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On the thermomechanics of continuous media with diffusion and/or weak nonlocality

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Abstract Working in parallel on the energy equation in a special form and the associated canonical equation of momentum, we focus attention on the case of deformable media which are basically finitely elastic, but which also admit the existence of thermodynamically irreversible phenomena by means of a diffusive internal variable of state, or alternately an additional degree of freedom, in any case presenting some weak nonlocality (gradient effects). Two descriptions follow thereof, one that can be called standard according to rational thermomechanics (there exists a generalized internal force or thermodynamically conjugated force for a variable and its gradient separately, and the entropy flux has its classical definition) or the so-called field-theoretic viewpoint in which only one generalized force (based on a variational derivative of the energy) is used. In the latter one, the entropy flux deviates from its classical definition but, simultaneously, by virtue of the space–time consistency, the Eshelby stress tensor has to be altered. Simple examples with diffusion of an internal variable illustrate these formulations that may be valuable in the description of some bio- and geomaterials.

Keywords Thermodynamics · Continua · Diffusion · Canonical equations · Eshelby tensor

1 Introduction

The formulation of a rational theory of continuous media with diffusive effects still presents a challenge in modern continuum thermomechanics. One reason for this is the recurring question of whether the field associated with the diffusive process of interest is an observable or an internal variable of state, whether it constitutes a true additional internal degree of freedom or merely a parameter compared to the main governing ingredients of the thermomechanical description, i.e., the deformation and the temperature fields. These questions have been posed for a long time, including in such classical works as the monograph of de Groot and Mazur [4] or in more rational approaches to fluid mixtures such as in Bowen [1, 2]. Furthermore, recent developments in the continuum mechanics of complex or microstructured media have led to considering gradients of certain variables, a consideration akin to introducing diffusive effects related to these variables as a sort of weak nonlocality concerning these variables (weak and strong nonlocalities were first distinguished in Maugin [24]). Among cases of particular interest along this line of development we note the case of *liquid crystals* [16, 17, 26], [27, pp.160–162] *damage* [9, 10, 18], *second-grade elastic materials* [7], *viscoplasticity* [8]. One specific point raised in some of these works is whether the entropy flux follows the standard imposed by the Coleman–Noll rational thermodynamics of the 1960s and 1970s [35] or its definition may be altered by the present diffusive effect (as shown in Maugin [26]). This alternative, together with the initial question raised, are critically

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examined in the present paper. A recent work by Ireman and Quoc-Son [15] addresses the same problem on the basis of Maugin [26].

It may also be reminded that a natural ingredient in diffusive theories in fluids is a tensor of *chemical potentials* [2, 14, 36] that was easily related to the Eshelby stress tensor (called the energy–momentum tensor in Eshelby’s original works; cf. the synthesis works of Maugin [27, 28]). As a matter of fact, the present work exploits this fruitful concept and clearly shows that alteration in the definition of the entropy flux goes along with a parallel alteration in the structure of the Eshelby stress tensor. The essential reason for this is the recognition of the complementary roles played by the balance of entropy and the balance of so-called canonical momentum in so far as thermomechanics is concerned. This was already emphasized in Maugin [33, 34]. The considerations in this paper, although presented in a somewhat abstract frame, are meant to apply to cases of interest in *geomaterials* (especially for weakly nonlocal damage and plasticity) and *biomaterials* (especially in the theory of growth as formulated – with diffusional effects – in Epstein and Maugin [6]).

Section 2 presents the theory of continua with a diffusive internal variable of state. Associated canonical balance laws of energy and momentum are derived in Sect. 3. The other view considering the additional variable as an additional degree of freedom is expanded in Sect. 4. Section 5 presents a comparison between the two approaches and reduction of the second approach to the first under appropriate conditions. Simple examples are briefly dealt with in Sect. 6, while Sect. 7 contains the conclusions.

2 Theory with diffusive internal variables of state

First we shall recall the basic equations of the finite-strain thermoelasticity of continua that, apart from heat conduction, may present dissipative effects through an internal variable of state, formally denoted by α . In agreement with Kestin’s definition (adopted in Maugin [32]) of internal variables of state, these cannot be controlled directly by any means either in the bulk or at the surface of the body so that they do not appear a priori in the balance of linear momentum, moment of linear momentum, energy and entropy; in particular, they produce no external work. As a consequence, all these basic laws should take on their classical form of the finite-strain thermoelasticity of conductors as they can be found in books on the subject matter, while the power expended by internal variables will be only of the *dissipated* type. The evolution of the internal variable is then possibly controlled by the local value of the classical fields of stresses and heat current. That is, at any regular material point \mathbf{X} in the body of volume V_0 in its reference configuration the following hold in the so-called Piola–Kirchhoff framework:

