Application of the Moment Equations to the Shock-tube Problem

Takeo Soga* , Takayuki Gamahara*1, Kazuhiro Ooue*1, and Naoki IIrose†

*Department of Aerospace Engineering, Nagoya University, Chikusa-ku, Furo-cho, Nagoya 464-8603 JAPAN
†National Aerospace Laboratory, Chofu, Tokyo 182-8522 JAPAN

Abstract. Moment equations derived from the Boltzmann equation were applied to the Riemann problem. A new closure method of the moment equations were proposed. It was demonstrated that supplemented moment equations were applicable to the analysis of moderately strong shock waves. Various higher order moments of the distribution function in the shock wave were obtained. Present result suggested that these higher order moments would not be simply expressed in terms of higher order derivatives of velocity, temperature, and pressure. If we include more higher moment equations present results may be considerably improved. Present method is expected for the analysis of nonequilibrium rarefied flow connecting with higher order moments demonstrated in this paper.

INTRODUCTION

The first Chapman-Enskog solution to the Boltzmann equation yields the Navier-Stokes equation, which is widely applied not only to the continuum flow but also to the rarefied flow with the aid of slip boundary conditions. The Burnett, and super-Burnett equations, pertinent to the higher Chapman-Enskog [1] [2] solutions, are respectively third order and fourth order differential equations with respect to the spatial derivatives of velocity, temperature and density. Signs of the highest derivatives change according to the level of approximation of the Chapman-Enskog solutions. Consequently, these equations occasionally yield unphysical solutions to the sound propagation [3] or to the heat transfer problem in a rarefied gas [4]. Quite different approach to the rarefied gas flow based upon the macroscopic equations such as the Burnett equation, i.e., “advanced” fluid dynamic equations, is the Grad’s method [5] of moment equations derived from the boltzmann equation: These moment equations are essentially equivalent to the Maxwell’s transfer equations. This method release one from applying the Newton’s law for the shear stress and the Fourier’s law for the heat flux, though these laws are very useful and have a robustness easy to apply. In the last symposium, one of the authors presented how to apply the moment equations to the rarefied flows with the aid of generalized slip boundary conditions. In this paper we treat the shock-tube (Riemann) problem, in which three different thermodynamic regions are included. Nonequilibrium shock wave, diffusive contact layer (surface), and thermally equilibrium rarefaction wave. Recently Beylich [6] has presented numerical solution of the kinetic equation for the Riemann problem, applying a splitting scheme for time and space and an idea of inter-cell integration where integrand in the path integral was properly approximated in accordance with the cell-Knudsen number. Instead of solving the kinetic equation, present approach applys an integrated version of such a scheme. Apparently truncation of higher moments in the integration of the kinetic equation causes us to lose the merit of the kinetic equation, i.e., spontaneous relaxation of every moments to a thermally equilibrium state. Taking all moments of the Boltzmann equation up to the third order, we obtain a set of 20 independent moment equations. We call this set as the full third order moment equations(F3OME). The full fourth order moment equations(F4OME) include 35 moment equations, and the full fifth order moment equations(F5OME) include 56 moment equations. In the one dimensional flow number of independent moment equations of F3OME, F4OME, and F5OME are 6, 9, and 9, respectively. Since above mentiond moment equations include three conservation equations of

1) Graduate student
mass, momentum, and energy and rate equations of higher moments, various CFD procedures are applicable
to the numerical analysis. However, we are not sure whether TVD scheme and/or similar flux limiting schemes
are adequate for the numerical analysis of the present equations. In this paper we apply the MacCormack’s
A method of truncation and a method of approximation of higher order moments will be described in the latter
section. Throughout in this paper we only treat the Maxwell molecular gas for simplicity but the extension
to the hard sphere gas and to other gases having different intermolecular potentials can be easily carried out

