A Study of Steady Flow of a Polyatomic Gas by Extended Thermodynamics with Six Fields

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Abstract. Steady flow of a polyatomic gas is studied by the extended thermodynamic theory with six independent fields (ET$_6$). It is shown that the ET$_6$ theory can describe the effects on a flow due to the relaxation process of the internal motion such as molecular rotation and vibration, which can not be predicted by the Euler perfect fluid theory. And thereby characteristic features of the ET$_6$ theory itself can be elucidated.

1. Introduction
Extended thermodynamics (ET) [1, 2, 3] is a theory for studying highly nonequilibrium phenomena, which are out of applicability range of thermodynamics of irreversible processes (TIP) with the local equilibrium assumption [4]. The ET theory of rarefied monatomic gases [1, 2, 5] adopts the same hierarchy structure of the balance equations as the moment theory based on the Boltzmann equation [6] such as Grad’s moment theory [7]. While the ET theory of rarefied polyatomic gases has been developed [3, 8, 9, 10, 11, 12, 13], where the binary hierarchy of the balance equations including the dynamic pressure (nonequilibrium pressure) as an independent field is adopted. The theory, in particular the theory with 14 independent fields, has been successfully confirmed by comparing the theoretical predictions to the experimental data of linear waves [14], shock waves [15], and light scattering [16] in the range where the TIP theory (in this case, the Navier-Stokes and Fourier theory) is invalid.

The role of the dynamic pressure can be highlighted in the ET theory with 6 fields (ET$_6$): mass density, velocity, specific internal energy, and dynamic pressure [17, 18, 19]. The correspondence relation between ET$_6$ and the Meixner theory of relaxation processes [20, 21] was established in [17, 22]. The theory with a nonlinear constitutive equation was also proposed and developed [22, 23, 24, 25]. Furthermore the ET theory with two relaxation processes was studied by introducing one more independent field [26].

Recently an ET theory of dense polyatomic gases with 6 independent fields was proposed by postulating a principle of duality between rarefied and dense gases in the paper [27] where two kinds of nonequilibrium temperature are introduced: One is related to the subsystem with the kinetic and potential energies and the other is related to the subsystem of the internal modes such as molecular rotation and vibration. The importance of the internal relaxation process due to the molecular energy exchange between two subsystems for understanding the nature of the dynamic pressure was also emphasized [27].

The purpose of the present paper is to study a steady flow of a polyatomic gas by the ET$_6$ theory. It is shown that, in contrast to the Euler perfect fluid theory, the ET$_6$ theory predicts
some remarkable effects on a flow due to the relaxation process of the internal molecular modes. And thereby characteristic features of the ET$_6$ theory itself can be elucidated.

2. Brief summary of the ET$_6$ theory of dense polyatomic gases

In this section, for the sake of completeness, we summarize briefly the ET$_6$ theory [27]. We study a gas with the Hamiltonian in the form:

$$H = H^{K+U} + H^I,$$

where $H^{K+U} (= K + U)$ is the Hamiltonian of the subsystem having the kinetic energy $K$ of molecular translational motion and the potential energy $U$ among molecules, and $H^I$ is the Hamiltonian of the subsystem of the internal motion of constituent molecules such as molecular rotation and vibration.

In an equilibrium state with the mass density $\rho$ and the temperature $T$, the pressure $p$ can be divided into two parts: the pressure $p^{K+U}$ due to the $(K + U)$-subsystem and the pressure $p^I$ due to the $I$-subsystem. However, as $p^I = 0$, we have the thermal equation of state:

$$p = p(\rho, T) \equiv p^{K+U}(\rho, T).$$

Similarly we have the caloric equation of state for the specific internal energy $\varepsilon$:

$$\varepsilon = \varepsilon(\rho, T) \equiv \varepsilon^{K+U}(\rho, T) + \varepsilon^I(T),$$

where $\varepsilon^{K+U}$ and $\varepsilon^I$ are, respectively, the specific internal energies of the $(K + U)$-subsystem and of the $I$-subsystem. Note that $\varepsilon^I$ depends only on $T$. The specific entropy density $s$ is obtained in the following form [28]:

