THEORIES OF RAREFIED GASES

R. KOVÁCS¹, D. MADJAREVIĆ⁴, S. SIMIĆ⁴ AND P. VÁN²,³

Abstract. Limits of classical constitutive laws such as Fourier and Navier-Stokes equations are discovered since decades. However, the proper extensions - generalizations of these are not evident. They differ in the underlying physical principles and in modelling capabilities. In this paper two different theories are discussed and compared to each other, namely the kinetic theory based Rational Extended Thermodynamics (RET) and non-equilibrium thermodynamics with internal variables (NET-IV).

First, the paper starts with the case of rigid heat conductors summarizing the result achieved so far. Then a typical example for compressible bodies is shown by presenting the first generalization for rarefied gases, called Meixner’s theory. It is further extended using generalized entropy current in the framework of NET-IV. It is shown how its structure is related to RET and how the compatibility between them can be acquired.

1. Introduction

The simplest and most widely applied classical continuum theory is related to isotropic fluids. They are based upon conservation laws of mass, momentum and energy, adjoined by appropriate constitutive equations for the heat flux $q_i$, deviatoric $\Pi_{(ij)}$ and spherical $\Pi^s$ part of the pressure:

\begin{align}
q_i &= -\lambda \partial_i T, \\
\Pi_{(ij)} &= -\nu \partial_{(i} v_{j)}, \\
\Pi^s &= -\mu \partial_i v_i,
\end{align}

where $\lambda$ is thermal conductivity, $\nu$ is shear viscosity and $\mu$ is bulk viscosity. The summation convention of Einstein is used and $(\cdot)$ denotes the deviatoric part. These equations are known as Fourier \cite{Fourier} and Navier-Stokes \cite{Navier-Stokes} constitutive relations.

Although widely accepted and applied in multitude of problems, there are numerous thermomechanical phenomena that constitutive relations \cite{Huang} are not capable to describe properly. In the sense of modelling, either linear relations between the constitutive quantities and gradients of field variables are inappropriate, or some kind of inertia of constitutive quantities has to be taken into account. Shortcomings of the classical model especially appear in processes under extreme thermomechanical conditions, or when the field variables are not restricted to a small neighborhood of local equilibrium state. These difficulties could be overcome in different ways. Here, in order to motivate our study, an example of modelling of the heat waves in solids will be presented.

Date: December 27, 2018.
1.1. Motivating example: the heat waves. In the case of heat conduction, the wave-like propagation of heat appeared as a non-Fourier phenomenon. It was first measured by Peshkov in superfluid He\textsuperscript{4} [1]. Later on, the ballistic heat conduction required the next level of modelling which still remains to be a theoretical challenge [2 3 4 5]. In current perspective, the most effective modelling frameworks, and at the same time thermodynamically consistent, are based upon Rational Extended Thermodynamics (RET) [6, 7] and non-equilibrium thermodynamics with internal variables and current multipliers (NET-IV) [8, 9, 10]. Their application to the heat waves modelling will be briefly described in the sequel.

In RET two different approaches to phonon gas can be taken to capture the propagating (wave) character of heat. The first one is continuum one, exposed in detail in [11], that describes the heat propagation using the energy conservation law and the balance law for the heat flux:

\[
\rho \dot{e} + \text{div} \mathbf{q} = 0, \quad (2)
\]

\[
\frac{d}{dt}(\alpha \mathbf{q}) + \nabla \nu = -\frac{\nu'}{\kappa} \mathbf{q},
\]

where dot indicates the material derivative and prime indicates the derivative with respect to temperature \(T\); \(\kappa(T)\) is the heat conductivity and \(\alpha(T)\) and \(\nu(T)\) are constitutive functions related to the second sound. The system of governing equations is closed by means of the compatibility with the entropy principle. The advantage of this model lies in its nonlinearity and wave speeds that depend on temperature. This enables the explanation of the shape changes of the second sound profile. For \(\alpha = \text{const.}\), governing equations (2) can be reduced to Cattaneo equation [13] which predicts the constant wave speed.

Another approach within RET is more closely related to the kinetic theory of gases, and phonon gas equations are obtained as proper moment equations of the Boltzmann-like equation for the phonon phase density function [7]. Closure of the governing equations, although trivial in this case, is based upon maximization of entropy. According to this approach, one has to define the way how the phonons interact with each other. Thus, two particularly interesting processes are introduced. One of them is the so called normal process, which leads to wave-like propagation, the Maxwell-Cattaneo-Vernotte (MCV) [12, 13, 14, 15, 16] equation is obtained in this case. The other one is the resistive process resulting in diffusive propagation where the Fourier equation holds. However, during ballistic heat conduction, there is no interaction between phonons, it is a propagation without any interaction among them, the phonons are scattered only on the boundary. The resulting system of moment equations in one-dimensional case reads as [6, 7]:

\[
\begin{align*}
\partial_t e + c^2 \partial_x p &= 0, \\
\partial_t p + \frac{1}{3} \partial_x e + \partial_x N &= -\frac{1}{\tau_R} p, \\
\partial_t N + \frac{4}{15} c^2 \partial_x p &= -\left(\frac{1}{\tau_R} + \frac{1}{\tau_N}\right) N,
\end{align*}
\]

where \(e\), \(p\) and \(N\) are the moments, i.e. the energy density, momentum density and the deviatoric part of the pressure tensor. The relaxation times \(\tau_R\) and \(\tau_N\) are related to the interacting processes. The other coefficients in the system (3) are
calculated according to the molecular structure, only the relaxation times are to be fitted for experiments.

In NET-IV, an analogous material model, called ballistic-conductive equation, can be derived for heat conduction using an extended entropy density and a generalized entropy current density with internal variables $q_i$ and $Q_{ij}$ \[8\]:

$$s(e, q_i, Q_{ij}) = s_{eq}(e) - \frac{m_1}{2} q_i q_i - \frac{m_2}{2} Q_{ij} Q_{ij}, \quad J_i = b_{ij} q_j,$$  \tag{4}

where $s_{eq}$ corresponds to term of local equilibrium, $m_1$ and $m_2$ are positive parameters. These functional assumptions characterise the deviation from local equilibrium according to thermodynamic requirements. The heat flux is identified as an internal variable as in Extended Irreversible Thermodynamics \[21\] and $Q_{ij}$ is interpreted as the current density of the heat flux, the dissipative pressure. In the entropy current $J_i$, the $b_{ij}$ is a current multiplier \[22\] allowing coupling between different tensorial order quantities such as the heat flux $q_i$ and the pressure $Q_{ij}$. This coupling stands as a requirement to appropriately describe ballistic effects \[5\]. That approach results in a compatible system in linearised one dimensional form:

$$\rho \partial_t e + \partial_x q = 0,$$

$$\tau_q \partial_t q + q + \lambda \partial_x T + \kappa \partial_x Q = 0,$$  \tag{5}

$$\tau_Q \partial_t Q + Q + \kappa \partial_x q = 0,$$

containing the same terms as \[3\], but with different coefficients. Although the coefficients can be compared to each other, and one can make a correspondence between them, it remains arbitrary since the coefficients in the NET-IV model are not constrained as in RET. There is more freedom for fitting with experimental data, but at the same time one has to deal with more parameters. This leads to another distinction between these two approaches in the case of ballistic propagation: the NET-IV model, with properly fitted parameters, may recover the exact propagation speed, whereas the RET model requires at least 30 moment equations for an accurate approximation. The difference in the interpretation in the fields is also remarkable.

All the models of heat waves presented here were tested against the experimental results. Continuum model \[2\] was used to determine the critical temperature at which the second sound in NaF and Bi was identified experimentally \[17\]. Kinetic-theory-based model \[3\] was used for numerical simulations which recover three different modes—the ballistic phonons, the second sound and the diffusive regime \[6\]. Finally the NET-IV model \[6\] is successfully tested on reconstructing the NaF experiments \[9\].

1.2. Aim and outline of the paper. The kinetic picture of ballistic propagation suggests the same behaviour in rarefied gases, too. The only difference is the type of the gas, instead of phonons we have real molecules like normal hydrogen. This fact is exploited in the framework of NET-IV when the coupled system of Fourier and Navier-Stokes equations is generalized. That is, the same form of entropy density and entropy current is applied, but the mass density $\rho$ is considered as a variable now. The goal of the extension of classical material laws is to study the irreversible processes that are coupled to the propagation of sound, especially close to a shock wave in rarefied gases. To that end, RET of polyatomic gases \[23\] and NET-IV
[10, 8] seem to be proper counterparts aimed to describe the same class of physical phenomena.

In this work we compare these two theories with the aim to find common theoretical background for them. This goal is going to be reached by seeking the answer to the following questions:

(1) How do we construct the system of governing (balance) equations?
(2) How do we close the governing system?
(3) How do we determine the material parameters (constitutive quantities)?
(4) Under what circumstances we obtain the equivalent systems?