**MOMENT EQUATIONS**

The one-dimensional Boltzmann equation for monatomic gas is given by

\[
\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} = \int \left( f' f'_1 - f f'_1 \right) g \sigma \sin \chi d\chi d\varphi d\varphi',
\]  

(1)

where \( f = f(\vec{c}) \) denotes the velocity distribution function, \( \vec{c} = (c_x, c_y, c_z) \) the molecular velocity, \( g = |g| \) the
relative velocity, \( \sigma = \sigma(g, \chi) \) the collision cross section, \( \chi \) the deflection angle, \( \epsilon \) the angle of inclination of the
plane of collision. According to Ikenberry and Truesdell [9], the distribution function can be expanded using
irreducible tensor \( Y_i(\vec{c}) \) and Sonine polynomials \( S_m^{(n)}(\vec{c}^2) \) where the \( Y_i(\vec{c}) \) represent any \( i \)th order irreducible
tensor and \( \vec{C}^2 = |\vec{C}|^2/2RT, \vec{C} = \vec{c} - \vec{v} \) denotes the peculiar velocity, \( \vec{v} \) the flow velocity, \( R \) the gas constant, and
\( T \) the temperature,

\[
f = f^{(0)} \left[ 1 + a_{p}_{ij} Y_{ij}(\vec{C}) + a_{Q_i} Q_i Y_{i}(\vec{C}) S_{i/2}^{(1)}(\vec{C}^2) + a_{Q_{ijk}} Q_{ijk} Y_{ijk}(\vec{C}) + a_{R_0} R_0 S_{1/2}^{(2)}(\vec{C}^2) + a_{R_{ijk}} R_{ijk} Y_{ijk}(\vec{C}) + a_{S_i} S_i Y_{i}(\vec{C}) S_{i/2}^{(2)}(\vec{C}^2) + a_{S_{ijk}} S_{ijk} Y_{ijk}(\vec{C}) S_{i/2}^{(2)}(\vec{C}^2) + a_{S_{ijk\ell m}} S_{ijk\ell m} Y_{ijk\ell m}(\vec{C}) \right] \quad (i, j, k, \ell, m = 1, 2, 3),
\]  

(2)

where moments are retained up to fifth order and the Maxwellian distribution function \( f^{(0)} \) is given by

\[
f^{(0)} = n(2\pi RT)^{-3/2} \exp(-\vec{C}^2),
\]

where \( n \) denotes the number density, and coefficients \( a_{p}_{ijk} \) and others are known functions of the temperature.
Macroscopic moments with respect to the thermal velocity \( \vec{C} \) included in the right hand side of Eq. (2) for the
one dimensional flow are defined by

\[
n = \langle f Y(\vec{c}) \rangle, \quad n u = \langle f Y_x(\vec{c}) \rangle, \quad 3p = m < C^2 f Y(\vec{c}) >, \quad p_{xx} = m C_m^2 < f Y_{xx}(\vec{C}) >
\]

\[
Q_x = -2q_x = m C_m^2 < f Y_x(\vec{C}) S_{i/2}^{(1)}(\vec{C}^2) >, \quad Q_{xxx} = m < f Y_{xxx}(\vec{C}) >, \quad R_0 = m C_m^4 < f S_{1/2}^{(2)}(\vec{C}^2) >,
\]

\[
R_{xx} = m C_m^2 < f Y_{xx}(\vec{C}) S_{i/2}^{(1)}(\vec{C}^2) >, \quad R_{xxx} = m < f Y_{xxx}(\vec{C}) >, \quad S_i = m C_m^4 < f Y_x(\vec{C}) S_{i/2}^{(2)}(\vec{C}^2) >,
\]

\[
S_{xx} = m C_m^2 < f Y_{xx}(\vec{C}) S_{i/2}^{(1)}(\vec{C}^2) >, \quad S_{xxx} = m < f Y_{xxx}(\vec{C}) >,
\]  