- *Balance of linear (physical) momentum* (no body force present for the sake of simplicity):

$$\left. \frac{\partial(\rho_0 \mathbf{v})}{\partial t} \right|_X - \operatorname{div}_R \mathbf{T} = \mathbf{0}; \quad (2.1)$$

- *Balance of energy* (first law of thermodynamics; no bulk energy supply for the sake of simplicity):

$$\left. \frac{\partial(K + E)}{\partial t} \right|_X - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v} - \mathbf{Q}) = 0; \quad (2.2)$$

- *Second law of thermodynamics* (no bulk entropy supply for the sake of simplicity):

$$\left. \frac{\partial S}{\partial t} \right|_X + \nabla_R \cdot \mathbf{S} \geq 0; \quad (2.3)$$

Here, if $\mathbf{x} = \bar{\mathbf{x}}(\mathbf{X}, t)$ is the sufficiently smooth (direct) deformation motion from a reference configuration K_R to the current configuration K_t , \mathbf{v} and \mathbf{F} are the physical velocity field and direct-motion gradient defined by

$$\mathbf{v} := \left. \frac{\partial \bar{\mathbf{x}}}{\partial t} \right|_X, \quad \mathbf{F} := \left. \frac{\partial \bar{\mathbf{x}}}{\partial \mathbf{X}} \right|_t \equiv \nabla_R \bar{\mathbf{x}}, \quad (2.4)$$

\mathbf{T} is the first Piola–Kirchhoff stress, and \mathbf{Q} is the material heat vector. E and S are the densities of internal energy and entropy per unit reference volume in K_R . Here we must distinguish between two possibilities:

A. Classical entropy flux–heat flux relationship

The entropy flux is a priori classically related to the heat flux by

$$\mathbf{S} = \theta^{-1} \mathbf{Q}, \tag{2.5}$$

where θ is the non-negative (nonvanishing, $\inf \theta = 0$) thermodynamical temperature. Accordingly, the free (Helmholtz) energy density is related (by definition) to E and S by the relationship

$$W = E - S \theta. \tag{2.6}$$

Here Eqs. (2.1) and (2.2) are strict conservation laws in the language of hyperbolic systems. We have not recalled the continuity equation (conservation of mass) which in fact has an integrated form as

$$\rho_0 = \rho J, \quad J := \det \mathbf{F}, \tag{2.7}$$

which equivalently yields a remarkably simple strictly conservative form

$$\left. \frac{\partial \rho_0}{\partial t} \right|_X = 0. \tag{2.8}$$

This means that here mass density ρ_0 in K_R is at most a function of the material point (the material coordinates) \mathbf{X} . In the rest of this work we assume that the body is *materially homogeneous* so that neither ρ_0 nor the energy density will depend explicitly on \mathbf{X} .

The undefined internal variable of state α appears only as an additional independent variable in the free energy (W) functional dependence. As a matter of fact, having in view a theory with a *diffusive* internal variable, both α and its material gradient $\nabla_R \alpha$, which do not contribute to the external working but will contribute to the dissipated power, will be present in W . Therefore, the latter has the following functional dependence for a homogeneous material (no explicit dependence on the material point \mathbf{X}):

$$W = \overline{W}(\mathbf{F}, \alpha, \nabla_R \alpha, \theta). \tag{2.9}$$

For thermoelasticity we have the following laws of state (given by Gibbs' equation):

$$\begin{aligned} \mathbf{T} &= \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \\ A &:= -\frac{\partial \overline{W}}{\partial \alpha}, \quad \mathbf{B} := -\frac{\partial \overline{W}}{\partial (\nabla_R \alpha)}, \end{aligned} \tag{2.10}$$

where the last two equations are mere definitions. On account of this and of Eqs. (2.5), (2.3) yields the following dissipation inequality:

$$\Phi = A \dot{\alpha} + \mathbf{B} \cdot \nabla_R \dot{\alpha} - \mathbf{S} \cdot \nabla_R \dot{\theta} \geq 0. \tag{2.11}$$