Although formal in their nature, these questions will help us to reveal the common ground and better understand the conceptual subtleties of the two approaches. To that end, the paper will be organized as follows. In Section 2, the comparative analysis of the Meixner theory, first extension of Navier-Stokes-Fourier (NSF) system, will be performed from the point of view of NET-IV and RET. Then, in Section 3 we move forward using the generalized entropy current density, together with the internal variables, to derive the generalized Navier-Stokes-Fourier equations. Subsequent Section 4, the 14 moments RET model of polyatomic gases is presented in the form amenable to comparison with NET-IV approach given in Section 3. A discussion about similarities and discrepancies of two approaches in the sense of governing equations, concepts and procedures is given in Section 5.

2. Meixner theory: precursor for generalized theories

In this Section we shall make a first step towards comparison of different theories of rarefied gases. Our aim is to compare the Meixner model, the simplest model of non-equilibrium processes that can be derived within the framework of internal variables theory, with the extended thermodynamic model with 6 fields (ET6) which takes into account only the dynamic pressure as non-equilibrium variable.

2.1. Internal variables—the Meixner model. In the following, the Meixner model with single internal variable will be presented. Appropriate background can be found in [24, 25]. The starting point is the usual set of conservation laws of mass, momentum and energy:

\begin{align}
\rho &\dot{\mathbf{v}} + \rho \mathbf{v} \cdot \mathbf{\nabla} \mathbf{v} = 0, \\
\rho \mathbf{\dot{v}}_i + \partial_j P_{ij} = 0, \\
\rho \mathbf{\dot{e}} + \partial_i q_i + P_{ij} \partial_j v_j = 0.
\end{align}

In (6) \( e \) is the specific internal energy, \( P_{ij} \) is the pressure tensor and \( q_i \) is the heat flux. \( P_{ij} \) and \( q_i \) can be regarded as non-convective (conductive) parts of momentum and energy flux, respectively. We shall assume that pressure tensor has the following representation:

\begin{align}
P_{ij} &= \Pi_{ij} + p \delta_{ij}; \quad \Pi_{ij} = \Pi_{(ij)} + \Pi \delta_{ij}, \quad \Pi = \frac{1}{3} \Pi_{kk},
\end{align}

where \( p \) is the hydrostatic pressure, \( \Pi_{(ij)} \) is the traceless deviatoric part of the viscous stress tensor and \( \Pi \) is the dynamic pressure (\( \delta_{ij} \) is the Kronecker symbol).

Meixner’s theory characterises the deviation from local equilibrium by a scalar internal variable. The entropy density is additively decomposed into an equilibrium
part and an internal variable dependent non-equilibrium part:

\[ s(e, \rho, \xi) = s_{eq}(e, \rho) - \frac{m_1}{2} \xi^2. \]  

(8)

It is assumed that equilibrium entropy density obeys the classical Gibbs relation:

\[ T d s_{eq} = d e - \frac{p}{\rho^2} d \rho. \]  

(9)

Crucial step in the analysis is exploitation of the entropy balance law,

\[ \rho \dot{s} + \partial_i J_i = \sigma_s \geq 0, \]  

with classical entropy current

\[ J_i = \frac{q_i}{T}, \]  

\[ \sigma_s = \rho \dot{s} + \partial_i J_i = \rho \left( s_{eq} - m_1 \xi \dot{\xi} \right) + q_i \partial_i \left( \frac{1}{T} \right) + \frac{1}{T} \partial_i q_i. \]

(10)

Taking into account Gibbs relation (9) and conservation laws (6) and (6)3, after straightforward calculation one arrives at:

\[ \sigma_s = -\frac{1}{T} \Pi_{(ij)} \partial_i v_j + q_i \partial_i \left( \frac{1}{T} \right) - \rho m_1 \xi \dot{\xi} \geq 0. \]  

(11)

Following the standard procedure, thermodynamic fluxes and forces are introduced [26, 27, 28], given in Table 1:

| Fluxes | Fluid—traceless | Fluid—spherical | Thermal | Internal |
|--------|----------------|----------------|---------|----------|
| \( \Pi_{(ij)} \) | \( \Pi \) | \( q_i \) | \( \rho \dot{\xi} \) |
| \( -\frac{1}{T} \partial_i v_j \) | \( -\frac{1}{T} \partial_k v_k \) | \( \partial_i \left( \frac{1}{T} \right) \) | \(-m_1 \xi \) |

TABLE 1. Thermodynamic fluxes and forces

To guarantee the non-negative entropy production rate \( \sigma_s \) in every thermodynamic process, proper linear relations between forces and fluxes are established, taking into account possible cross-effects between the terms of the same tensorial order:

\[ \Pi_{(ij)} = -\frac{\mu}{T} \partial_i v_j, \]

\[ q_i = \lambda \partial_i \left( \frac{1}{T} \right), \]  

(12)

\[ \rho \dot{\xi} = -l_{11} \xi - \frac{l_{12}}{T} \partial_k v_k, \]

\[ \Pi = -l_{21} \xi - \frac{l_{22}}{T} \partial_k v_k. \]

First two relations represent the classical constitutive relations of Navier-Stokes-Fourier theory, the third one determines the evolution of the internal variable and the last is a constitutive relation for dynamic pressure. Also, from (12)4 one may observe the physical interpretation of internal variable \( \xi \)—it is a linear combination of dynamic pressure \( \Pi \) and divergence of velocity (divided by temperature). In the
special case, $l_{22} = 0$, we have $\Pi = -l_{21}m_1\xi$ and $\xi$ is directly related to dynamic pressure.

Due to scalar character of internal variable and linear relations between forces and fluxes in (12), it is possible to eliminate $\xi$ and obtain a single constitutive relation of the rate type for dynamic pressure $\Pi$. Therefore, the final set of equations for rarefied gases, obtained by means of single internal variable, reads:

$$\begin{align*}
\dot{\rho} + \rho \partial_t v_i &= 0, \\
\rho \dot{v}_i + \partial_j P_{ij} &= 0, \\
\rho \dot{e} + \partial_i q_i + P_{ij} \partial_j v_j &= 0
\end{align*}$$

(13)

$$\begin{align*}
\rho \dot{\Pi} + l_{11}m_1 \Pi &= -(l_{11}l_{22} - l_{12}l_{21})m_1 \frac{\partial_k v_k}{T} - l_{22}\rho \frac{d}{dt} \left( \frac{\partial_k v_k}{T} \right) \\
\Pi_{(ij)} &= -\frac{\mu}{T} \partial_i(v_j), \\
q_i &= \lambda \partial_i \left( \frac{1}{T} \right),
\end{align*}$$

where (7) has to be taken into account.

2.2. Extended thermodynamics with 6 fields. Within the realm of RET of polyatomic gases [23], the theory with 6 fields (ET6) is the simplest possible theory that captures non-equilibrium effects [36]. It contains only one non-equilibrium variable—the dynamic pressure $\Pi$. Its development was fostered by two facts: first, experimental evidence shows that in polyatomic gases dynamic pressure has greater influence than shear stresses and heat flux (see [38]); second, it can be easily compared with the simplest version of Meixner’s theory [39]. In this Section it will be presented only in the simplest possible form, without the details of its derivation.

The governing equations of ET6 have the following form:

$$\begin{align*}
\dot{\rho} + \rho \partial_k v_k &= 0, \\
\rho \dot{v}_i + \partial_i (p + \Pi) &= 0, \\
\rho \dot{e} + (p + \Pi) \partial_k v_k &= 0
\end{align*}$$

(14)

$$\begin{align*}
\frac{d}{dt} \left[ \frac{p + \Pi}{\rho} - \frac{2}{3} e \right] &= -\frac{1}{\tau} \frac{\Pi}{\rho},
\end{align*}$$

where we assumed linearized form of the source term in (14). In general case, ET6 theory is peculiar extended theory which admits the possibility of non-linear closure [39]. However, for the purpose of comparison with internal variables approach it is sufficient to keep only the linear approximation. Entropy density and entropy flux are:

$$s = s_{eq} - \frac{\Psi(\rho, e)}{\rho} \Pi^2, \quad J_i = 0,$$

(15)

whereas the entropy balance law reads:

$$\frac{d}{dt} \left[ s_{eq} - \frac{\Psi(\rho, e)}{\rho} \Pi^2 \right] = \frac{2\Psi}{\rho \tau} \Pi^2.$$

(16)

2.3. Comparison of IV with ET6. The aim of this part of our study is to compare the equations (13) of internal variables approach with ET6 equations (14). It is obvious that the model (13) contains more field variables than (14). It consists of conservation laws of mass, momentum and energy, and constitutive relations for
dynamic pressure $\Pi$, pressure deviator $\Pi_{ij}$ and heat flux $q_i$. The only non-classical part of the model is equation (13). It came out as a consequence of the second law of thermodynamics, but has the form of the balance law rather than classical constitutive relation. On the other hand, ET6 model comprises the same conservation laws, but only one additional equation—balance law for dynamic pressure $\Pi$. Pressure deviator and heat flux are neglected. Moreover, formal procedure of RET assumes from the outset the form of balance laws for all the state variables—$\Pi$ belongs to this set. Compatibility with entropy inequality yields the form of the unknown non-convective fluxes and the source terms. This will be thoroughly discussed in Section 4.