(3)

where \( C_m = \sqrt{2RT} \) and \( < > \) denotes

\[
< Q(\vec{C}) f > = \int \int \int_{-\infty}^{\infty} Q(\vec{C}) f d\vec{c}
\]

and irreducible tensors are given as

\[
Y(\vec{c}) = 1, \quad Y_x(\vec{c}) = C_x, \quad Y_{xx}(\vec{C}) = C_x^2 - \frac{1}{3} C^2, \quad Y_{xxx}(\vec{C}) = C_x C_x^2 - \frac{3}{5} C^2,
\]

\[
Y_{xxxx}(\vec{C}) = C_x^4 - \frac{6}{7} C^2 C_x^2 - \frac{3}{35} C^4, \quad Y_{xxxx}(\vec{C}) = C_x C_x^4 - \frac{10}{9} C^2 C_x^2 + \frac{5}{21} C^4.
\]
Sonine polynomials are given by
\[ S^{(0)}_m(y) = 1, \quad S^{(1)}_m(y) = m + 1 - y, \quad S^{(2)}_m(y) = (m + 1)(m + 2)/2 - (m + 1)y + y^2/2. \]

Since the irreducible tensors satisfy a contraction relation \( Y_{11i1k...} + Y_{22j2k...} + Y_{33k3k...} = 0 \), the macroscopic moments in the same order satisfy contraction relations such as \( p_{xx} + p_{yy} + p_{zz} = 0 \).

Let \( Q_{mn} \) and \( \Delta Q_{mn} \) be respectively \( Q_{mn} = \langle mc_{x}^m c_{2n} \rangle \) and \( \Delta Q_{mn} = \langle mc_{x}^m c_{2n} J_{coll} \rangle \) where \( J_{coll} \) denotes the reighthand side of Eq. (1); \( Q_{mn} \) and \( \Delta Q_{mn} \) are the moment with respect to the molecular velocity rather than the thermal velocity. Substituting Eq. (2) into Eq. (1), multiplying the equation by \( mc_{x}^m c_{2n} \), and integrating with respect to the molecular velocity, we obtain

\[
\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}}{\partial x} = \frac{p}{m\mu} \Delta \vec{Q},
\]

where
\[
\vec{U} = (Q_{00}, Q_{10}, Q_{01}, Q_{20}, Q_{11}, Q_{30}, Q_{21}, Q_{40}, Q_{31}, Q_{50}),
\vec{F} = (Q_{10}, Q_{20}, Q_{11}, Q_{21}, Q_{30}, Q_{22}, Q_{31}, Q_{40}, Q_{41}, Q_{50}),
\Delta \vec{Q} = (0, 0, 0, \Delta Q_{20}, \Delta Q_{11}, \Delta Q_{30}, \Delta Q_{22}, \Delta Q_{21}, \Delta Q_{40}, \Delta Q_{31}, \Delta Q_{50}).
\]

Defining \( \vec{Q} = (\rho, u, p, p_{ex}, Q_{x}, Q_{exx}, R_{0}, R_{ex}, R_{exxx}, S_{x}, S_{exx}, S_{exxx}) \) where \( \rho = mn \), the vectors \( \vec{U}, \vec{F}, \) and \( \Delta \vec{Q} \) are expressed as
\[
\vec{U} = A \vec{Q}, \quad \vec{F} = B \vec{Q}, \quad \Delta \vec{Q} = \Gamma \vec{Q},
\]

where the elements of the three matrices are simple functions of \( n, u, \) and \( p \).