B. Nonclassical entropy flux–heat flux relationship

Had we considered from the beginning that $\mathbf{S} = \tilde{\mathbf{S}} \neq \mathbf{Q}/\theta$ or $\tilde{\mathbf{S}} = \theta^{-1} \mathbf{Q} + \mathbf{K}$, while (2.9) is kept, the dissipation inequality (2.11) would be replaced by

$$\tilde{\Phi} = \tilde{A} \dot{\alpha} - \tilde{\mathbf{S}} \cdot \nabla_R \dot{\theta} \geq 0, \tag{2.12}$$

on the condition that we define the generalized conjugate force \tilde{A} and the new entropy flux $\tilde{\mathbf{S}}$ by

$$\tilde{A} \equiv -\frac{\delta \overline{W}}{\delta \alpha} = -\left(\frac{\partial \overline{W}}{\partial \alpha} - \nabla_R \cdot \frac{\partial \overline{W}}{\partial (\nabla_R \alpha)} \right) = A - \nabla_R \cdot \mathbf{B}, \quad \tilde{\mathbf{S}} := \theta^{-1} (\mathbf{Q} - \mathbf{B} \dot{\alpha}), \tag{2.13}$$

i.e., $\mathbf{K} = -\theta^{-1} \mathbf{B} \dot{\alpha}$ – see similar developments in Eq. (4.16) and paragraph 4.3.1 here below. That is, although we could have considered that the extra entropy flux \mathbf{K} in all generality requires a constitutive equation in terms perhaps of α , $\nabla_R \alpha$, and $\dot{\alpha}$, we simply admit an expression of \mathbf{K} that is sufficient for the satisfaction of the dissipation inequality.

By the same token, we show that the energy equation yields the entropy equation [obviously not a strict conservation law according to Eq. (2.3)]:

$$\theta \left. \frac{\partial S}{\partial t} \right|_X + \nabla_R \cdot \mathbf{Q} = A\dot{\alpha} + \mathbf{B} \cdot \nabla_R \dot{\alpha}, \quad (2.14)$$

or, equivalently, with the formulation (2.12)

$$\theta \left. \frac{\partial S}{\partial t} \right|_X + \nabla_R \cdot (\theta \tilde{\mathbf{S}}) = \tilde{A}\dot{\alpha}. \quad (2.15)$$

Remark Each of the formulations (2.11) and (2.12) epitomize a different conceptual vision of continuum thermodynamics. The first of these may be called the *Coleman–Noll* – nowadays standard in continuum mechanics circles – *thermomechanical view*, where (2.5) is assumed as a basic premise, and α and $\nabla_R \alpha$ may essentially be considered to vary in time independently of one another so that the conjugate thermodynamical forces A and \mathbf{B} can also be determined independently of one another, although being both derived from the energy density W via Eqs. (2.10)_{3–4}. The second line of thought may be called the *field-theoretic view* as it would certainly be the one more akin to analytical mechanics and field theory on the one hand, and to more classical irreversible thermodynamics on the other. The analytical mechanics character here relates to the appearance of a functional derivative (Euler–Lagrange derivative) in the definition of the effective conjugate force \tilde{A} by Eq. (2.13)₁. The second point relates to that fact that the entropy flux takes on a more general form than (2.5), including an additional entropy flux [cf. Eq. (2.13)₂] that is not a priori set forth. Such a generalized entropy flux appears in the classical irreversible thermodynamics of fluid mixtures [4]. We advocated a similar approach in Maugin [26], and this was implemented in Maugin ([29,30]; the last reference unfortunately practically inaccessible). Although we consider that the present formulation embodied in Eqs. (2.12), (2.13) and (2.15) is the one that least deviates from the standards set forth by Kestin’s definition of internal variables of state, there still remains the ultimate fact that in the evolution equation (see an example in Sect. 6) governing α there will arise the need to specify a boundary value problem. Then we may question the interpretation of α as a true internal variable of state.

3 Canonical balance laws

Canonical balance laws are those that are expressed in a framework that does not depend on the observer and they do relate to the entire physical system under consideration and not only to one particular degree of freedom. The energy equation, because of the inclusive multiform notion of energy itself, is such an equation. It may be written in more or less self-explanatory or cognitive manners (see below). The *canonical balance of momentum* is another one that is not often exploited in continuum mechanics. In the field theory of *thermodynamically reversible processes* both canonical energy and momentum balance are obtained via a straightforward application of Noether’s invariance theorem related to the variation of the time–space parametrization of fields (see, in particular, Maugin [27]), here Newtonian time and material coordinates. While the canonical expression of the energy equation compatible in form with the canonical momentum equation is easily obtained through mere manipulations, in the absence of Hamiltonian variational formulation due to the presence of dissipative effects, the canonical balance of momentum can only be obtained here by a canonical projection of the physical momentum balance (2.1) onto the material manifold, i.e., by multiplying (2.1) to the right by \mathbf{F} and seeing what happens. This direct and simple method is applicable here because the classical motion $\bar{\mathbf{x}}(\mathbf{X}, t)$ is the only true degree of freedom present since α is *not* an additional degree of freedom in a classical sense, but merely a parameter in so far as the canonical projection is concerned (α is not governed by a *field* equation, i.e., its own balance law; compare the case of α as a true additional degree of freedom in Sect. 4 below). Still it will leave a print, like all dissipative processes, in the final expression of the canonical momentum equation, granting to the terms resulting from α the nature of so-called *pseudo-inhomogeneity* effects (cf. [34] for this notion).