At this level of approximation, the internal variable approach yields the system which is inherently parabolic. Not only because of the constitutive relations (13)\textsuperscript{5,6}, but the balance law (13)\textsuperscript{4} as well, since it contains the material derivative of $\partial_k v_k/T$ which brings second order derivatives. On the other hand, ET6 model (14) is hyperbolic by construction.

To be comparable with ET6 model, it is necessary to reduce the number of field variables in the internal variable model (13) by neglecting the pressure deviator, i.e. $P_{ij} = (p + \Pi)\delta_{ij}$, $\Pi = (1/3)\Pi_{ii}$, and the heat flux by taking $\mu = 0$, $\lambda = 0$. Also one must assume $l_{22} = 0$, which altogether leads to the following reduced system:

$$
\dot{\rho} + \rho \partial_i v_i = 0,
\rho \dot{v}_i + \partial_i (p + \Pi) = 0_i,
\rho \dot{e} + (p + \Pi) \partial_i v_i = 0,
\frac{\rho}{l_{11} m_1} \dot{\Pi} + \Pi = \frac{1}{T} l_{12} l_{21} \partial_k v_k.
$$

On the other hand, equation (14)\textsuperscript{4} has to be adapted by using the ideal gas equations of state, $e = p/\rho(\gamma - 1)$, and taking into account the conservation laws for mass and energy. After certain straightforward calculations, the resulting system reads:

$$
\dot{\rho} + \rho \partial_k v_k = 0,
\rho \dot{v}_i + \partial_i (p + \Pi) = 0_i,
\rho \dot{e} + (p + \Pi) \partial_k v_k = 0,
\tau \dot{\Pi} + \tau \left[ \Pi - \left( \gamma - \frac{5}{3} \right)(p + \Pi) \right] \partial_k v_k = -\Pi.
$$

Comparison of the reduced IV-Meixner model (17) with ET6 model (18) yields the following equivalence conditions:

$$
\tau \Pi := \frac{\rho}{l_{11} m_1} = \tau; \quad \frac{1}{T} \frac{l_{12} l_{21}}{l_{11}} = \tau \left[ \Pi - \left( \gamma - \frac{5}{3} \right)(p + \Pi) \right]; \quad \mu = 0; \quad \lambda = 0.
$$

Further comparison of IV and RET approach to rarefied gases will be postponed until more refined theories are developed in the next two Sections.

3. NET-IV: generalized Navier-Stokes-Fourier equations

As it is demonstrated, the extension of entropy density itself is not enough to obtain coupling between the heat flux and the pressure tensor. However, the Nyirimultipliers [22] open further possibilities within a generalized entropy current. Let us choose the same set of extension of the state space together with the identification
entropy production for isotropic materials is of the compatibility with kinetic theory \[6, 21\]. Then the most general form of the entropy production for isotropic materials is

\[
s(e, \rho, q_i, \Pi_{ij}) = s_e(e, \rho) - \frac{m_1}{2} q_i q_i - \frac{m_2}{2} \Pi_{(ij)} \Pi_{(ij)} - \frac{m_3}{6} \Pi_{ii} \Pi_{jj},
\]

where the spherical and deviatoric parts are distinguished, \(m_1\), \(m_2\) and \(m_3\) are strictly positive parameters. This is not a Taylor series expansion, but a consequence of Morse lemma, as long as the internal variables are abstract fields that characterize the deviation from local equilibrium \[28, 18\]. The entropy current is a consequence of Gibbs relation for the equilibrium specific entropy, \(de = T ds + \frac{d}{d\rho} d\rho\):

\[
J_i = (b_{(ij)} + b_{kk} \delta_{ij}/3) q_j,
\]

where the current multiplier, \(b_{ij} = b_{(ij)} + b_{kk} \delta_{ij}/3\), is split into deviatoric and spherical parts, too. Then one can calculate the entropy production, considering the usual Gibbs relation for the equilibrium specific entropy, \(de = T ds + \frac{d}{d\rho} d\rho\):

\[
\sigma_s = \rho \dot{s} + \partial_i J_i = \\
= \rho \left( \partial_e \dot{s} + \partial_{\rho} \dot{s} \rho + \partial_{q_i} \dot{q}_i + \partial_{\Pi_{ij}} s_{\Pi_{(ij)}} + \partial_{\Pi_{ii}} s_{\Pi_{ii}} \right) + \partial_i \left[ (b_{(ij)} + \frac{1}{3} b_{kk} \delta_{ij}) q_j \right] = \\
= \partial_i q_i \left( \frac{b_{kk}}{3} - \frac{1}{T} \right) + q_i \left( \partial_{i} b_{kk} / 3 + \partial_{k} b_{(ki)} - \rho m_1 q_i \right) + b_{(ij)} \partial_i q_j - \\
- \frac{\Pi_{kk}}{3} \left( \frac{1}{T} \partial_j v_j + \rho m_3 \Pi_{jj} \right) - \Pi_{(ij)} \left( \frac{1}{T} \partial_i v_j + \rho m_2 \Pi_{(ij)} \right) \geq 0.
\]

Assuming linear relations between thermodynamic fluxes and forces one realizes coupling between the quantities of same tensorial order in the case of isotropic materials, too:

\[
-\rho m_1 q_i + \frac{1}{3} \partial_i b_{kk} + \partial_j b_{(ij)} = n q_i,
\]

\[
-\frac{1}{T} \partial_i v_j - \rho m_2 \Pi_{(ij)} = l_{11} \Pi_{(ij)} + l_{12} \partial_i q_j,
\]

\[
b_{(ij)} = l_{21} \Pi_{(ij)} + l_{22} \partial_i q_j,
\]

\[
-\frac{1}{T} \partial_j v_j - \rho m_3 \Pi_{ii} = k_{11} \frac{\Pi_{ii}}{3} + k_{12} \partial_i q_i,
\]

\[
b_{kk} - \frac{1}{T} = k_{21} \frac{\Pi_{ii}}{3} + k_{22} \partial_i q_i.
\]

Here isotropy is interpreted in a restricted sense, including spatial reflections \[19\]. It is also remarkable, that we did not assume any symmetry of the reciprocity relations. A similar assumption turned out to be extremely fruitful in the case of internal variables \[10\]. The positive definiteness of entropy production constraints the sign of the coefficients:

\[
n > 0, \quad l_{11} l_{22} - (l_{12} + l_{21})^2/4 > 0, \quad k_{11} k_{22} - (k_{12} + k_{21})^2/4 > 0.
\]
Let us assume constant coefficients, that is a strictly linear theory, and eliminate the current multipliers to obtain the constitutive relations:

\[
\begin{align*}
\tau_1 \hat{q}_i + q_i + \lambda \partial_i T - \alpha_{21} \partial_i \Pi_{kk} - \beta_{21} \partial_i \Pi_{(ij)} &= \gamma_1 \partial_i (\partial_k q_k) + \gamma_2 \partial_j (\partial_{ij} q_i), \\
\tau_2 \hat{\Pi}_{(ij)} + \Pi_{(ij)} + \nu \partial_i \langle v_j \rangle + \beta_{12} \partial_i \langle q_j \rangle &= 0, \\
\tau_3 \hat{\Pi}_{ii} + \Pi_{ii} + \eta \partial_i v_i + \alpha_{12} \partial_i q_i &= 0,
\end{align*}
\]

(29)

Coefficients have the following meaning: \( \tau_m \) \((m = 1, 2, 3)\) are the relaxation times, \( \lambda \) is the heat conductivity, \( \eta \) is the shear viscosity, \( \nu \) denotes the bulk viscosity, \( \alpha_{ab}, \beta_{ab} \) \((a, b = 1, 2)\) are the coupling parameters between the heat flux and the pressure and \( \gamma_c \) \((c = 1, 2)\) are the relaxation times of RET, whose equations are hyperbolic by construction, let us consider the case \( \gamma_1 = \gamma_2 = 0 \), i.e. \( l_{22} = k_{22} = 0 \). Its consequence is that the reciprocity is antisymmetric and \( l_{12} = -l_{21} \) and \( k_{12} = -k_{21} \). This way, one can simplify the resulting parabolic system to a hyperbolic one:

\[
\begin{align*}
\tau_1 \hat{q}_i + q_i + \lambda \partial_i T - \alpha_{21} \partial_i \Pi_{kk} - \beta_{21} \partial_i \Pi_{(ij)} &= 0, \\
\tau_2 \hat{\Pi}_{(ij)} + \Pi_{(ij)} + \nu \partial_i \langle v_j \rangle + \beta_{12} \partial_i \langle q_j \rangle &= 0, \\
\tau_3 \hat{\Pi}_{ii} + \Pi_{ii} + \eta \partial_i v_i + \alpha_{12} \partial_i q_i &= 0,
\end{align*}
\]

(30)

and in 1D:

\[
\begin{align*}
\tau_1 \hat{q} + q + \lambda \partial_x T - \alpha_{21} \partial_x \Pi_s - \beta_{21} \partial_x \Pi_d &= 0, \\
\tau_2 \hat{\Pi}_d + \Pi_d + \nu \partial_x v + \beta_{12} \partial_x q &= 0, \\
\tau_3 \hat{\Pi}_s + \Pi_s + \eta \partial_x v + \alpha_{12} \partial_x q &= 0,
\end{align*}
\]