$$s = s^{K+U}(\rho, T) + s^I(T), \quad (1)$$

where $s^{K+U}$ and $s^I$ are the specific entropy densities of the two subsystems. The Gibbs relations of the subsystems are expressed as

$$Tds^{K+U} = d\varepsilon^{K+U} - \frac{p}{\rho^2} d\rho,$$

$$Tds^I = d\varepsilon^I. \quad (2)$$

In the ET$_6$ theory, a nonequilibrium state is specified by the quantities $\{\rho, v_i, \vartheta, \Theta\}$, where $v_i$ is the velocity, $\theta$ and $\Theta$ are the nonequilibrium temperatures of the $(K + U)$-subsystem and of the $I$-subsystem, respectively [27]. Then the time-evolution of a gas is governed by the following system of balance equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0,$$

$$\frac{\partial \rho v_j}{\partial t} + \frac{\partial}{\partial x_i} \{p(\rho, \vartheta) \delta_{ij} + \rho v_i v_j\} = 0,$$

$$\frac{\partial}{\partial t} \left\{2\rho \varepsilon^{K+U}(\rho, \vartheta) + 2\rho \varepsilon^I(\Theta) + \rho v_i^2\right\} +$$

$$+ \frac{\partial}{\partial x_i} \left\{\left[2p(\rho, \vartheta) + 2\rho \varepsilon^{K+U}(\rho, \vartheta) + 2\rho \varepsilon^I(\Theta) + \rho v^2\right] v_i\right\} = 0,$$

$$\frac{\partial}{\partial t} \left\{2\rho \varepsilon^I(\Theta)\right\} + \frac{\partial}{\partial x_i} \left\{2\rho \varepsilon^I(\Theta) v_i\right\} = -\dot{p}_l,$$
where $-\hat{P}_l$ is the production term. The first three equations are conservation laws of mass, momentum, and energy. The last equation expresses the irreversible energy exchange between the two subsystems.

The entropy balance equation is given by

$$\frac{\partial h}{\partial t} + \frac{\partial h_i}{\partial x_i} = \Sigma \geq 0,$$

where $h (= \rho \eta)$ is the entropy density, $h_i$ is the entropy flux, and $\Sigma$ is the entropy production. In the ET$_6$ theory, we can prove $h_i = hv_i$. The nonequilibrium specific entropy density $\eta$ is given as follows:

$$\eta = \eta(\rho, \vartheta, \Theta) = s^K + U(\rho, \vartheta) + s^I(\Theta).$$

If $\vartheta = \Theta = T$ with $T$ being the (local) equilibrium temperature, equation (5) coincides with (1).

### 3. Basic equations of a steady flow

From (3), a steady flow is governed by the following system of equations:

$$\frac{\partial}{\partial x_i}(\rho v_i) = 0,$$

$$\frac{\partial p(\rho, \vartheta)}{\partial x_j} + \rho v_i \frac{\partial v_j}{\partial x_i} = 0,$$

$$v_i \frac{\partial}{\partial x_i} \left( \frac{2p(\rho, \vartheta)}{\rho} + 2\varepsilon^K + U(\rho, \vartheta) + 2\varepsilon^I(\Theta) + v^2 \right) = 0,$$

$$2\rho v_i \frac{\partial \varepsilon^I(\Theta)}{\partial x_i} = -\hat{P}_l.$$

And the entropy balance equation (4) now reduces to

$$\rho v_i \frac{\partial \eta}{\partial x_i} = \Sigma \geq 0.$$

Let us pay attention to the variation of quantities along a streamline. From (6), we have

$$\delta p(\rho, \vartheta) + \rho v \delta v = 0,$$

$$v \delta \left( \frac{2p(\rho, \vartheta)}{\rho} + 2\varepsilon^K + U(\rho, \vartheta) + 2\varepsilon^I(\Theta) + v^2 \right) = 0,$$

$$2\rho v \delta \varepsilon^I(\Theta) = -\hat{P}_l,$$

where

$$\delta \equiv \frac{v_i}{v} \frac{\partial}{\partial x_i} \quad (v \equiv \sqrt{v_i v_i})$$