**TRUNCATION PROCEDURE**

It is well known that the Grad’s thirteen moment equations is valid only for the analysis of weak shock waves. The range of applicability is given by \( 1 \leq M_s \leq 1.5 \). The full fourth order moment equation (F4OME) includes three fifth order moments, \( S_{x}, S_{exx}, \) and \( S_{exxx} \) in the last three components of \( \vec{F} \). If these fifth order moments are extracted from the moment equations (we call this as TF4OME), we have,

\[
\det B = \frac{1080}{w^5}(\frac{p}{\rho} - u^2)(\frac{3p}{\rho} - u^2).
\]

So, in the steady state problem, Eq. (4) may yield discontinuous solution of plane shock waves for \( M_s > \sqrt{9/5} = 1.34 \ldots \). The \( \det B \) for F5OME with extraction of sixth order moments also include the factor \( (3p/\rho - u^2) \). Since this factor related to the degeneration of the highest moment equations in Eq. (4), the simple truncation of the highest moments mentioned above strongly restrict the applicability of the system of moment equations. Although there may be various method to remedy this defect, we propose in this paper one of the most simple manner. The method is as follows: The \((i + 1)\)th moments in the \(i\)th order moment equations are evaluated applying supplemented \((i + 1)\)th moment equations. In the supplemented moment equations \((i + 1)\)th order moments and \((i + 2)\)th order moments in the convective term, \( \vec{F} \), are extracted. Using this approximation, the supplemented F4OME yields

\[
\det B = -(432/35)\rho u^5(17p/\rho + 5u^2).
\]

Thus, \( \det B \) does not change the sign for any value of the \( M_s \). Present method implies that in the steady state \((i + 1)\)th order moments are approximated by the derivatives of lower order moments. So, the present method is similar to the Navier-Stokes approximation for the thirteen moment equations. Hereafter, we call these supplemented moment equations as “the supplemented full \(i\)th order moment equations (SF\(i\)OME).
FIGURE 1. Riemann problem using TF5OME and SF4OME. Parameters: Mach = 1.2(left), Mach = 2.0(right), \( \lambda_1 = \sqrt{\gamma \mu / \rho U_c}, \lambda_c = \lambda_1 / C_{m1} \). Upper panel: \( x-t \) plot of shock wave, contact surface, and rarefaction wave. The second panel: Moments \( (\rho, p) \). The third panel: Moments \( (T, T_x, T_n) \), Lower panel: Heat flux \( q_x \) and shear stress \( p_{xx} \).
SHOCK-TUBE PROBLEM

We consider the following Riemann problem in the shock-tube: The driver (high pressure) gas at pressure $p_4$ and temperature $T_4$ and the driven (low pressure) gas at pressure $p_1$ and temperature $T_1 = T_4$ are separated by a diaphram and the diaphram is suddenly ruptured at time $t = 0$. We assume that the both driver and driven gases are composed of Maxwell molecules, i.e., the ratio of the specific heats $\gamma = 5/3$. We study the time and space evolution of this Riemann problem for $p_4/p_1$ before a shock wave or a rarefaction wave hits the end walls. The shock waves is moving to the right with a speed $W = M_1a_1$ where $a_1$ denotes the sound velocity in the driven gas. An adequate ratio of the pressure $p_4/p_1$ for $M_1$ is evaluated using conventional shock-tube relations. Introducing dimensionless variables of time, length, and moments as, $\tau = t/t_c$, $\xi = x/\lambda_1$, and $\tilde{Q}_{mn} = Q_{mn}/mC_m^{n+2m}$ where $t_c = \lambda_1/C_m$ and $\lambda_1$ denotes the mean free path defined by $\lambda_1 = \sqrt{\pi}p_1/p_1C_m$ where the subscript 1 denotes values pertinent to the driven gas, Eq. (4) can be expressed in the nondimensional form,

$$\frac{\partial \tilde{U}}{\partial \tau} + \frac{\partial \tilde{F}}{\partial \xi} = \frac{\sqrt{\pi}}{2} \tilde{n} \tilde{\Delta} \tilde{Q},$$