(31)

where the lower indices \( d \) and \( s \) denote the deviatoric and spherical parts, respectively.

| Fluxes  | Thermal | Fluid—traceless | Fluid—spherical |
|---------|---------|-----------------|-----------------|
| Forces  | \( -\rho m_1 \hat{q}_j + \partial_j b_{kk} + \partial_j b_{(ij)} \) | \( \hat{\Pi}_{(ij)} \) | \( \hat{\Pi}_{ii} \) |
|         | \( 4\dot{\partial}_j v_j + \rho m_2 \hat{\Pi}_{(ij)} \) |                 |                 |
|         | \( \frac{4}{n} \dot{\partial}_j v_j + \rho m_3 \hat{\Pi}_{jj} \) |                 |                 |

Table 2. Thermodynamic fluxes and forces of NET-IV I.
TABLE 3. Thermodynamic fluxes and forces of NET-IV II.

| Fluxes                        | Entropical coupling - traceless | Entropical coupling - spherical |
|-------------------------------|---------------------------------|---------------------------------|
| Forces                        | \( b_{ij} \)                     | \( b_{kk} - \frac{1}{T} \)      |
| \( \partial_i q_j \)          |                                 | \( \partial_i q_i \)            |

4. THE 14 MOMENTS MODEL OF RATIONAL EXTENDED THERMODYNAMICS

Rational extended thermodynamics of polyatomic gases with 14 moments \[40, 23\] presents a different route to description of viscous, heat-conducting gases. It fits within the general framework of RET, to be described briefly in the sequel, and inherits the basic principles of modern continuum theories.

4.1. Formal structure of RET. There are four basic principles in this approach \[6\]:

(a) governing equations are of balance type;
(b) constitutive relations are of local type;
(c) governing equations are invariant with respect to Galilean transformations;
(d) governing equations are compatible with the entropy inequality with convex entropy.

Assumptions (a) and (b) are the specific mathematical requirements introduced with the aim to obtain the system of governing equations in the form of hyperbolic system of balance laws. Moreover, they allow the existence of weak solutions and shocks. Assumptions (c) and (d) are basic physical requirements, fully consistent with modern continuum theories. In the sequel, the basic structure of RET will be described following \[6\].

Since the equations of RET have the structure of balance laws, they can be recast into the following form:

\[
\partial_t \mathbf{F}^0(\mathbf{u}) + \partial_i \mathbf{F}^i(\mathbf{u}) = \mathbf{f}(\mathbf{u}), \quad i = 1, 2, 3. \tag{32}
\]

In \( \mathbf{u} \in \mathbb{R}^N \) denotes the vector of state variables, \( \mathbf{F}^0(\mathbf{u}) \in \mathbb{R}^N \) is the vector of densities, \( \mathbf{F}^i(\mathbf{u}) \in \mathbb{R}^N \) are the components of fluxes, and \( \mathbf{f}(\mathbf{u}) \in \mathbb{R}^N \) is the vector of source (production) terms. Certain components of \( \mathbf{F}^0(\mathbf{u}) \) and \( \mathbf{F}^i(\mathbf{u}) \) are determined by the physical laws, but some of the fluxes are constitutive quantities, as well as the source terms \( \mathbf{f}(\mathbf{u}) \). Since the dependence of the densities and fluxes on \( \mathbf{u} \) is of local type (in accordance with assumption (b)), the system turns into a quasi-linear system of PDE’s:

\[
\mathbf{A}^0(\mathbf{u}) \partial_t \mathbf{u} + \mathbf{A}^i(\mathbf{u}) \partial_i \mathbf{u} = \mathbf{f}(\mathbf{u}), \tag{33}
\]

where \( \mathbf{A}^0 = \partial \mathbf{F}^0 / \partial \mathbf{u} \) and \( \mathbf{A}^i = \partial \mathbf{F}^i / \partial \mathbf{u} \). If all the eigenvalues \( \lambda(\mathbf{u}) \) of the eigenvalue problem \( (\lambda \mathbf{A}^0 + n_i \mathbf{A}^i) \mathbf{d} = \lambda \mathbf{d} \) are real, where \( n_i \) are the components of the unit-normal vector, the system \[33\] is hyperbolic in \( t \)-direction.

For any thermodynamic process described by \[32\], in accordance with assumption (d) the state variables \( \mathbf{u} \) must satisfy the entropy inequality:

\[
\partial_t h^0(\mathbf{u}) + \partial_i h^i(\mathbf{u}) = \Sigma(\mathbf{u}) \geq 0, \tag{34}
\]

\[1\] It is quite common to adopt \( \mathbf{F}^0(\mathbf{u}) \equiv \mathbf{u} \).
where \(h^0\) is the entropy density, \(h^i\) are the components of the entropy flux, and \(\Sigma\) is the entropy production rate. Due to local dependence, the entropy inequality can be put into quasi-linear form:

\[
\frac{\partial h^0}{\partial u} \cdot \partial_t u + \frac{\partial h^i}{\partial u} \cdot \partial_i u = \Sigma(u). \tag{35}
\]

The entropy principle states \([49]\) that for any thermodynamic process the state variables \(u\) must obey the entropy law (34), provided they satisfy the balance laws (32). In other words, the balance laws are regarded as constraints. Since both the balance laws (33) and the entropy law (35) are quasi-linear with respect to \(u\), the problem with constraints can be transformed into a problem without constraints at the expense of introduction of the Lagrange multipliers \(u' \in \mathbb{R}^N\):

\[
\partial_t h^0 + \partial_i h^i - \Sigma = u' \cdot (\partial_t F^0 + \partial_i F^i - f). \tag{36}
\]

As a consequence, the following relations must hold:

\[
dh^0 = u' \cdot dF^0, \quad dh^i = u' \cdot dF^i, \tag{37}
\]

or equivalently:

\[
\frac{\partial h^0}{\partial u} = u' \cdot \frac{\partial F^0}{\partial u}, \quad \frac{\partial h^i}{\partial u} = u' \cdot \frac{\partial F^i}{\partial u}. \tag{38}
\]

Moreover, the residual inequality has to be satisfied as well:

\[
\Sigma = u' \cdot f \geq 0. \tag{39}
\]

Equations (36)–(39) require some comments. Since certain components of the fluxes are constitutive quantities, equations (38) can serve for determination of the multipliers \(u'\), as well as constitutive components fluxes. Moreover, one of the legacies of RET is the assumption that entropy flux \(h^i\) is not necessarily proportional to the heat flux, i.e. it is not defined as \(h^i = q_i/T\). Instead, it is treated as a constitutive quantity, which brings certain freedom in its derivation. Finally, once the multipliers \(u'\) are determined, one may choose the source terms \(f(u)\) in such a way that the residual inequality (39) is satisfied for all thermodynamic processes. Although this statement introduces the flavor of arbitrariness, it is usually reduced to the similar arguments as those used in classical TIP, or as in NET-IV in previous Section. Namely, the components of the source terms \(f\) are chosen as linear forms of \(u'\) (in the appropriate way which takes into account their tensorial order), so that \(\Sigma\) becomes quadratic form in \(u'\).

Another property of the method of multipliers—the possibility to transform the system (32) into symmetric hyperbolic form—is substantial for the mathematical analysis, but it will not be studied here. The details, including an account on its historical development, may be found in [23] (pp. 39–40).

### 4.2. Hierarchical structure of governing equations

One of the basic properties of the governing equations of RET is that they have a hierarchical structure with an increasing tensorial order of densities, fluxes and production terms. The equations for monatomic gas can be put into a single hierarchy:

\[
\partial_t F_{k_1 \ldots k_n} + \partial_i F_{k_1 \ldots k_n,i} = P_{k_1 \ldots k_n}. \tag{40}
\]

The system (40) is fully compatible with Grad’s moment equations obtained in the kinetic theory of gases [34]. However, in contrast to Grad’s approach which is relied on approximation of non-equilibrium distribution function, closure procedure
in RET is purely macroscopic and relies on the application of entropy principle and exploitation of the Liu’s method of multipliers \[^{[49]}\].

The hierarchical structure (with the assumption of convex entropy density) facilitated introduction of the concept of subsystems \[^{[50]}\] with nice structural properties. For example, Lagrange multipliers used in exploitation of the entropy principle could be used as new state variables, so-called main field \[^{[51]}\], and the system is transformed into a symmetric hyperbolic form.

To the abstract form of equations \[^{(40)}\] one may adjoin the proper physical interpretation, at least at the level of 13 moments. In this case the equations have the following form:

\[
\begin{align*}
\partial_t F + \partial_i F_i &= 0, \\
\partial_t F_k + \partial_i F_{ki} &= 0, \\
\partial_t F_{kk} + \partial_i F_{kki} &= 0, \\
\partial_t F_{k1} + \partial_i F_{k1i} &= P_{k1k2}, \\
\partial_t F_{kJ} + \partial_i F_{kji} &= P_{kJ}.
\end{align*}
\]

(41)

The densities can be written in usual physical notation:

\[
F^0 = \begin{pmatrix}
F \\
F_k \\
F_{kk} \\
F_{ij} \\
F_{kij}
\end{pmatrix} = \begin{pmatrix}
\rho \\
\rho v_k \\
\rho v^2 + 2\rho e \\
\rho v_i v_j + p \delta_{ij} + \Pi_{(ij)} \\
\rho v^2 v_j + 2(\rho e + p) v_j + \Pi_{(kj)} v_k + 2q_j
\end{pmatrix},
\]

(42)

where \(\langle \cdots \rangle\) denotes the traceless part of the tensor.

