Shock wave structure in rarefied polyatomic gases with large relaxation time for the dynamic pressure

Shigeru Taniguchi\textsuperscript{1}, Takashi Arima\textsuperscript{2}, Tommaso Ruggeri\textsuperscript{3} and Masaru Sugiyama\textsuperscript{4}

\textsuperscript{1} Department of Creative Engineering, National Institute of Technology, Kitakyushu College, Kitakyushu, Japan
\textsuperscript{2} Department of Mechanical Engineering, Faculty of Engineering, Kanagawa University, Yokohama, Japan
\textsuperscript{3} Department of Mathematics and Alma Mater Research Center on Applied Mathematics AM\textsuperscript{2}, University of Bologna, Bologna, Italy
\textsuperscript{4} Graduate School of Engineering, Nagoya Institute of Technology, Nagoya, Japan

E-mail: taniguchi.shigeru@kct.ac.jp, arima@kanagawa-u.ac.jp, tommaso.ruggeri@unibo.it, sugiyama@nitech.ac.jp

Abstract. The shock wave structure in rarefied polyatomic gases is analyzed based on extended thermodynamics (ET). In particular, the case with large relaxation time for the dynamic pressure, which corresponds to large bulk viscosity, is considered by adopting the simplest version of extended thermodynamics with only 6 independent fields (ET\textsubscript{6}); the mass density, the velocity, the temperature and the dynamic pressure. Recently, the validity of the theoretical predictions by ET was confirmed by the numerical analysis based on the kinetic theory in [S Kosuge and K Aoki: Phys. Rev. Fluids, Vol. 3, 023401 (2018)]. It was shown that numerical results using the polyatomic version of ellipsoidal statistical model agree with the theoretical predictions by ET for small or moderately large Mach numbers. In the present paper, first, we compare the theoretical predictions by ET\textsubscript{6} with the ones by kinetic theory for large Mach number under the same assumptions, that is, the gas is polytropic and the bulk viscosity is proportional to the temperature. Second, the shock wave structure for large Mach number in a non-polytropic gas is analyzed with the particular interest in the effect of the temperature dependence of specific heat and the bulk viscosity on the shock wave structure. Through the analysis of the case of a rarefied carbon dioxide (CO\textsubscript{2}) gas, it is shown that these temperature dependences play important roles in the precise analysis of the structure for strong shock waves.

1. Introduction
In polyatomic gases, in addition to the translational modes, the rotational and vibrational modes (microscopic internal modes) play important roles. In particular, in some temperature range, the internal modes are partially excited and relax much more slowly than the translational modes. Due to the presence of the slowly relaxing modes, the shock wave structure in rarefied polyatomic gas shows different features from the ones in rarefied monatomic gases\textsuperscript{[1,2]}. The thickness of a shock wave is several orders larger than the mean free path, which is typical length of the thickness in the case of rarefied monatomic gases. Moreover, as the Mach number increases from unity, the profile of the shock wave structure changes from the nearly symmetric profile (Type A) to the asymmetric profile (Type B), and then changes further to the profile composed of
thin and thick layers (Type C) [3–8]. Schematic profile of the mass density of the shock wave structure of Type C is shown in Figure 1. The previous approaches by Gilbarg & Paolucci [9] based on the Navier-Stokes, Fourier equations and by Bethe & Teller [10] based on the Meixner theory [11,12] are not able to explain these features in a unified way. A unified explanation of these peculiar shock wave structures has remained a long-standing problem. Although the experimental results were obtained in the 1950s, only recently, unified explanation was made.

A promising phenomenological approach is the one based on extended thermodynamics (ET) theory [13–15]. It was shown that the features of the shock wave structure are explained in a unified way by ET with 14 independent variables (ET$^{14}$); the mass density, the velocity, the temperature, the dynamic pressure (nonequilibrium pressure), the shear stress and the heat flux [16,17]. The agreement between the theoretical predictions and the experimental data for small or moderately large Mach numbers is quite good [16,17]. Moreover, it was shown that, when the relaxation time for the dynamic pressure is much larger than other relaxation times, the shock wave structure can be explained satisfactorily [18] based on the simplified ET theory with only 6 independent fields (ET$^{6}$) [19,20]; the mass density $\rho$, the velocity $v \equiv (v_i)$, the temperature $T$ and the dynamic pressure $\Pi$. The nonlinear version ET$^{6}$ theory was also derived only from the general principles without adopting near equilibrium assumption and therefore nonlinear of ET$^{6}$ is valid even far from equilibrium [21]. It was shown that the predictions of the shock wave structure based on linear and nonlinear ET$^{6}$ theories are substantially the same for small or moderately large Mach numbers and the only small difference appears even for large Mach numbers [22]. Therefore, we expect to analyze safely the structure of a strong shock wave for large Mach numbers by using ET$^{6}$.