where tilde implies dimensionless values. For $t = 0$ quiescent gas for $\xi \leq 0$ is expressed by $\tilde{Q}(\xi \leq 0) = (p_{41}, 0, p_{41}, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T$ and the quiescent gas for $\xi > 0$ is expressed by $\tilde{Q}(\xi > 0) = (1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T$. For $t > 0$ $\tilde{Q}(\xi \leq 0)$ and $\tilde{Q}(\xi > 0)$ yield boundary conditions for $\xi \to -\infty$ and for $\xi \to \infty$, respectively. Substituting these initial and boundary conditions for $\tilde{Q}$ into Eq. (8) we obtain the initial and boundary conditions of $\tilde{U}$. A conventional difference scheme in connection with a splitting scheme for inhomogeneous simultaneous partial differential equations is given by,

$$\frac{\partial \tilde{U}}{\partial \tau} + \frac{\partial \tilde{F}}{\partial \xi} = 0, \quad \frac{\partial \tilde{U}}{\partial \tau} = \Delta \tilde{Q}.$$  

Knowing $\tilde{U}(\xi, \tau)$, we obtain value of the next step at $\tau = \tau + \Delta \tau$ by $\tilde{U}(\xi, \tau + \Delta \tau) = L_xL_t\tilde{U}(\xi, \tau)$. As the operator $L_x$ we applied the MacCormack’s predictor corrector method and as the latter operator $L_t$ we applied two-step Runge-Kutta time integration.

![FIGURE 2. Density $\rho$ for Mach = 1.2(left) and for Mach = 2.0(right) at different time levels. Parameters as in Fig. 2. Calculated ratios for Mach = 1.2; $\rho_4/\rho_1 = 2.51, \rho_2/\rho_1 = 1.88, \rho_4/\rho_1 = 1.30$. Calculated ratios for Mach = 2.0; $\rho_4/\rho_1 = 49.8, \rho_2/\rho_1 = 12.1, \rho_2/\rho_1 = 2.29$.](image)

RESULTS AND DISCUSSION

Equation (7) were reduced to TFiOME and SFiOME. These equations with aforementioned relevant initial and boundary conditions were solved. In order to obtain stable solution a small Courant number was chosen. The value $\Delta \tau/\Delta \xi = 0.1$ where $\Delta \xi$ was chosen as 0.2, i.e., $\Delta x/\lambda_1 = 0.2$. TFiOME and SFiOME were solvable.
in the range $p_4/p_1 \lesssim 7.8$ but this upper limit was dependent upon the order of moment equation. In the numerical simulation for $p_4$ beyond this upper limit strong numerical oscillation set up in the early stage of numerical simulation at the contact surface (layer) and this oscillation broke down the numerical simulation. In order to control this oscillation we employed an artificial viscosity [10].

\begin{equation}
D = \epsilon \Delta x^2 \frac{C_m}{p} \left[ \partial^2 \frac{p}{\partial x^2} \right],
\end{equation}

in the $L_x$ operator where $\epsilon$ is an adjustable numerical parameter. The solvable range of SF4OME extended to $p_4/p_1 \approx 70 \sim 100$, while the solvable upper limit of TF5OME with the artificial viscosity was $p_4/p_1 \approx 10$. For $p_4/p_1 > (p_4/p_1)_{\text{upper limit}}$ a Gibbs'-like numerical oscillation emerged and diverged in the contact layer, resulting in the break down of the simulation. The observed oscillation may be due to the central difference scheme and a small Courant number. It is required to find more adequate CFD procedure so as to extend the solvable range of the moment equations. It should be noted that an unsteady conservative numerical scheme yielded the solution for TF5OME beyond the applicable range mentioned in Sec III.

FIGURE 3. Shock structure for Mach=1.2. Temperature $T$, density $\rho$ (left), heat flux $q_x$, and shear stress $p_{xx}$ (right) as function $x$.

FIGURE 4. Shock structure for Mach=2.0. Temperature $T$, density $\rho$ (left), heat flux $q_x$, and shear stress $p_{xx}$ (right) as function $x$.