3.1 Case A of Section 2

Proceeding now to the establishment of the canonical momentum balance, we indeed apply \mathbf{F} to the right in Eq. (2.1) while accounting for Eqs. (2.9) and (2.10). We note the following partial results:

$$\begin{aligned} \left(\frac{\partial(\rho_0 \mathbf{v})}{\partial t} \right) \cdot \mathbf{F} &= \frac{\partial(\rho_0 \mathbf{v} \cdot \mathbf{F})}{\partial t} - (\rho_0 \mathbf{v}) \cdot (\nabla_R \mathbf{v})^T \\ &= - \frac{\partial \mathbf{P}}{\partial t} \Big|_X - \nabla_R \left(\frac{1}{2} \rho_0 \mathbf{v}^2 \right), \end{aligned} \quad (3.1)$$

$$\begin{aligned} (\operatorname{div}_R \mathbf{T}) \cdot \mathbf{F} &= \operatorname{div}_R (\mathbf{T} \cdot \mathbf{F}) - \mathbf{T} \cdot (\nabla_R \mathbf{F})^T \\ &= \operatorname{div}_R (\mathbf{T} \cdot \mathbf{F}) - \frac{\partial \bar{W}}{\partial \mathbf{F}} : (\nabla_R \mathbf{F})^T, \end{aligned} \quad (3.2)$$

and

$$\begin{aligned} \nabla_R \bar{W} &\equiv \operatorname{div}_R (W \mathbf{1}_R) = \frac{\partial \bar{W}}{\partial \mathbf{F}} : (\nabla_R \mathbf{F})^T + \frac{\partial \bar{W}}{\partial \theta} \nabla_R \theta + \frac{\partial \bar{W}}{\partial \alpha} \nabla_R \alpha + \frac{\partial \bar{W}}{\partial (\nabla_R \alpha)} : (\nabla_R (\nabla_R \alpha))^T \\ &= \mathbf{T} : (\nabla_R \mathbf{F})^T - S \nabla_R \theta - A \nabla_R \alpha - \mathbf{B} : (\nabla_R (\nabla_R \alpha))^T. \end{aligned} \quad (3.3)$$

The reader untrained in using the intrinsic notation can make the evaluation using Cartesian tensorial indices where this applies. We have introduced the *material* linear momentum \mathbf{P} per unit reference volume by the pull back, changed of sign, of the physical linear momentum:

$$\mathbf{P} := -\rho_0 \mathbf{v} \cdot \mathbf{F}. \quad (3.4)$$

The meaning of this material co-vectorial quantity becomes clear if we introduce the inverse motion $\bar{\mathbf{X}}$, the inverse-motion gradient \mathbf{F}^{-1} , the material velocity field \mathbf{V} , and the Cauchy–Green finite strain tensor \mathbf{C} by

$$\begin{aligned} \bar{\mathbf{X}} &= \bar{\mathbf{x}}^{-1} = \bar{\mathbf{X}}(\mathbf{x}, t), \\ \mathbf{F}^{-1} &\equiv (\mathbf{F})^{-1} = \frac{\partial \bar{\mathbf{X}}}{\partial \mathbf{x}} \Big|_t = \nabla \bar{\mathbf{X}}, \quad \mathbf{V} := \frac{\partial \bar{\mathbf{X}}}{\partial t} \Big|_x = -\mathbf{F}^{-1} \cdot \mathbf{v}, \\ \mathbf{C} &= \mathbf{F}^T \cdot \mathbf{F}. \end{aligned} \quad (3.5)$$