Two remarks have to be given. First, the system \[^{(41)}\] can be split into conservative part, consisted of conservation laws of mass, momentum and energy, and non-conservative part, consisted of balance laws for the fluxes of momentum and energy, i.e. the pressure tensor \(\Pi_{(ij)}\) and the heat flux \(q_i\). Actually, conservation laws \[^{(41)}\]_1−3, with \(\Pi_{(ij)} = 0\) and \(q_i = 0\), represent an equilibrium subsystem in the sense defined in \[^{[50]}\]. Thus, the balance laws \[^{(41)}\]_4−5 are supposed to capture the non-equilibrium effects and bring the dissipation into the system. Dissipative character is preserved by the fact that the source terms \(P_{k1k2}\) and \(P_{kJ}\) are determined through the compatibility with residual inequality \[^{(39)}\], i.e. they are responsible for the non-negativity of the entropy production rate.

Second remark is concerned with the restriction that naturally appears in the hierarchical structure of equations \[^{(10)}\], in which the fluxes in the moment equation of tensorial order \(k\) become the densities in the moment equation of tensorial order \(k+1\). Since \(F_{kk}\) is the trace of the density \(F_{ij}\), there exists the constraint among the state variables, \(2\rho e = 3p\), which restricts the application of the model to monatomic gases. There were several attempts to derive the equations for 14 moments, with intention to capture the behaviour of polyatomic gases. A brief review of these attempts may be found in \[^{[23]}\] (pp. 109–110).

Recently \[^{(40)}\], a natural and physically convincing hierarchical structure of equations for dense and polyatomic gases was discovered. Main feature of this system is

\[^{2}\]In mathematical community these state variables are often called entropic variables.
that a single-hierarchy structure of (40) is replaced with double-hierarchy structure, which in the case of 14 moments reads:

\[\begin{align*}
    \partial_t F + \partial_k F_k &= 0, \\
    \partial_t F_i + \partial_k F_{ik} &= 0, \\
    \partial_t F_{ij} + \partial_k F_{ijk} &= P_{ij}, \\
    \partial_t G_{ll} + \partial_k G_{llk} &= 0, \\
    \partial_t G_{lli} + \partial_k G_{lli} &= Q_{lli},
\end{align*}\]  

(43)

where the densities have the following physical interpretation:

\[\begin{align*}
    F &= \rho, \\
    F_i &= \rho v_i, \\
    F_{ij} &= \rho v_i v_j + (p + \Pi) \delta_{ij} + \Pi_{(ij)}, \\
    G_{ll} &= \rho v^2 + 2pe, \\
    G_{lli} &= \rho v^2 v_i + 2(p + \Pi) v_i + 2\Pi_{(ki)} v_i + 2q_i.
\end{align*}\]

The main feature of hierarchy (43) is lack of relation between energy density and momentum flux, \(G_{ll} \neq F_{kk}\), i.e. \(2pe \neq 3p\). Thus, dynamic pressure \(\Pi\) naturally appears as fourteenth state variable. It is convenient to identify the \(F\)-hierarchy as the momentum hierarchy and \(G\)-hierarchy as the energy hierarchy, according to leading non-zero order moments that appear in them.

As it was mentioned above, the hierarchical structure of RET equations for monatomic gases is compatible with Grad’s moment equations. The case of polyatomic gases more delicate due to internal degrees of freedom of molecules. Nevertheless, it was shown [41] that double hierarchy (43) can be recovered within the framework of kinetic theory (by the application of maximum entropy principle) with a single scalar variable capturing all the internal degrees of freedom (for the origin of this approach one have to consult [45, 46]). This result was further developed in [47] and summarized in [23].

4.3. Constitutive relations near equilibrium. Except in rare situations, closure problem in RET cannot be generally solved. Its solution is usually restricted to a neighborhood of local equilibrium state. Since the constitutive relations are determined by the application of entropy principle, it is common to assume the following general form of entropy density and entropy flux:

\[\begin{align*}
    h^0 &= \rho s = \rho s_{eq} + \rho k, \\
    h^i &= h^0 v_i + J^i
\end{align*}\]  

(44)

where \(s_{eq}(\rho, e)\) is the specific entropy in equilibrium; \(k(\rho, e, \Pi, \Pi_{(ij)}, q_i)\) is the non-equilibrium part of the entropy density, and \(J^i(\rho, e, \Pi, \Pi_{(ij)}, q_i)\) is the non-convective part of the entropy flux; they both must obey the equilibrium conditions, \(k(\rho, e, 0, 0, 0) = 0, J^i(\rho, e, 0, 0, 0) = 0\). It is shown [40, 23] that in the case of 14 moments equations Lagrange multipliers are completely determined by the non-equilibrium specific entropy density \(k\). The results of these detailed studies, that can be of use in comparison of ET with the method of internal variables, will be summarized in the sequel.
The approximate form (up to second order in non-equilibrium variables) of the entropy density and entropy flux reads:

\[ h^0 = \rho s_{eq} - \frac{1}{2T} \Pi^2 - \frac{1}{4\rho T} \Pi_{(ij)} \Pi_{(ij)} + \rho z_3 q_i q_i + O(3), \]

\[ J^k = \frac{1}{T} q_k - \beta_2 \Pi q_k - \beta_3 q_i \Pi_{(ik)} + O(3), \]

where:

\[ \Gamma = \frac{5}{3} p - \rho p - \frac{\rho}{\rho} p_k - \frac{5}{3} p - \rho \left( \frac{\partial p}{\partial \rho} \right), \]

and \( O(N) \) denotes the lowest order non-equilibrium terms that are neglected. Convexity arguments yield the following inequalities:

\[ \Gamma > 0, \quad z_3 < 0. \]

The source terms are expressed as linear forms of non-equilibrium variables:

\[ \dot{P}_t = \frac{3}{T} \Pi + O(2), \quad \dot{P}_{(ij)} = -\frac{1}{\tau_S} \Pi_{(ij)} + O(2), \quad \dot{Q}_{lii} = -\frac{2}{\tau_q} q_i + O(2). \]

Using the source terms and Lagrange multipliers up to first order in non-equilibrium variables, the entropy production rate becomes:

\[ \Sigma = \frac{1}{T} \Pi^2 + \frac{1}{2\rho T \tau_S} \Pi_{(ij)} \Pi_{(ij)} - \frac{2\rho z_3}{\tau_q} q_i q_i \geq 0 \]

whose definiteness is secured by the following inequalities:

\[ T T \tau_t > 0, \quad p T \tau_S > 0, \quad \frac{\tau_q}{z_3} < 0, \]

They eventually impose the constraints on the relaxation times:

\[ \tau_t > 0, \quad \tau_S > 0, \quad \tau_q > 0. \]

Finally, the unknown non-convective fluxes have the following form:

\[ \dot{F}_{ijk} = \frac{3}{2} f_2 q_i (\delta_j k) + O(2) \Leftrightarrow \]

\[ \Leftrightarrow \dot{F}_{ijk} = \frac{5}{2} f_2 q_k + O(2), \quad \dot{F}_{(ij)k} = f_2 q_i (\delta_j k) + O(2) \]

\[ \dot{G}_{lii} = g_1 \delta_{ij} - g_2 \Pi \delta_{ij} + g_3 \Pi_{(ij)} + O(2), \]

One important feature of RET approach to 14 moments equations must be emphasized: all the functions \( k_t, \beta_m, f_n \) and \( g_r \) are expressed in terms of the state variables, i.e. they are determined once the thermal and caloric equations of state are fixed (see pp. 120–123 in [23]). Only the relaxation times remain undetermined. However, their values may be estimated using more refined theories like kinetic theory of gases (see [42]) or experimental data [48], since they are related to transport coefficients, i.e. viscosities and heat conductivity (see Eq. (5.62) in [23]).
4.4. **14 moments equations (ET14).** Once the constitutive relations are determined, and the closure problem is resolved in accordance with the principles of ET, the complete set of governing (field) equations can be written. Although the field equations are given in conservative form, for the purpose of comparison with generalized NSF equations we shall give them in the sequel in material form. The \( F \)-hierarchy consists of the conservation laws of mass and momentum, and the balance laws (evolution equations) for the dynamic pressure \( \Pi \) and the deviatoric part of the pressure tensor \( \Pi_{(ij)} \) are:

\[
\dot{\rho} + \rho \partial_k v_k = 0,
\]

\[
\rho \dot{v}_i + \partial_j \left[ (p + \Pi) \delta_{ij} + \Pi_{(ij)} \right] = 0, 
\]

\[
\Pi + \left[ \Gamma + \left( \frac{5}{3} - \frac{1}{\rho c_v} \left( \frac{\partial p}{\partial T} \right)_\rho \right) \Pi \right] \partial_k v_k + \left( \frac{2}{3} - \frac{1}{\rho c_v} \left( \frac{\partial p}{\partial T} \right)_\rho \right) \Pi_{(jk)} \partial_k v_j 
+ \frac{5}{6} g_k \Pi_{(ij)} f_2 + \left( \frac{5}{6} f_2 - \frac{1}{\rho c_v} \left( \frac{\partial p}{\partial T} \right)_\rho \right) \partial_k q_k = - \frac{1}{\tau_i} \Pi, 
\]

\[
\Pi_{(ij)} + \Pi_{(ij)} \partial_k v_k + 2 \Pi_{(k(j)} \partial_k v_{j)} + 2(p + \Pi) \partial_j v_i 
+ q_i \partial_j f_2 + f_2 \partial_j q_i = - \frac{1}{\tau_S} \Pi_{(ij)}. 
\]