In Fig. 1, x-t diagrams of shock tube for $M_1 = 1.2$ (left) and $M_1 = 2.0$ (right), $\rho$, $p$, $u$, $T$, $T_{xx}$, $T_n$, $p_{xx}$, and $q_x$ at $t = 48t_c$ are present, where $T_{xx} = (p + p_{xx})/\rho$, and $T_n = (2p - p_{xx})/\rho$, respectively. This time stage $t = 48t_c$ is close to that of Beylich [6] at $t = 0.307$ in Figs. 11 and 12. For the case $M_1 = 2.0$ we employed SF4OME with Eq. (9), while for the case when $M_1 = 1.2$ we employed TF4OME without the artificial viscosity. The time development of density distributions in the shock tube is shown in Fig. 2 for $M_1 = 1.2$ (left) and for $M_1 = 2.0$ (right).
FIGURE 5. distribution of twelve moments in the shock tube at three time stages for \( M_1 = 1.4 \)

Shock structures at \( t/t_c = 120 \) for \( M_1 = 1.2 \) and for \( M_1 = 2.0 \) are shown in Figs. 3 and 4, respectively, density and temperature distributions in the left side and shear stress and heat flux distributions in the right side. In the figure left-hand side is the upstream. Thickness of the shock wave \( \delta \) defined by,

\[
\delta = \frac{\rho_2 - \rho_1}{(dp/dx)_{max}} \lambda_1
\]

for \( M_1 = 1.2 \) was evaluated from Fig. 3 as \( 15\lambda_1 \). Present shock-profiles of density and temperature show an excellent agreement with the results of the Navier-Stokes equation and DSMC simulation [11] when we rescale the mean free path \( \lambda_1 = 0.79\lambda_1 \) according to the definition of VSS model [12]. As shown in Fig. 4, the density profile for \( M_1 = 2 \) has a slight hollow in the supersonic part following to the foot of the shock wave.
Comparing this profile with the ones of Navier-Stokes equation and DSMC simulation [11], we found that as a whole density increased along the Mott-Smith solution but, in the intermediate region, it touched to the Navier-Stokes solution. This results may be partly attributed to the order of approximation of the moment equations. The distribution of the shear stress shown in Fig. 4 shows an apparent deviation from the Mott-Smith results near the peak point, while the distribution of heat flux shows a good agreement with the Mott-Smith result. Even though the Mott-Smith results are not so correct, we may remove such discrepancy by taking into account further moment equations.

For $M_t = 1.4$ F5OME was solved without artificial viscosity. Obtained distributions of twelve moments in the shock tube are shown in Fig. 5 at three time stages. The third Chapman-Enskog solution includes the third order derivatives of $u$, $T$ and $p$ and these derivatives are connected not only with the Burnett or the super-Burnett equation but also with the moments those as $S_x$, $S_{xxx}$, and $S_{xxxx}$. If these are so related to the higher derivatives of $u$, $T$ and $p$, distributions of these moments will exhibit more oscillatory variations in the shock wave. Present results shown in Fig. 5 did not exhibit such oscillatory features. Furthermore, we found from Fig. 5 that,

$$|Q_x| \approx |S_x| \gg |Q_{xxx}|,$$

while the second order Chapman-Enskog solution yields,

$$|S_x|, |S_{xxx}| \approx |p_{xx}| \cdot |Q_x| \ll |Q_{xx}|.$$

Present results demand us to examine the range of validity of the second order Chapman-Enskog solution.

**CONCLUDING REMARKS**

Moment equations derived from the Boltzmann equation were applied to the Riemann problem. A new closure method of the moment equations were proposed. It was demonstrated that supplemented moment equations were applicable to the analysis of moderately strong shock waves. Present result suggested that higher order moments of the velocity distribution function would not simply be expressed in terms of the higher order derivatives of velocity, temperature, and pressure. Present results also suggested that if we include more higher moment equations results of the present method may be considerably improved. Present method is expected for the nonequilibrium rarefied flow connecting with higher order moments demonstrated in the present analysis. To extend the moment method to various gases with different intermolecular potentials may be one of an urgent task to be done.

**REFERENCES**