On account of these, we obtain

$$\mathbf{P} = \rho_0 \mathbf{C} \cdot \mathbf{V}. \quad (3.6)$$

Gathering the partial results (3.1)–(3.4), we obtain the canonical momentum balance in the following form

$$\frac{\partial \mathbf{P}}{\partial t} \Big|_X - \operatorname{div}_R \mathbf{b} = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}}, \quad (3.7)$$

where we have defined the dynamical *Eshelby material stress* tensor \mathbf{b} , the *thermal material force* \mathbf{f}^{th} , and the *intrinsic material force* \mathbf{f}^{intr} by

$$\mathbf{b} := -(\mathbf{L} \mathbf{1}_R + \mathbf{T} \cdot \mathbf{F}),$$

and

$$\mathbf{f}^{\text{th}} := S \nabla_R \theta, \quad \mathbf{f}^{\text{intr}} := A \nabla_R \alpha + \mathbf{B} \cdot \nabla_R (\nabla_R \alpha), \quad (3.8)$$

and an energy scalar identified as a Lagrangian density quantity L [13], although we did not (and could not) use any variational principle:

$$L := K - W, \quad K = \frac{1}{2} \rho_0 \mathbf{v}^2. \quad (3.9)$$

At this point it is salient to note that Eq. (2.14) is immediately rewritten as

$$\left. \frac{\partial(\theta S)}{\partial t} \right|_X + \nabla_R \cdot \mathbf{Q} = h^{\text{th}} + h^{\text{intr}}, \quad (3.10)$$

where we have defined source terms on the right-hand side by

$$h^{\text{th}} := S\dot{\theta}, \quad h^{\text{intr}} := A\dot{\alpha} + \mathbf{B} \cdot \nabla_R \dot{\alpha}. \quad (3.11)$$

One easily recognizes the space–time symmetry between Eqs. (3.7) and (3.10) by acknowledging that the material gradients in expressions (3.8) for the material momentum are replaced by material time derivative for the energy in expressions (3.11). Accordingly, Eqs. (3.7) and (3.10) are but the space-like and time-like components of a unique four-dimensional conservation law, that of energy–momentum. Such a true four-dimensional formalism is discussed in Maugin [33].

Remark The internal-variable nature of α is comforted in the present thermomechanical vision by the facts that: (i) the internal variable is not involved in the definition of \mathbf{P} (it does not carry momentum) and (ii) the Eshelby stress \mathbf{b} here is expressed just as in pure elasticity [27] or in the thermoelasticity of conductors [28, 32]. The presence of the diffusive internal variable is materialized in the functional dependence of W and the appearance of the source term (3.8)₂ which is directly the space analogue of the intrinsic dissipated power given in (3.11)₂.

3.2 Case B of Section 2

The following transformation of Eq. (3.7) is straightforward. One obtains

$$\left. \frac{\partial \mathbf{P}}{\partial t} \right|_X - \text{div}_R \tilde{\mathbf{b}} = \mathbf{f}^{\text{th}} + \tilde{\mathbf{f}}^{\text{intr}}, \quad (3.12)$$

wherein

$$\tilde{\mathbf{b}} = -(\mathbf{L}\mathbf{1}_R + \mathbf{T}\cdot\mathbf{F} - \mathbf{B} \cdot (\nabla_R \alpha)^T), \quad \tilde{\mathbf{f}}^{\text{intr}} := \tilde{A} \nabla_R \alpha, \quad (3.13)$$

but both \mathbf{P} and \mathbf{f}^{th} are left unchanged. Simultaneously, the energy equation (3.10) takes on the form

$$\left. \frac{\partial(\theta S)}{\partial t} \right|_X + \nabla_R \cdot \tilde{\mathbf{Q}} = h^{\text{th}} + \tilde{h}^{\text{intr}}, \quad (3.14)$$

wherein

$$\tilde{\mathbf{Q}} := \mathbf{Q} - \mathbf{B}\dot{\alpha}, \quad \tilde{h}^{\text{intr}} := \tilde{A}\dot{\alpha}. \quad (3.15)$$

We could stop at this point concerning internal variables of state per se, remarking that the first of (3.15) agrees with Eq. (2.13)₂. Not only does the field-theoretic view require the introduction of an effective heat flux and of an extra entropy flux as already met in previous works [26], but it also requires a simultaneous alteration in the definition of the Eshelby stress tensor (3.13)₁. This alteration is not so surprising when we remember that the Eshelby stress is a kind of machinery to capture gradients of fields [28], but usually this is reserved to those related to a true degree of freedom, i.e., an observable variable. This is one more opportunity where a *diffusive* internal variable of state exhibits an ontological ambiguity in its definition. This necessarily leads us to a thorough comparison with the case of a true additional degree of freedom.