After the successful explanation about the shock wave structure by ET theories, the confirmation of the results of ET theories was also made by the numerical analysis of kinetic theory. Previously, the approaches based on the Boltzmann equation such as the Direct Simulation Monte Carlo (DSMC) method [23], the Chapman-Enskog method [24] and the moment method [25–28] has encountered the difficulty in an appropriate modeling of the collision term due to the complexity of the collisional processes. Very recently, it was shown that the polyatomic version of the ellipsoidal statistical (ES) model can explain the features of the shock wave structure [29,30] by adopting large bulk viscosity, which corresponds to the large relaxation time for the dynamic pressure (See the equation (2) in the next section). The prediction by kinetic theory agrees quite well with the one by ET$^{14}$ for moderately large Mach number; $M_0 = 1.47$, where $M_0$ represents the unperturbed Mach number. In these papers [29,30], systematic numerical computations on the shock wave structure were carried out even for strong shock waves.

The purpose of the present paper is to make clear the structure of a strong shock wave in
rarefied polyatomic gases in which the relaxation time for the dynamic pressure is much larger than other relaxation times. First, we compare the theoretical predictions by ET$_6$ with the ones obtained by the numerical calculations based on the kinetic theory for large Mach number under the same assumptions, that is, the gas is polytropic and the bulk viscosity is proportional to the temperature. Second, we clarify the effect of the temperature dependence of the specific heat and bulk viscosity on the shock wave structure by considering non-polytropic gases with the general temperature dependence of the bulk viscosity. Through the analysis of the case of a rarefied CO$_2$ gas, we show the important role of these temperature dependences in the analysis of the structure of strong shock waves.

2. Field equations of ET$_6$

Let us consider plane shock waves propagating in $x$ direction such that the velocity is expressed as $v \equiv (v, 0, 0)$. The field equations of ET$_6$ are summarized in the following balance form with the independent field variables $u = (\rho, v, T, \Pi)$ [19, 21, 22, 31]:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) &= 0, \\
\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x} \left[ (p + \Pi) + \rho v^2 \right] &= 0, \\
\frac{\partial}{\partial t} \left( 2\rho \varepsilon + \rho v^2 \right) + \frac{\partial}{\partial x} \left\{ \left[ 2(p + \Pi) + 2\rho \varepsilon + \rho v^2 \right] v \right\} &= 0, \\
\frac{\partial}{\partial t} \left[ 3(p + \Pi) - 2\rho \varepsilon \right] + \frac{\partial}{\partial x} \left\{ [3(p + \Pi) - 2\rho \varepsilon] v \right\} &= -\frac{3\Pi}{\tau_{\Pi}},
\end{align*}
\]

where $\varepsilon$, $p$ and $\tau_{\Pi}$ are, respectively, the specific internal energy, the (equilibrium) pressure and the relaxation time for the dynamic pressure. In general, the relaxation time for the dynamic pressure $\tau_{\Pi}$ is a function of the mass density $\rho$ and the temperature $T$. As it was discussed in the Introduction, it was shown that the difference between the theoretical predictions by linear and nonlinear ET$_6$ theories is not so drastic [22]. For simplicity, we adopt linear ET$_6$ in the present study. The following caloric and thermal equations of state for rarefied polyatomic gases are adopted:

\[
\varepsilon \equiv \varepsilon(T), \quad p = \frac{k_B}{m} \rho T,
\]

where $k_B$ and $m$ are, respectively, the Boltzmann constant and the mass of a molecule. The temperature dependence of $\varepsilon$ may be determined by the dependence of the specific heat $c_v$ on the temperature through the following relation:

\[
\varepsilon(T) = \frac{k_B}{m} \int_{T_R}^{T} \hat{c}_v(\theta) \, d\theta
\]

with $\hat{c}_v = (m/k_B)c_v$ being the dimensionless specific heat and $T_R$ represents an inessential reference temperature. By using the Maxwellian iteration [13], we obtain the following relation between the relaxation time for the dynamic pressure $\tau_{\Pi}$ and the bulk viscosity $\nu$:

\[
\nu = \left( \frac{2}{3} - \frac{1}{\hat{c}_v} \right) \rho \tau_{\Pi}.
\]

We can determine the functional forms of $\varepsilon(T)$ and $\tau_{\Pi}(\rho, T)$ once we have the temperature dependence of $\hat{c}_v$ and the dependence of $\nu$ on the mass density and the temperature from the kinetic theoretical consideration and/or experimental data.

It should be noted that the systems of field equations of the ET theory of rarefied polyatomic gases are consistent with kinetic theoretical consideration. The kinetic theory gives the same
systems of field equations as the moment equations via Maximum entropy principle for the case of polytropic gases [19,32–34] and also for non-polytropic gases [35].