is the directional derivative along a streamline. And, from (7), we have

$$\rho v \delta \eta = \Sigma.$$

Equations (8) are rewritten in terms of $\{\delta v, \delta \rho, \delta \vartheta, \delta \Theta\}$ as follows:

$$\rho v \delta v + p_\rho(\rho, \vartheta) \delta \rho + p_\vartheta(\rho, \vartheta) \delta \vartheta = 0,$$

$$v \delta v + \left( -\frac{p(\rho, \vartheta)}{\rho^2} + \frac{p_\rho(\rho, \vartheta)}{\rho} + \varepsilon^K + U(\rho, \vartheta) \right) \delta \rho + \left( \frac{p_\vartheta(\rho, \vartheta)}{\rho} + \varepsilon^K + U(\rho, \vartheta) \right) \delta \vartheta + \varepsilon^I(\Theta) \delta \Theta = 0,$$

$$2\rho v c^I_v(\Theta) \delta \Theta = -\hat{P}_l.$$
where the suffix indicates the partial derivative, for example, \( p_{\rho}(\rho, \vartheta) \equiv \partial p(\rho, \vartheta)/\partial \rho \), and \( c_{v}^{K+U} \) and \( c_{v}^{I} \) are the specific heats of the subsystems defined by
\[
c_{v}^{K+U}(\rho, \vartheta) = \frac{\partial \varepsilon^{K+U}(\rho, \vartheta)}{\partial \rho}, \quad c_{v}^{I}(\Theta) = \frac{d \varepsilon^{I}(\Theta)}{d \Theta}.
\]
These specific heats are positive, and the total specific heat is given by \( c_{v} = c_{v}^{K+U} + c_{v}^{I} \).

4. Discussions

From (10)\(_1,2\), the variation of the mass flux \( \delta(\rho v) \) is expressed in terms of \( \delta v \) and \( \delta \Theta \) as follows:
\[
\delta(\rho v) = \rho \left( 1 - \frac{u^2}{u^2_E} \right) \delta v + \frac{v}{u^2_E} \frac{p_{\rho}(\rho, \vartheta)c_{v}^{I}(\Theta)}{c_{v}^{K+U}(\rho, \vartheta)} \delta \Theta,
\]
where \( u \) is the characteristic velocity [27] given by
\[
u^2 = p_{\rho}(\rho, \vartheta) + \frac{p_{\rho}(\rho, \vartheta)}{c_{v}^{K+U}(\rho, \vartheta)} \left\{ \frac{p^{K+U}(\rho, \vartheta)}{\rho^2} - \varepsilon^{K+U}(\rho, \vartheta) \right\}
= p_{\rho}(\rho, \vartheta) + \frac{\partial p_{\rho}(\rho, \vartheta)}{\rho^2 c_{v}^{K+U}(\rho, \vartheta)}.
\]
In particular, in an equilibrium case with the condition \( \vartheta = \Theta = T \), the velocity \( u \) is given by
\[
u^2_E = p_{\rho}(\rho, T) + \frac{T p_{r}^2(\rho, T)}{\rho^2 c_{v}(\rho, T)}.
\]

It is interesting to remind that the counterpart of equation (11) in the Euler theory is given by
\[
\delta(\rho v) = \rho \left( 1 - \frac{u^2}{u^2_{Euler}} \right) \delta v,
\]
where \( u_{Euler} \) is the sound velocity given by
\[
u^2_{Euler} = p_{\rho}(\rho, T) + \frac{T p_{r}^2(\rho, T)}{\rho^2 c_{v}(\rho, T)}.
\]

Because the system of ET\(_6\) includes the Euler system as the subsystem [29], we have the following subcharacteristic condition:
\[
u^2_E - \nu^2_{Euler} = \frac{T p_{r}^2(\rho, T)}{\rho^2} \frac{c_{v}(\rho, T)c_{v}^{K+U}(\rho, T)}{c_{v}(\rho, T)} > 0.
\]

Other interesting relations along a streamline are as follows: From (10)\(_1,2\), we have
\[
\delta \varepsilon = \frac{p_{\rho}(\rho, \vartheta)}{\rho^2} \delta \rho
\]
and, from (5), (2), (13) and (9), we have
\[
\delta \eta = c_{v}^{I}(\Theta) \left( \frac{1}{\Theta} - \frac{1}{\vartheta} \right) \delta \Theta = \frac{\Sigma}{\rho v},
\]
Some noticeable points are summarized as follows:

(i) In the Euler theory, as seen from (12), we notice the well-known result that the mass flux \( \rho v \) reaches the maximum value at the place where the velocity \( v \) is equal to the local velocity of sound \( u_{Euler} \) [30, 31].