The \( G \)-hierarchy consists of the conservation law of energy, and the balance law (evolution equation) for the heat flux \( q_i \):

\[
\rho \dot{e} + \left[ (p + \Pi) \delta_{ij} + \Pi_{(ij)} \right] \partial_i v_j + \partial_i q_i = 0, 
\]

\[
\dot{q}_i + \left( 1 + \frac{f_2}{2} \right) q_i \partial_k v_k + \left( 1 + \frac{f_2}{2} \right) q_k \partial_k v_i 
+ \frac{f_2}{2} q_k \partial_k v_k 
- \left\{ \left[ \frac{1}{\rho} \left( \frac{\partial p}{\partial \rho} \right)_T - \frac{1}{2} \left( \frac{\partial g_2}{\partial \rho} \right)_T \right] \Pi \delta_{ik} + \left[ \frac{1}{\rho} \left( \frac{\partial p}{\partial \rho} \right)_T - \frac{1}{2} \left( \frac{\partial g_2}{\partial \rho} \right)_T \right] \Pi_{(ik)} \right\} \partial_k \rho 
- \frac{1}{2 T^2 \rho c_2} + \left[ \frac{1}{\rho} \left( \frac{\partial p}{\partial T} \right)_\rho - \frac{1}{2} \left( \frac{\partial g_2}{\partial T} \right)_\rho \right] \Pi \delta_{ik} 
+ \left[ \frac{1}{\rho} \left( \frac{\partial p}{\partial T} \right)_\rho - \frac{1}{2} \left( \frac{\partial g_2}{\partial T} \right)_\rho \right] \Pi_{(ik)} \right\} \partial_k T 
- \left\{ \left( e - \frac{p}{\rho} \right) \frac{1}{2} g_2 + \frac{\Pi}{\rho} \right\} \delta_{ik} + \frac{1}{\rho} \Pi_{(ik)} \right\} \partial_k \Pi 
- \left\{ \left( e - \frac{p}{\rho} \right) \frac{1}{2} g_3 - \frac{\Pi}{\rho} \right\} \delta_{ij} + \frac{1}{\rho} \Pi_{(ij)} \right\} \partial_k \Pi_{(jk)} = - \frac{1}{\tau_q} q_i. 
\]

Our aim is to compare ET14 field equations with generalized NSF equations obtained in Section \( \text{[3]} \). However, their structure is substantially different. The differential part of ET14 equations is quasi-linear, whereas the constitutive equations of NET-IV model have linear differential part with constant coefficients. To facilitate the comparison, we shall linearize the balance laws of ET14 model in the neighborhood of stationary equilibrium state \( \mathbf{u}^{(0)} = (\rho^{(0)}, v_i^{(0)}, T^{(0)}, 0, 0, 0, 0) = \text{const} \). Field variables will be regarded as perturbations of the equilibrium state,
\[
\mathbf{u} = (\rho^{(0)} + \rho, v_i^{(0)} + v_i, T^{(0)} + T, \Pi, \Pi_{(ij)}, q_i).
\]
Linearized balance laws then read:

\[
\begin{align*}
\dot{q}_i - \frac{1}{2(T^{(0)})^2} \rho^{(0)} z_3^{(0)} \partial_k T - \left( e - \frac{p}{\rho} - \frac{1}{2} g_3 \right)^{(0)} \partial_i \Pi \\
- \left( e - \frac{p}{\rho} - \frac{1}{2} g_3 \right)^{(0)} \partial_k \Pi_{(ik)} = -\frac{1}{\tau_q} q_i,
\end{align*}
\]

\[
\Pi_{(ij)} + 2 \rho^{(0)} \partial_j v_i + \eta^{(0)} \partial_j q_i = -\frac{1}{\tau_S} \Pi_{(ij)},
\]

\[
\Pi + \Gamma^{(0)} \partial_k v_k + \left( \frac{5}{6} f_2 - \frac{1}{\rho c v} \left( \frac{\partial p}{\partial T} \right)^{(0)} \right) \partial_i q_i = -\frac{1}{\tau_\Pi} \Pi.
\]

We did not linearize the conservation laws since they are completely equivalent. Note that we ordered linearized balance laws (54) in the same way as in (50) for the sake of easier comparison.

5. COMPARISON AND SUMMARY

In this Section we shall compare the equations, the procedure of their derivation and the underlying assumptions of two approaches in the modeling of rarefied gases. First, the governing equations will be compared at formal level. After that, two approaches will be compared for the concepts and procedures used in the study of non-equilibrium rarefied gases.

5.1. Comparison of the governing equations. Governing equations of NET-IV model consist of conservation laws of mass, momentum and energy (13) and constitutive relations (30). The latter have the form of balance laws describing the time rate of change of heat flux \(q_i\), pressure deviator \(\Pi_{(ij)}\), and dynamic pressure \(\Pi_{ii}\). On the other hand, ET14 model is structured in two hierarchies. \(F\)-hierarchy (52) consists of the conservation laws mass and momentum, and the balance laws for dynamic pressure \(\Pi = (1/3) \Pi_{ii}\) and stress deviator \(\Pi_{(ij)}\). \(G\)-hierarchy (53) consists of the conservation law of energy and the balance law for heat flux \(q_i\).

Conservation laws in both models are completely equivalent. The difference appears in the structure of balance laws. NET-IV balance laws (29) are linear by construction, while balance laws in ET14 model are quasi-linear, with state dependent coefficients. Balance laws have different structure for other reasons as well:

(a) balance law (29) contains second order parabolic terms on the right hand side which are not present in (53);
(b) balance law (53) is coupled with velocity gradient field through \(\partial_k v_k\) and \(\partial_k v_i\), and with density gradient field \(\partial_k \rho\); none of them is present in (29);
(c) balance law (52) has rather complex coupling with other fields; e.g. it is explicitly coupled with divergence of velocity \(\partial_k v_k\), whereas coupling with gradients of \(\rho\) and \(T\) comes due to \(\partial_j f_2\); none of these terms is present in (29);
(d) finally, balance law (52) is coupled with deviatoric part of velocity gradient \(\partial_k v_j\), as well as gradients of \(\rho\) and \(T\) due to \(\partial_j f_2\), while they do not appear in (29).
We would like to find, if possible, the common ground for NET-IV and ET14 models. To that end the following simplifications are needed:

1. balance laws (29) of NET-IV model have to be reduced to hyperbolic form; therefore, it has to be assumed $\gamma_1 = \gamma_2 = 0$ which reduces the system to (30);
2. balance laws of ET14 model have to be linearized; linearization in the neighborhood of constant equilibrium state leads the balance laws in the form (54).

Simple comparison of the reduced systems of balance laws leads to the following identification of the coefficients:

$$
\begin{align*}
\tau_1 &= \tau_q, \quad \tau_2 = \tau_S, \quad \tau_3 = \tau_\Pi, \\
\lambda &= -\frac{\tau_q}{2(T^{(0)})^2 \rho^{(0)} z_3^{(0)}}, \quad \nu = 2\rho^{(0)} \tau_S, \quad \eta = 3\Gamma^{(0)} \tau_\Pi, \\
\alpha_{12} &= 3 \left( \frac{5}{6} f_2 - \frac{1}{\rho c_v} \left( \frac{\partial p}{\partial T} \right) \right)^{(0)} \tau_\Pi, \quad \alpha_{21} = -\frac{\tau_q}{3} \left( e - p \rho - \frac{1}{2} g_2 \right)^{(0)}, \\
\beta_{12} &= f_2^{(0)} \tau_S, \quad \beta_{21} = \tau_q \left( e - \frac{p}{\rho} - \frac{1}{2} g_3 \right)^{(0)}.
\end{align*}
$$

Note that this comparison leads to equivalent results for transport coefficients as thermodynamic limit analysis in RET [40, 23].