3. Shock wave structure

3.1. Settings and numerical method

Due to the Galilean invariance, without loss of generality, we adopt the frame moving with the shock wave such that the shock wave is considered as stationary. It is assumed that both the unperturbed state (the state at \( x = -\infty \) before and far from a shock wave) and the perturbed state (the state at \( x = \infty \) after and far from a shock wave) are in thermal equilibrium. Hereafter, the quantities with subscript 0 represent the quantities evaluated in the unperturbed state \( \mathbf{u}_0 = (\rho_0, v_0, T_0, 0) \) and the quantities with subscript 1 represent the quantities evaluated in the perturbed state \( \mathbf{u}_1 = (\rho_1, v_1, T_1, 0) \). The Mach number in the unperturbed state is defined by

\[
M_0 = \frac{v_0}{c_0}
\]

with \( c_0 \) being the sound velocity in the unperturbed state. The relationship between \( \mathbf{u}_1 \), \( \mathbf{u}_0 \) and \( M_0 \) is given by the Rankine-Hugoniot (RH) conditions for the system of the Euler equations. When the shock velocity is larger than the maximum characteristic velocity, the sub-shock appears [36]. In this case, we incorporate the analytical result on the strength of the sub-shock predicted by the RH condition for the system of ET_6 [18]. The algebraic equations obtained by replacing the differentiation in space by the central difference are solved numerically by Newton’s method [16,18,37].

3.2. Case of a polytropic gas with \( \nu \propto T \)

In [30], it was shown that theoretical prediction by kinetic theory agrees with the one of ET_14 for moderately large Mach number \( M_0 = 1.47 \). In this subsection, we compare the theoretical predictions by ET_6 with the ones by kinetic theory shown in [30] for large Mach number under the same assumptions. We assume that \( \hat{c}_v \) is independent of the temperature [30] and we introduce the following notation:

\[
\hat{c}_v = \frac{D}{2}
\]

where \( D(>3) \) is a constant, which represents the degrees of freedom of a molecule. In other words, we consider a polytropic gas in this subsection. In the case of a rarefied monatomic gas, \( D = 3 \). We also assume that [30]

\[
\nu \propto T
\]

and therefore the relaxation time \( \tau_\Pi \) is independent of temperature and inversely proportional to the mass density.

The following dimensionless quantities are introduced for the analysis based on ET_6 [16,18,22]:

\[
\hat{\rho} \equiv \frac{\rho}{\rho_0}, \quad \hat{v} \equiv \frac{v}{c_0}, \quad \hat{T} \equiv \frac{T}{T_0}, \quad \hat{\Pi} \equiv \frac{\Pi}{\rho_0 \frac{k_B}{m} T_0}, \quad \hat{x} \equiv \frac{x}{\tau_\Pi (\rho_0, T_0) c_0}
\]

and for comparison, we also introduce the following dimensionless position \( x_1 \) adopted in the numerical analysis of kinetic theory [30]:

\[
x_1 \equiv x \frac{3(3 + \delta)}{2\delta} \sqrt{\frac{\pi \delta + 5}{8 \delta + 3}} \frac{Pr \nu}{\mu}
\]
Figure 2. Profiles of the normalized mass density (red curves), normalized velocity (green curves) and normalized temperature (blue curves) predicted by ET$_6$ (left) for $M_0 = 5$. Four cases with $D = 6$ (solid curves), $D = 7$ (dashed curves), $D = 8$ (dot-dashed curves) and $D = 11$ (dotted curves) are shown. The vertical dashed lines at $x_1 = 0$ represent the jumps of physical quantities across the sub-shock. For comparison, the corresponding theoretical predictions by kinetic theory using ES model (right) are also shown. The right figure is a reproduction of Fig. 6 (a) in [30] (courtesy of K. Aoki).

3.3. Case of a non-polytropic gas with $\nu \propto T^n$

In the previous subsection, in order to compare the predictions by ET$_6$ with the one by kinetic theory, we adopt the assumptions of a polytropic gas and $\nu \propto T$. However, the experimental data [38, 39] indicate that these assumptions are not justified in several kinds of rarefied polyatomic gases in some temperature range. In fact, the dependence of $c_v$ on the temperature $T$ K for a rarefied carbon dioxide (CO$_2$) gas is expressed as [22]

$$c_v = 1.412 + 8.697 \times 10^{-3} T - 6.575 \times 10^{-6} T^2 + 1.987 \times 10^{-9} T^3$$

within the third order polynomial by fitting the experimental data [38] in the following temperature range: $220 \text{K} < T < 1100 \text{K}$. Moreover, in order to consider the more realistic case, we need to assume the following temperature dependence of $\nu$ [9]:

$$\nu \propto T^n,$$
where the exponent $n$ depends on gases and is determined from the fitting with the experimental data. The value of $n$ is expected to be $n = -1.3$ [22], which is opposite dependence to the case of $\nu \propto T$, through the comparison with the experimental data for a rarefied CO$_2$ gas [39].