4 The variable α as an additional degree of freedom

Had we considered α as an *observable* field endowed with both inertia and flux, where the latter is not necessarily purely dissipative (on the contrary, it could be purely *non-dissipative*), we would have started with:

- A global statement of the *principle of virtual power* (PVP) following Germain [11, 12] and Maugin [25], and
- A global statement of the *first and second laws* of thermodynamics (following any standard book on continuum mechanics).

The first statement (PVP) would read for a body B_0 occupying the regular region V_0 with regular boundary surface ∂V_0 (of outward pointing unit normal \mathbf{N}) in its reference configuration K_R

$$P_{(\text{inertia})}^* = P_{(i)}^* + P_{(\text{data})}^* \quad (4.1)$$

with

$$P_{(\text{inertia})}^* = \int_{V_0} (\rho_0 \mathbf{v} \cdot \mathbf{v}^* + \rho_0 (\mathbf{I} \cdot \dot{\alpha}) \cdot (\dot{\alpha})^*) dV_0, \quad (4.2)$$

$$P_{(\text{data})}^* = \int_{V_0} (\hat{\mathbf{f}} \cdot \mathbf{v}^* + \hat{A} \cdot (\dot{\alpha})^*) dV_0 + \int_{\partial V_0} (\hat{\mathbf{T}}_{\mathbf{n}} \cdot \mathbf{v}^* + \hat{\mathbf{B}}_{\mathbf{n}} \cdot (\dot{\alpha})^*) dS_0, \quad (4.3)$$

and

$$P_{(i)}^* = - \int_{V_0} (\mathbf{T} : \nabla_R \mathbf{v}^* - A \cdot (\dot{\alpha})^* - \mathbf{B} \cdot \nabla_R (\dot{\alpha})^*) dV_0, \quad (4.4)$$

where

$$\hat{\mathbf{f}}, \hat{A}, \hat{\mathbf{T}}_{\mathbf{n}}, \hat{\mathbf{B}}_{\mathbf{n}} \quad (4.5)$$

are prescribed – hence the subscript “*data*” in the corresponding power – and

$$A, \mathbf{T}, \mathbf{B} \quad (4.6)$$

are *generalized internal forces* to be given by (nondissipative or dissipative, or both) *constitutive equations*.

Remark In Eqs. (4.1)–(4.4) an asterisk means that the expression or the field to which it is attached is a virtual field at our choice disposal. Deleting the asterisk means that the expression or the field in question takes its actual value in the initial-value boundary-value problem to be solved. Prescriptions to formulate the various virtual powers, once the basic fields such as the motion of the body and the variable α are chosen, have been clearly enunciated in Maugin [25]. In particular, the virtual power of internal forces $P_{(i)}^*$ must be written as a linear continuous form on a set of *objective* generalized velocity fields in order that the internal forces introduced by the inherent duality as the set (4.6) are objective fields (i.e., invariant under superimposed rigid-body motions in the current configuration K_t). If α is simply a scalar under such transformations, there are no problems in writing directly the linear form (4.4). For instance this is done by Frémond and Nedjar [9, 10] when α is a scalar damage variable. Then the inertia I in the expression of the virtual power of inertia force is also a scalar, if it exists at all. The objectivity requirement does not apply to the other virtual powers since neither inertial forces nor externally applied forces need be objective. Whenever α is a field of higher tensorial order (e.g., a vector field such as in the cases of liquid crystals, internally electrically polarized materials – cf. Maugin, [21–23] – , or internally magnetized material – cf. Maugin, [20]), one has to be more thoughtful in writing down $P_{(i)}$; in particular the objective (convected or Jaumann) time derivatives of α and its gradient must be introduced. This remark obviously holds true if α is a tensor of second order (e.g., representative of a rigid or deformable microstructure). The tensorial order of the inertia I is accordingly formulated. The dots between symbols in Eqs. (4.1) through (4.4) take their full meaning of contractors of indices or inner products in the appropriate space. These technicalities are more or less obvious. The formulation given in Eqns.(4.2)–(4.4) is called a *first-gradient theory* in so far as both the classical continuum motion and the variable α are concerned. Higher-order gradient theories, i.e., stronger non-local theories, may be constructed

following the same generalized pattern and rules [25,31]. First order is enough to compare with the foregoing diffusive internal variable theory. Note that there is no obligation that the theory be of the same order for the classical motion and for the additional variable α . This choice is at our disposal and depends essentially on our apprehending of the spatial range of interactions.

