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Overshoot of the non-equilibrium temperature in the shock wave structure of a rarefied polyatomic gas subject to the dynamic pressure

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ABSTRACT

The shock wave structure in a rarefied polyatomic gas is analyzed on the basis of non-linear extended thermodynamics with 6 independent fields (ET6); the mass density, the velocity, the temperature and the dynamic pressure, which permits us to study the shock profile also for large Mach numbers. The first result of this paper is that the shock wave structure is substantially the same as that obtained previously from the linear theory for small or moderately large Mach numbers. Only for very large Mach numbers there exist some differences in the relaxation part of the profile between the model with a non-linear production term and the one with a linear production term. The mathematical reason of this behavior is due to the fact that the non-linear differential system has the same principal part of the linear one.

The classical Meixner theory of relaxation processes with one internal variable is fully compatible with the ET6 theory and this fact gives us the explicit expressions of the internal variable and the non-equilibrium temperature in the Meixner theory in terms of the 6 fields, especially, of the dynamic pressure. By using the correspondence relation, the shock wave structure described by the ET6 theory is converted into the variables described by the Meixner theory. It is shown that the non-equilibrium Meixner temperature overshoots in a shock wave in contrast to the kinetic temperature. This implies that the temperature overshoot is a matter of definition of the non-equilibrium temperature.

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1. Introduction

Highly non-equilibrium and non-linear features of shock wave phenomena with steep gradient and rapid change in space and time have been attracting many theoretical and experimental researchers [1,2]. The study of the phenomena is also pivotal for developing many applications in various fields, for examples, the reentry problem of a spacecraft in aerospace engineering, extra corporeal shock wave lithotripsy (ESWL) in medical science.

For shock waves in rarefied polyatomic gases, the following features have been reported [1–8]: (1) The thickness of a shock wave is several orders larger than the mean free path of a constituent molecule. (2) When the Mach number increases from unity, the shock wave structure changes from the nearly symmetric profile (type A) to the asymmetric profile (type B) and further to the structure composed of thin and thick layers (type C). These features are never observed in rarefied monoatomic gases.

The previous approach to such peculiar shock wave structure is the one based on the Navier–Stokes Fourier (NSF) equations with a large value of the bulk viscosity [9]. This is, however, applicable only to type A.

The other previous approach by Bethe and Teller [10] is the one based on the Meixner theory [11,12]. Let us then consider the Meixner theory with only one relaxation parameter (internal variable) ξ, which, in the present case, indicates the behavior of internal modes in a polyatomic molecule. The system of basic equations of the Meixner theory is prescribed by the following relaxation equation:

$$\dot{\xi} = -\beta\mathcal{A}$$

together with the Euler equations in which the pressure and the internal energy depend also on the internal variable ξ. Here $\mathcal{A}$ and β represent the affinity of the relaxation process, which is a kind of the thermodynamic force, and a positive phenomenological coefficient, respectively. And a dot stands for the material time derivative. The Bethe–Teller theory has been used to explain the shock

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wave structure of Type C in such a way that, for the explanation of the thin layer, only the Euler equations are assumed, while for the thick layer, the Meixner theory is utilized. The Bethe–Teller theory is composed of two qualitatively different systems of equations.

As for the Meixner theory, however, we usually encounter a difficulty in determining the functional forms of the affinity and of the phenomenological coefficients. Moreover the theoretical consistency of the Meixner theory composed of the Euler equations and the relaxation equation is not clear enough as is pointed out in the previous paper [13] of the present authors.

The kinetic approaches on the basis of the Boltzmann equation such as the Direct Simulation Monte Carlo (DSMC) method [14], the Chapman–Enskog method [15] and the moment method [16–19] also encounter the difficulty. Due to the complexity of the collisional processes between polyatomic molecules with slowly relaxing internal modes, some simplifications are needed and appropriate modeling of the collision term still remains as an open problem.

More promising approach to shock wave phenomena is the one based on extended thermodynamics (ET) that is capable to describe non-equilibrium phenomena out of local equilibrium [20]. In the ET theory, in addition to the equilibrium quantities, the dissipative quantities are adopted as independent variables. The closed system of field equations is derived by imposing the general principles: (1) Material frame indifference principle, (2) Entropy principle, and (3) Causality.

Recently extended thermodynamics for polyatomic gases was established [21–25]. The usefulness of the ET theory was demonstrated through the analysis of ultrasonic sound [26,27], and the kinetic-theoretical basis of ET was made clear [28,29]. The present authors succeeded to explain the features (1) and (2) of the shock wave structure in a rarefied polyatomic gas in a unified way [30,31] by using the extended thermodynamics theory with 14 independent fields [21,22] (ET14), which is the most natural extension of the NSF theory. Moreover, the authors analyzed the shock wave structure based on the simplified ET theory with 6 independent fields (ET6) [13,32]; the mass density ρ, the velocity $\mathbf{v} \equiv (v_i)$, the temperature T and the dynamic pressure (non-equilibrium pressure) Π. The system of the ET6 theory is a principal sub-system [33] of the ET14 theory. It is shown that the ET6 theory also can explain the shock wave structure satisfactorily [34].