The theoretical predictions of the shock wave structure with some values of $n$ has been reported: The shock wave structure in a rarefied CO$_2$ gas with $n = 0.935$ was analyzed based on ET by taking non-polytropic effect into account [16,18] and similarly the case of a polytropic gas with $n = 0.935$ was analyzed by kinetic theory [30]. In [22], the shock wave structure in a rarefied CO$_2$ gas with $n = -1.3$ is analyzed up to $M_0 = 5$. However, the experimental determination of the value of the relaxation time for the dynamic pressure (or the bulk viscosity) is extremely difficult and in this reason a reliable value of $n$ has not yet been known. It was also shown that the shock wave structure based on ET$_{14}$ is not sensitive to the change of $n$ for small or moderately large Mach numbers; $1 < M_0 < 1.47$ [17]. In the present subsection, we adopt $\hat{c}_v$ (3) for a rarefied CO$_2$ gas and analyze the effect of the value of $n$ on the structure of a strong shock wave.

Let us consider the shock wave structure for $T_0 = 295$ K and $M_0 = 5$. By using RH conditions for the system of Euler equations, we have $T_1 = 1098$ K. The dimensionless specific heat changes from $\hat{c}_v(T_0) = 3.46$ to $\hat{c}_v(T_1) = 5.66$ and we conclude that the change of $\hat{c}_v$ across the shock wave is not negligible. The non-polytropic effect should be considered for precise calculations on the shock wave structure for $M_0 = 5$. As a typical example, in Figure 3, we show the profiles of the dimensionless mass density, velocity, temperature and dynamic pressure for $M_0 = 5$ and $n = 1, 0, -1$. The thin layer of the shock wave structure of Type C is expressed by a sub-shock within the limited resolution of ET$_6$ [18] and the strength of a sub-shock is determined by RH conditions for the system of ET$_6$, which are derived from the left-hand side of (1). Therefore the strength of the sub-shock is independent of the values of $n$ and the difference between the predictions with the different values of $n$ appears only in the thick-layer region. Even though, we see the large difference between predictions with different $n$. The profiles in the thick layer strongly depend on the value of $n$. It is concluded that the temperature dependences of the specific heat and the bulk viscosity become important in the analysis of strong shock waves for large Mach numbers such as $M_0 = 5$.

4. Summary and concluding remarks

In the present paper, we have analyzed the shock wave structure on the basis of extended thermodynamics (ET) of rarefied polyatomic gases in which the relaxation time for the dynamic pressure is much larger than other relaxation times. We have adopted the ET theory with 6 independent fields (ET$_6$) and have shown the usefulness of ET$_6$ through the comparison with the numerical results obtained from the kinetic theory under the same assumptions, that is, the gas is polytropic and the bulk viscosity is proportional to the temperature. It has also been shown that the temperature dependences of the specific heat and the bulk viscosity strongly affect the structure of strong shock waves. The phenomenological approach based on ET enables us to incorporate these temperature dependences in a consistent way.

Lastly, we make the following remarks:

(I) In the present analysis, the simplest extended thermodynamics theory with only 6 independent variables is adopted. Although the thin layer of the shock wave structure of Type C is obtained as the sub-shock within the resolution of ET$_6$, it is shown that ET with 14 independent variables can describe the fine structure in the thin layer at least for moderate Mach numbers [16]. Detailed analysis of the fine structure by using ET with more independent variables are the future subject.

(II) In the case of ET$_6$, there exists only one characteristic velocity propagating in the positive direction and the characteristic value of the shock velocity for the sub-shock formation is determined analytically. However, ET theories with more independent variables have several
Figure 3. Profiles of the dimensionless mass density, velocity, temperature and dynamic pressure predicted by ET$_6$ for $M_0 = 5$. Three cases with $n = 1$ (black thin curves), $n = 0$ (blue dot-dashed curves) and $n = -1$ (red thick curves) are shown. The vertical dashed lines at $\hat{x} = 0$ represent the jumps of physical quantities across the sub-shock.

characteristic velocities propagating in the positive direction. In these cases, the determination of the characteristic value of the shock velocity for the sub-shock formation still remains as an open problem. The recent development on this issue including the peculiar feature of the sub-shock formation based on ET$_{14}$ was reported in [40].

(III) Another ET theories for polyatomic gases have been proposed such as a refined version of ET$_6$ which is expected to be valid also for dense gases [41], ET$_7$ dealing with rotational and vibrational modes individually [42] and the ET theory for mixtures of polyatomic gases [43]. The analysis of the shock wave structure based on these ET theories is now in progress. The results will soon be reported elsewhere.

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