Remark Here we call α an observable field. We could as well say a *controllable* field, meaning by this that, contrary to internal variables of state, their values can be adjusted by a proper action in the bulk and at the surface of the body by the introduced generalized forces present in $P_{(\text{data})}$. Note also that Frémond and Nedjar [9,10], while not considering any inertia, seem to believe they are dealing with an internal variable of state for α . But the very introduction of a working for α contradicts Kestin's original definition, to which we adhere. These authors are just working in the general framework devised by the author (1980) where a statement of the principle of virtual power is strictly equivalent to the statement of balance laws, including for additional degrees of freedom, to the status of which α is now reduced.

The two laws of thermodynamics are now set forth in the following global form:

4.1 First law of thermodynamics

$$\frac{d}{dt} \int_{V_0} (K + E) dV_0 = P_{(\text{data})} + \dot{Q}, \quad \dot{Q} = - \int_{\partial V_0} \hat{Q}_{\mathbf{n}} dS_0 \quad (4.7)$$

where \mathbf{K} is introduced for the sake of generality.

4.2 Second law of thermodynamics

$$\frac{d}{dt} \int_{V_0} S dV_0 + \int_{\partial V_0} \mathbf{N} \cdot \tilde{\mathbf{S}} dS_0 \geq 0, \quad \tilde{\mathbf{S}} = \theta^{-1} \mathbf{Q} + \mathbf{K}, \quad (4.8)$$

where \mathbf{K} is introduced for the sake of generality.

In these two equations, K , E , and S are the kinetic energy, internal energy, and entropy density per unit reference volume. \dot{Q} is the energy rate supply to the body through its boundary. This occurs through heat. We introduce no energy supply per unit volume. In writing the second law, we have somewhat anticipated by introducing an entropy flux with a more general relationship to heat and dissipative processes since, while θ is the standard thermodynamical temperature, we have admitted the possible existence of an extra entropy flux \mathbf{K} (which vanishes in most cases in continuum theories). The kinetic energy here is given by

$$K = \frac{1}{2} \rho_0 \mathbf{v}^2 + \frac{1}{2} \rho_0 \dot{\alpha} \cdot \mathbf{I} \cdot \dot{\alpha}. \quad (4.9)$$

As a first outcome from the application of (4.1) for any virtual fields (\mathbf{v}^* , $(\dot{\alpha})^*$) in any volume and surface element, we obtain the following balance laws and natural boundary conditions:

$$\left. \frac{\partial(\rho_0 \mathbf{v})}{\partial t} \right|_X - \text{div}_R \mathbf{T} = \hat{\mathbf{f}} \text{ in } V_0, \quad \hat{\mathbf{T}}_{\mathbf{n}} = \mathbf{N} \cdot \mathbf{T} \text{ at } \partial V_0, \quad (4.10)$$

$$\left. \frac{\partial(\rho_0 \mathbf{I} \cdot \dot{\alpha})}{\partial t} \right|_X = \hat{A} + A - \nabla_R \cdot \mathbf{B} \text{ in } V_0, \quad \hat{\mathbf{B}}_{\mathbf{n}} = \mathbf{N} \cdot \mathbf{B} \text{ at } \partial V_0. \quad (4.11)$$

A second result is obtained for real virtual velocity fields (no asterisks), on account of (4.9). It is the so-called equation of kinetic energy in global form:

$$\frac{d}{dt} \int_{V_0} K dV_0 = P_{(i)} + P_{(\text{data})} \quad (4.12)$$

On combining this with the first law (4.7), we obtain the so-called *equation of internal energy* in global form:

$$\frac{d}{dt} \int_{V_0} E \, dV_0 + P_{(i)} = \dot{Q}, \quad (4.13)$$

the localization of which yields

$$\begin{aligned} \left. \frac{dE}{dt} \right|_X &= \mathbf{T} : \nabla_R \mathbf{v} - A \dot{\alpha} - \mathbf{B} \cdot \nabla_R \dot{\alpha} - \nabla_R \cdot \mathbf{Q} \quad \text{in } V_0, \\ \dot{Q}_{\mathbf{n}} &= \mathbf{N} \cdot \mathbf{Q} \quad \text{at } \partial V_0 \end{aligned} \quad (4.14)$$

