Stokes solutions I: Maxwell molecules, $M_1 = 1.05, 1.2, 1.5$ and 2.0.

**FIGURE 6.** Comparison between the number density profiles $n(x)$ for the present model and Navier-Stokes solutions II: Maxwell, helium gas and hard sphere molecules, $M_1 = 1.2$.

**CONCLUSION**

The important matter of the present study is to open a computational way for the comprehensive kinetic model. In this point of view, the present paper exhibits some reasonable numerical solutions for different inverse-power-law potentials in a plane shock wave structure problem. The present results suggest us the present kinetic model is applicable to various problems on rarefied gas dynamics in weakly rarefied situations.
FIGURE 7. Inverse shock thickness plotted against $M_1 - 1$: Maxwell molecules.
[* Erwin, A. D., Muntz, E. P. and Pham-Van-Diep, G. (1989) [10]]

FIGURE 8. Normal stress and heat flux profiles $p_{xx}(x)$ and $q_{x}(x)$: Maxwell molecules, $M_1 = 1.2$,

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APPENDIX: EQUATIONS FOR THE REDUCED DISTRIBUTION FUNCTIONS G AND H

In one-dimensional flow analysis, the reduced distribution functions $G$ and $H$ are obtained as

$$G = \int \int F dv_x dv_y, \quad H = \int \int (V_x^2 + V_y^2) F dv_x dv_y.$$  

Then, the kinetic model equation (9) is converted to

$$\frac{\partial G}{\partial t} + v_x \frac{\partial G}{\partial x} = G_c, \quad \frac{\partial H}{\partial t} + v_x \frac{\partial H}{\partial x} = H_c,$$

where $F_c$ is the collision term of Eq. (9). In the present kinetic model equation, the collision terms $G_c$ and $H_c$ are generally obtained as functions of $V_x$ for arbitrary inverse power law potentials through numerical integration over the velocity space $v_x$ and $v_y$. In a case of Maxwell molecules, analytic formulae of $G_c$ and $H_c$ are obtained in normalized forms as functions of $V_x$ as follows

$$G_c = -v \frac{G_x}{T} \left[ \frac{3}{4} \left( \frac{V_x^2}{T} - \frac{1}{2} \right) + \frac{2}{5} \left( \frac{V_x^2}{T} - \frac{3}{2} \right) \right],$$

$$H_c = -v G_x \left[ \frac{3}{4} \left( \frac{V_x^2}{T} - \frac{1}{2} \right) + \frac{2}{5} \left( \frac{V_x^2}{T} - \frac{1}{2} \right) \right],$$

where

$$G_0 = \frac{n}{(\pi T)^{\frac{3}{2}}} \exp \left( -\frac{V_x^2}{T} \right).$$

The five moments $n$, $u$, $T$ (or $p$), $p_{xx}$ and $q_x$ are obtained in normalized forms as follows

$$n = \int G dv_x, \quad nu = \int v_x G dv_x, \quad p = nT = \frac{2}{3} \int (V_x^2 G + H) dv_x,$$

$$p_{xx} = 2 \int v_x^2 G dv_x - p, \quad q_x = \int V_x (V_x^2 G + H) dv_x.$$

REFERENCES