While, in the ET\( _{\theta} \) theory, from (11), mass flux attains the maximum value at the place where the following condition is satisfied:

\[
\rho \left( 1 - \frac{v^2}{u^2} \right) \delta v = - \frac{v}{u^2} \frac{p_{\theta}(\rho, \vartheta)}{c_v^2 R U^v} \delta \Theta.
\]

It is interesting to note that the sign of \( \delta v/\delta \Theta \) depends on the condition whether \( v \) is greater than the local characteristic speed \( u \) or not.

(ii) At the place where the condition \( v = u \) is fulfilled, we have the relation:

\[
\delta(\rho v) = \frac{1}{u} \frac{p_{\theta}(\rho, \vartheta)}{c_v^2 R U^v} \delta \Theta = \frac{1}{u^2} \frac{p_{\theta}(\rho, \vartheta)}{\rho c_v^2 R U^v} \frac{\Sigma}{(1 - \frac{1}{\vartheta})}.
\]

Therefore, if \( p_{\theta} > 0 \), the quantities \( \delta(\rho v) \), \( \delta \Theta \), and \( \vartheta - \Theta \) have the same sign.

(iii) When we take the monatomic gas limit by letting \( \varepsilon \) tend to zero, it is easy to see that the relation (11) reduces to (12).

(iv) Let us study a steady flow in a nozzle parallel to the \( x \)-direction. We adopt the approximation of a quasi-one-dimensional flow. Then, in addition to the system of equations (8), we have an equation that comes from the conservation law of mass:

\[
\delta(\rho v A) = 0,
\]

where \( A \) is the cross section of a nozzle, and \( \delta \) in this case is

\[
\delta \equiv \frac{d}{dx}.
\]

From (11) and (15), we have the relation:

\[
\frac{1}{v} \left( 1 - \frac{v^2}{u^2} \right) \delta v = - \frac{1}{A} \delta A - \frac{1}{u^2} \frac{p_{\theta}(\rho, \vartheta)}{\rho c_v^2 R U^v} \delta \Theta = - \frac{1}{A} \delta A - \frac{1}{u^2} \frac{p_{\theta}(\rho, \vartheta)}{\rho c_v^2 R U^v} \frac{\Sigma}{(1 - \frac{1}{\vartheta})}.
\]

Therefore, if \( p_{\theta} > 0 \), the quantities \( \delta(\rho v) \), \( \delta \Theta \), and \( \vartheta - \Theta \) have the same sign.

(v) From the relation (14), we notice that the quantities \( \delta \Theta \) and \( \vartheta - \Theta \) have the same sign at all places on a streamline.

The above qualitative analysis is valid for any production term \( \dot{P}_{li} \), provided that it is compatible with the entropy principle (\( \Sigma > 0 \)). While in the case of a quantitative analysis, for example numerical analysis, the choice of an explicit expression for \( \dot{P}_{li} \) is required. Its simplest expression may be given by [27]

\[
\dot{P}_{li} = \frac{2\rho}{\varepsilon} \Delta,
\]
where $\tau_\Delta(\rho, T) (> 0)$ is the relaxation time for the energy exchange between two subsystems:

$$\Delta = \varepsilon^I(\Theta) - \varepsilon^I(T).$$

The final remarks are as follows: i) In a rarefied-gas limit where the intermolecular potential $U$ can be neglected, we have more explicit expressions of the relations obtained above. ii) It is interesting to study real-gas effects by adopting, for example, van der Waals equations of state. iii) Numerical analysis of typical nozzle flows is necessary to obtain quantitative results. Detailed analysis on these subjects will be reported soon elsewhere.

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