Concerning the extended thermodynamics theories, the present authors have recently constructed the non-linear ET6 theory without the near-equilibrium approximation due to the simplicity of the structure of the ET6 theory [35]. The non-linear ET6 theory is valid even far from equilibrium as far as the relaxation time of the dynamic pressure is much larger than other relaxation times. This is the first example of the extended thermodynamics with non-linear constitutive equations and is expected to play an important role for analyzing highly non-equilibrium phenomena. In the case of polytropic gases the theory is in perfect agreement with the one obtained by using kinetic considerations and the closure based on the Maximum Entropy Principle (MEP) [36].

The present authors also found that, if the Meixner theory has only one internal variable, there exists a rigorous correspondence relation between the ET6 theory and the Meixner theory [35]. From this relation, the internal variable and the non-equilibrium temperature in the Meixner theory are explicitly expressed in terms of the independent variables of the ET6 theory, especially, of the dynamic pressure. More details concerning the new approach of ET beyond the monoatomic gas are presented in the recent book by Ruggeri and Sugiyama [25].

The purpose of the present paper is twofold: Firstly, we show the reliability of the previous analysis of the shock wave structure based on the linear production term in the light of the non-linear ET6. Secondly, we describe the results based on the ET6 theory in terms of the physical quantities of the Meixner theory by using the correspondence relation. Physical implications of the results obtained by this transformation are discussed.

Significance to have two different descriptions of a shock wave is summarized as follows:

(a) The study of shock wave structure from various viewpoints gives us deep understandings of the complex phenomena. For example, as we see below, the temperature overshoots after a shock front predicted in the references [1,2] depends, in reality, on the definition of the non-equilibrium temperature. If we adopt the kinetic temperature of the ET6 theory, the overshoot never occurs [34] (see also the reference [30] for 14 moments).

(b) Because the Meixner theory has been frequently used for analyzing not only relaxation processes of the internal degrees of freedom of polyatomic molecules but also many kinds of phenomena such as chemical reactions and because many experimental data have been accumulated on the basis of the Meixner theory [4–8,37], the comparison between the two theories enables us to understand the experimental data from the viewpoint of the ET6 theory. This must be useful for enriching the ET theory itself.

(c) Conversely we can enrich the Meixner theory by using the ET6 theory. In the Meixner theory, it is sometimes difficult to pick up an appropriate internal variable ξ and to determine the explicit forms of the physical quantities. We can prove that these tasks can be carried out through the analysis by the ET6 theory. We can also critically reexamine the relaxation equation itself that has been frequently adopted in the literature [1,2].

2. Basic equations

We adopt the following caloric and thermal equations of state for a rarefied polyatomic gas:

$$\varepsilon \equiv \varepsilon(T), \quad p = \rho \frac{k_B}{m} T, \tag{1}$$

where ε, T, p, ρ, k_B, m are, respectively, the specific internal energy, the temperature, the pressure, the mass density, the Boltzmann constant and the mass of a molecule. In the present paper we consider a *non-polytropic* rarefied polyatomic gas where the specific heat $c_v = d\varepsilon/dT$ is not constant but is a function of the temperature T. As c_v can be measured by experiments as a function of the temperature T we can obtain the specific internal energy ε as

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

where $\hat{c}_v = (m/k_B)c_v$ is the dimensionless specific heat and T_R is an inessential reference temperature. The sound velocity c is given by

$$c = \sqrt{\frac{k_B}{m} T \gamma(T)},$$

where the ratio of the specific heat is given by $\gamma(T) = (1 + \hat{c}_v(T))/\hat{c}_v(T)$.

2.1. Field equations of the ET6 theory and non-equilibrium entropy

The field equations for the non-linear ET6 theory are summarized as follows [35]:

$$\begin{aligned}
&\dot{\rho} + \rho \frac{\partial v_k}{\partial x_k} = 0, \\
&\rho \dot{v}_i + \frac{\partial}{\partial x_i}(p + \Pi) = 0, \\
&\rho \dot{\varepsilon} + (p + \Pi) \frac{\partial v_k}{\partial x_k} = 0, \\
&\left(\frac{p + \Pi}{\rho} - \frac{2}{3}\varepsilon \right)^{\bullet} = \frac{\alpha k_\Pi}{3\rho}.
\end{aligned} \tag{2}$$

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