Comparative analysis given above revealed common points of the models, as well as their differences. However, this kind of analysis could be extended in the way which put Meixner theory into common perspective with NET-IV and ET14 models. It was already shown in Section 2 that IV-Meixner model (13) can be reduced to form (17) compatible with (18) by neglecting pressure deviator ($\mu = 0$) and heat flux ($\lambda = 0$). On the other hand, it is common procedure in RET [52, 23] to study classical thermodynamic limit using so-called Maxwellian iteration—an asymptotic procedure which is akin to expansion in powers of relaxation time. It leads to the recovery of classical constitutive relations for pressure tensor and heat flux. However, in the case of polyatomic gases the situation is more delicate because of the fact that relaxation time for dynamic pressure is several orders of magnitude greater than relaxation times for pressure deviator and heat flux (see [48]). Therefore, it seems reasonable to partially apply Maxwellian iteration to the ET14 system (52)-(53), i.e. to apply it to linearized balance laws (54) for heat flux and (54) for pressure deviator and reduce them to constitutive relations (13) for pressure and heat flux (see [48]). Assuming $l_{22} = 0$, almost complete compatibility is reached with with (13)—there only one extra term in (54), $\partial_t q_i$, which does not appear in (13).

5.2. Comparison of concepts and procedures. Aim of this Section is to analyze the concepts which stand behind the NET-IV and RET. Since concepts are closely related to the procedures applied for derivation of equations, they will be compared as well.

The formalism of NET-IV is based upon the following premises:

(IV-a) The governing equations are standard conservation laws of mass, momentum and energy, with undetermined non-convective fluxes.
(IV-b) Non-equilibrium effects are included through internal variables, as constitutive elements of the non-equilibrium entropy density, and current multipliers, which are the non-equilibrium counterparts of the entropy flux.

(IV-c) Entropy balance law provides the entropy production rate in bilinear form—as the sum of products of thermodynamic forces and fluxes. Definiteness of the entropy production is achieved through linear relations between forces and fluxes.

(IV-d) Elimination of internal variables and current multipliers yield constitutive relations for physical variables, e.g. non-convective fluxes. These relations may have the form of balance laws.

On the other hand, formalism of RET provides different setting:

(ET-a) The governing equations consist of two finite hierarchies of balance laws, with an increasing tensorial order. They have a nested structure—fluxes in the equation of order \( n \) become densities in the equation of order \( n + 1 \).

(ET-b) The state variables are the densities. Unknown fluxes and source terms are local functions of state variables.

(ET-c) The closure problem is resolved through the compatibility of balance laws and the entropy inequality using the method of multipliers.

(ET-d) Compatibility conditions lead to the (approximate) form of non-equilibrium entropy density and entropy flux, and (approximate) closure for the unknown fluxes and source terms, which yield the definiteness of the entropy production rate.

It is clear from the procedures described above that there are two common pillars on which both approaches stand—standard conservation laws and the entropy balance law. The differences emerge in strategy chosen to capture the non-equilibrium phenomena. NET-IV starts with the non-equilibrium entropy density and the entropy flux, which inherit internal variables and current multipliers, and get the constitutive relations—balance laws—from the entropy production rate. Instead, RET proceeds in a bit opposite direction: it starts with an extended list of state variables governed by the appropriate balance laws. By means of compatibility with entropy balance law, one determines the structure of entropy density and entropy flux, as well as the non-convective fluxes, while residual inequality serves for determination of the source terms in balance laws. It is, however, interesting that both approaches in the end provide equivalent entropy densities and entropy fluxes—compare Eqs. (13) and (15) for Meixner theory, and Eqs. (20), (21) and (45) for generalized NSF/14 moments equations.

We also compare the conceptual differences in a different way.

1. **Universality.** NET-IV is based on general assumptions. Beyond the second law there was no assumption regarding the structure of the material. The internal variables and current multipliers are convenient representations of the deviation from local equilibrium. For example, instead of the multiplier structure one can use the additive extension of the entropy flux with \( k \) vector, but in that form the simple linear solution of the entropy inequality is less apparent \([20, 22, 10]\). On the other hand the assumed hierarchical structure of the RET governing equations, and their compatibility with kinetic theory, introduces formal restrictions on the structure of balance laws for extended set of state variables.
(2) **Balance structure.** In case of RET it is inherited from kinetic theory and due to the balance form of the Boltzmann equation. For NET-IV it is the consequence of the second law.

(3) **Locality.** The locality of RET is required from the outset and leads to the quasi-linear hyperbolic structure of equations. They are compatible with the moment equations of kinetic theory as well [41, 42, 47]. Then the usual gradient terms in the constitutive equations emerge by elimination of the higher moments [54]. In our case the missing Fourier term in eqs. [53] is remarkable.

(4) **Spacetime embedding.** In RET it is based on the particular transformation rules of the balances under Galilean transformations (scalars are invariant, etc.). With this starting point the transformation rules of the particular physical quantities can be derived [55, 6]. It is remarkable, that Galilean relativity of fluids, that is a reference frame independent covariant treatment, leads to the same transformation rules in the special Galilean or Euclidean transformations. In that treatment the balances are natural four-divergences [56]. Then the doubled hierarchy is not necessary but generalisation of the entropy four-vector with internal variables and the role of current multipliers is not clear.

(5) **Second law.** The assumption of quadratic entropy density is common in both theories. RET assumes a more particular entropy flux, as it is required by the Lagrange multipliers.

(6) **Nonlinearity.** The apparent nonlinearity of the RET equations is mostly due to state dependent transport coefficients. The assumed particular nonlinear thermodynamic coefficients can be calculated.

(7) **Further extension.** It is possible in both theories. However, with further extensions the differences are seemingly increasing. See e.g. the treatment of NET-IV with the Nyíri multiplier related to the tensor internal variable. A complete treatment requires higher order isotropic representations and the number of coefficients is increasing. It is given in [57].

(8) **Experiments.** In case of ballistic heat conduction, with a single hierarchical structure, NET-IV seems to reproduce the data better [8, 9]. However, then the 14 momentum equations are not applied yet, because phonons can be hardly polyatomic.

The last point in the comparison of conceptual differences provides also the strong motivation for further simultaneous analysis of the NET-IV and and RET approach to polyatomic gases. Namely, there are numerous studies of experimental character in the literature, showing the non-classical behaviour of rarefied gases. Sluijter et al. [29, 30] measured the sound absorption at low temperatures (77K and 90K) and at room temperature also, with different types of molecules. Similar measurements are made by Rhodes [31], Greenspan [32] and Sette et al. [33]. From the kinetic theory point of view, these experimental results were investigated in detail by Arima et al. [35, 36, 37, 39]. The next step is to compare the modelling capabilities of different theories to each other based upon the measurement data.

Another line of research will be related to a paradigmatic problem in non-equilibrium processes—the shock structure problem. It was studied in the framework of RET for 14 moments equations [48], for ET6 model [38, 39] and from the point of view of kinetic theory of gases [44]. There remains an open problem of
the application of NET-IV approach in this context, which will certainly bring new insights.

As a summary we want to emphasize that the two theoretical approaches must be concordant. Second law based approximations are promising and kinetic theory should provide a mechanism to obtain universal evolution equations. In this study we have shown that the compatibility is valid, but there are still several points of deviations where the relation of the two approaches are not really clear. This comparative analysis can be helpful in future improvements.

6. Acknowledgments

The work was supported (R. Kovács and P. Ván) by the grants of National Research, Development and Innovation Office – NKFIH 116197(116375), NKFIH 124366(124508), NKFIH 123815 and NKFIH 130378, and (D. Madjarević and S. Simić) by the Ministry of Education, Science and Technological Development, Republic of Serbia, within the project “Mechanics of nonlinear and dissipative systems—contemporary models, analysis and applications”, Project No. ON174016.

REFERENCES

[1] V. Peshkov. Second sound in Helium II. J. Phys. (Moscow), 381(8), 1944.
[2] K. Frischmuth and V. A. Cimmelli. Numerical reconstruction of heat pulse experiments. *International Journal of Engineering Science*, 33(2):209–215, 1995.
[3] K. Frischmuth and V. A. Cimmelli. Hyperbolic heat conduction with variable relaxation time. *Journal of Theoretical and Applied Mechanics*, 34(1):57–65, 1996.
[4] K. Frischmuth and V. A. Cimmelli. Coupling in thermo-mechanical wave propagation in NaF at low temperature. *Archives of Mechanics*, 50(4):703–713, 1998.
[5] R. Kovács and P. Ván. Models of Ballistic Propagation of Heat at Low Temperatures. *International Journal of Thermophysics*, 37(9):95, 2016.
[6] I. Müller and T. Ruggeri. Rational Extended Thermodynamics, volume 37 of Springer Tracts in Natural Philosophy. Springer Verlag, New York-etc., 2nd edition, 1998.
[7] W. Dreyer and H. Struchtrup. Heat pulse experiments revisited. *Continuum Mechanics and Thermodynamics*, 5:3–50, 1993.
[8] R. Kovács and P. Ván. Generalized heat conduction in heat pulse experiments. *International Journal of Heat and Mass Transfer*, 83:613 – 620, 2015.
[9] R. Kovács and P. Ván. Second sound and ballistic heat conduction: NaF experiments revisited. *International Journal of Heat and Mass Transfer*, 117:682–690, 2018. arXiv:1708.09770.
[10] A. Berezovsky and Ván P. *Internal Variables in Thermoelasticity*. Springer, 2017.
[11] T. Ruggeri, A. Murachini and L. Seccia. Continuum Approach to Phonon Gas and Shape Changes of Second Sound via Shock Waves Theory. *Il Nuovo cimento D*, 16(1):15–44, 1994.
[12] J. C. Maxwell. On the dynamical theory of gases. *Philosophical Transactions of the Royal Society of London*, 157:49–88, 1867.
[13] C. Cattaneo. Sur une forme de l’equation de la chaleur éliminant le paradoxe d’une propagation instantanée. *Comptes Rendus Hebdomadaires Des Sciences De L’Academie Des Sciences*, 247(4):431–433, 1958.
[14] P. Vernotte. Les paradoxes de la théorie continue de l’équation de la chaleur. *Comptes Rendus Hebdomadaires Des Sciences De L’Academie Des Sciences*, 246(22):3154–3155, 1958.
[15] D. D. Joseph and L. Preziosi. Heat waves. *Reviews of Modern Physics*, 61(1):41, 1989.
[16] D. D. Joseph and L. Preziosi. Addendum to the paper on heat waves. *Reviews of Modern Physics*, 62(2):375–391, 1990.
[17] T. Ruggeri, A. Murachini and L. Seccia. Shock Waves and Second Sound in a Rigid Heat Conductor: A Critical Temperature for NaF and Bi. *Physical Review Letters*, 64(22):2640–2643, 1990.
[18] P. Ván and T. Fülöp. Universality in heat conduction theory: weakly nonlocal thermodynamics. *Annalen der Physik*, 524(8):470–478, 2012. arXiv:1108.5689.
[19] I. Müller. *Thermodynamics*. Pitman, Toronto, 1985.
[20] J. Vérhás. On the entropy current. *Journal of Non-Equilibrium Thermodynamics*, 8:201–206, 1983.
[21] J. Jou, J. Casas-Vázquez, and G. Lebon. Extended irreversible thermodynamics. *Reports on Progress in Physics*, 51(8):1105, 1988.
[22] B. Nyíri. On the entropy current. *Journal of Non-Equilibrium Thermodynamics*, 16(2):179–186, 1991.
[23] T. Ruggeri, M. Sugiyama, *Rational Extended Thermodynamics beyond the Monatomic Gas* (Springer, Heidelberg, 2015).
[24] J. Meixner. Absorption und Dispersion des Schalles in Gasen mit Chemisch Reagierenden und Anregbaren Komponenten. I. Teil. *Annalen der Physik*, 435(6-7):470–487, 1943.
[25] S. R. de Groot and P. Mazur. *Non-Equilibrium Thermodynamics*. Dover Publications, 1963.
[26] Lars Onsager. Reciprocal relations in irreversible processes. I. *Physical Review*, 37(4):405, 1931.
[27] Lars Onsager. Reciprocal relations in irreversible processes. II. *Physical Review*, 38(12):2265, 1931.
[28] J. Vérhás. *Thermodynamics and Rheology*. Akadémiai Kiadó-Kluwer Academic Publisher, 1997.
[29] C. G. Sluijter, H. F. P. Knaap, and J. J. M. Beenakker. Determination of rotational relaxation times of hydrogen isotopes by sound absorption measurements at low temperatures. I. *Physica*, 30(4):745–762, 1964.
[30] C. G. Sluijter, H. F. P. Knaap, and J. J. M. Beenakker. Determination of rotational relaxation times of hydrogen isotopes by sound absorption measurements at low temperatures II. *Physica*, 31(6):915–940, 1965.
[31] J. E. Rhodes Jr. The velocity of sound in hydrogen when rotational degrees of freedom fail to be excited. *Physical Review*, 70(11-12):932, 1946.
[32] M. Greenspan. Propagation of sound in five monatomic gases. *The Journal of the Acoustical Society of America*, 28(4):644–648, 1956.
[33] D. Sette, A. Busala, and J. C. Hubbard. Energy transfer by collisions in vapors of chlorinated methanes. *The Journal of Chemical Physics*, 23(5):787–793, 1955.
[34] H. Grad. On the kinetic theory of rarefied gases. *Comm. Pure Appl. Math.*, 2:331–407, 1949.
[35] T. Arima, S. Taniguchi, T. Ruggeri, and M. Sugiyama. Extended thermodynamics of dense gases. *Continuum Mechanics and Thermodynamics*, 24(4-6):271–292, 2012.
[36] T. Arima, S. Taniguchi, T. Ruggeri, and M. Sugiyama. Extended thermodynamics of real gases with dynamic pressure: An extension of Meixner’s theory. *Physics Letters A*, 376(44):2799–2803, 2012.
[37] T. Arima, S. Taniguchi, T. Ruggeri, and M. Sugiyama. Dispersion relation for sound in rarefied polyatomic gases based on extended thermodynamics. *Continuum Mechanics and Thermodynamics*, 25(6):727–737, 2013.
[38] S. Taniguchi, T. Arima, T. Ruggeri, and M. Sugiyama. Effect of the dynamic pressure on the shock wave structure in a rarefied polyatomic gas. *Physics of Fluids*, 26:016103, 2014.
[39] T. Arima, T. Ruggeri, M. Sugiyama, and S. Taniguchi. Non-linear extended thermodynamics of real gases with 6 fields. *International Journal of Non-Linear Mechanics*, 72:6–15, 2015.
[40] T. Arima, S. Taniguchi, M. Sugiyama, T. Ruggeri, Extended thermodynamics of dense gases. *Contin. Mech. Thermodyn.* 24, 271 (2011).
[41] M. Pavić, T. Ruggeri, and S. Simić. Maximum entropy principle for rarefied polyatomic gases. *Physica A*, 392:1302–1317, 2013.
[42] M. Pavić-Čolić, S. Simić, Moment Equations for Polyatomic Gases. *Acta Applicandae Mathematicae* 132 (1), 469 (2014)
[43] M. Pavić-Čolić, D. Madjarević, S. Simić, Polyatomic gases with dynamic pressure: Kinetic non-linear closure and the shock structure. *International Journal of Non-Linear Mechanics* 92:160–175 (2017).
[44] S. Kosuge, K. Aoki, Shock-wave structure for a polyatomic gas with large bulk viscosity. *Physical Review Fluids* 3:023401 (2018).
[45] C. Borgnakke and P.S. Larsen. Statistical Collision Model for Monte Carlo Simulation of Polyatomic Gas Mixture. *J. Comput. Phys.* 18:405—420, 1975.
[46] J.-F. Bourgat, L. Desvilletes, P. Le Tallec, B. Perthame. Microreversible collisions for polyatomic gases. *Eur. J. Mech. B Fluids* 13(2):237—254, 1994.
[47] T. Arima, A. Mentrelli and T. Ruggeri. Molecular extended thermodynamics of rarefied polyatomic gases and wave velocities for increasing number of moments. *Annals of Physics* 345:111–140, 2014.

[48] S. Taniguchi, T. Arima, T. Ruggeri, M. Sugiyama, Thermodynamic theory of the shock wave structure in a rarefied polyatomic gas: Beyond the Bethe-Teller theory. *Physical Review E* 89, 013025 (2014)

[49] I.-S. Liu, Method of Lagrange multipliers for exploitation of the entropy principle. *Arch. Ration. Mech. Anal.* 46, 131 (1972)

[50] G. Boillat, T. Ruggeri, Hyperbolic principal subsystems: entropy convexity and subcharacteristic conditions. *Arch. Ration. Mech. Anal.* 137, 305 (1997)

[51] T. Ruggeri, A. Strumia, Main field and convex covariant density for quasi-linear hyperbolic systems. Relativistic fluid dynamics. *Ann. Inst. H. Poincaré, Sect. A* 34, 65 (1981).

[52] I. Müller, T. Ruggeri, *Extended Thermodynamics*, Springer Tracts in Natural Philosphy, vol. 37, 1st Ed. (Springer, New York, 1993)

[53] C. Truesdell, *Rational Thermodynamics* (McGraw-Hill, New York, 1969)

[54] T. Ruggeri. Can constitutive equations be represented by non-local equations? *Quarterly of Applied Mathematics*, LXX(3):597–611, 2012.

[55] T. Ruggeri. Galilean invariance and entropy principle for systems of balance laws. *Continuum Mechanics and Thermodynamics*, 1(1):3–20, 1989.

[56] P. Ván. Galilean relativistic fluid mechanics. *Continuum Mechanics and Thermodynamics*, 29(2):585–610, 2017. [arXiv:1508.00121]v1- Hungarian; v2- English.

[57] A. Fama, L. Restuccia, and P. Ván. Internal variables for ballistic heat conduction in isotropic materials. 2018. under preparation.

1Department of Energy Engineering, Faculty of Mechanical Engineering, BME, Budapest, Hungary and 2Department of Theoretical Physics, Institute for Particle and Nuclear Physics, MTA Wigner Research Centre for Physics, Budapest, Hungary and 3Montavd Thermodynamic Research Group and 4University of Novi Sad, Novi Sad, Serbia.