Introducing now the Helmholtz free energy per unit reference volume W by

$$W = E - S\theta, \quad (4.15)$$

and combining with the local form of the inequality (4.8)₁, we arrive at the following Clausius–Duhem inequality:

$$-\left(\frac{dW}{dt} + S \frac{d\theta}{dt} \right) + p_{(i)} + \nabla_R \cdot (\theta \mathbf{K}) - \tilde{\mathbf{S}} \cdot \nabla_R \theta \geq 0; \quad (4.16)$$

while evaluating $\theta \, dS/dt$ from (4.14)₁ on account of (4.15) we obtain the entropy equation, which will ultimately provide the heat propagation equation, in the form

$$\theta \frac{dS}{dt} = -\left(\frac{dW}{dt} + S \frac{d\theta}{dt} \right) + p_{(i)} - \nabla_R \cdot \mathbf{Q}. \quad (4.17)$$

We have introduced the following notation

$$p_{(i)} := \mathbf{T} : \dot{\mathbf{F}} - A \dot{\alpha} - \mathbf{B} \cdot \nabla_R \dot{\alpha}, \quad (4.18)$$

and accounted for the fact that

$$\nabla_R \mathbf{v} \equiv \dot{\mathbf{F}}. \quad (4.19)$$

Now we consider three cases of exploitation of the scheme developed above.

4.2.1 The only dissipative process is heat conduction

We have the following obvious reduction:

$$\mathbf{K} \equiv \mathbf{0}, \quad \tilde{\mathbf{S}} \equiv \frac{\mathbf{Q}}{\theta}, \quad (4.20)$$

$$-\left(\frac{dW}{dt} + S \frac{d\theta}{dt} \right) + p_{(i)} = 0, \quad \Phi^{\text{th}} := -\tilde{\mathbf{S}} \cdot \nabla_R \theta \geq 0, \quad (4.21)$$

$$\theta \frac{dS}{dt} + \nabla_R \cdot \mathbf{Q} = 0. \quad (4.22)$$

The last of these can also be written as (since $\theta > 0$ always)

$$\frac{dS}{dt} + \nabla_R \cdot \tilde{\mathbf{S}} = \sigma^{\text{th}}, \quad \sigma^{\text{th}} = \theta^{-1} \Phi^{\text{th}}. \quad (4.23)$$

With a functional dependence $W = \overline{W}(\mathbf{F}, \theta, \alpha, \nabla_R \alpha)$, a classical reasoning applied to the first of (4.21) yields the constitutive equations:

$$S = -\frac{\partial W}{\partial \theta}, \quad \mathbf{T} = \frac{\partial W}{\partial \mathbf{F}}, \quad A = -\frac{\partial W}{\partial \alpha}, \quad \mathbf{B} = -\frac{\partial W}{\partial (\nabla_R \alpha)}. \quad (4.24)$$

It remains to give an expression to the heat flux \mathbf{Q} in order to arrive at a fully explicit expression for Eq. (4.22).

4.2.2 The Coleman–Noll continuum thermodynamics viewpoint

In this case Eqs. (4.20) are valid a priori, independently of any deformation and time internal evolution of α , i.e.,

$$\mathbf{K} \equiv \mathbf{0} \Rightarrow \tilde{\mathbf{S}} \equiv \frac{\mathbf{Q}}{\theta}. \quad (4.25)$$

The generalized internal forces (4.6) are each the sum of a thermodynamically reversible part and a *dissipative* thermodynamically irreversible part, i.e.,

$$A = A_{\text{rev}} + A_{\text{irrev}}, \quad \mathbf{T} = \mathbf{T}_{\text{rev}} + \mathbf{T}_{\text{irrev}}, \quad \mathbf{B} = \mathbf{B}_{\text{rev}} + \mathbf{B}_{\text{irrev}}. \quad (4.26)$$

The dependent functions $\{W, S, A_{\text{rev}}, \mathbf{T}_{\text{rev}}, \mathbf{B}_{\text{rev}}\}$ depend all on the same set as

$$W = \bar{W}(\mathbf{F}, \theta, \alpha, \nabla_R \alpha), \quad (4.27)$$

while the remaining dissipative fields $\{\tilde{\mathbf{S}}, A_{\text{irrev}}, \mathbf{T}_{\text{irrev}}, \mathbf{B}_{\text{irrev}}\}$ depend on the same set as *also* on the set $\{\nabla_R \theta, \dot{\mathbf{F}}, \dot{\alpha}, \nabla_R \dot{\alpha}\}$. Here classical reasoning also yields constitutive equations similar to those in Eqs. (4.24) for the nondissipative contributions, i.e.,

$$\begin{aligned} \mathbf{T}_{\text{rev}} &= \frac{\partial \bar{W}}{\partial \mathbf{F}}, & A_{\text{rev}} &= -\frac{\partial \bar{W}}{\partial \alpha}, & \mathbf{B}_{\text{rev}} &= -\frac{\partial \bar{W}}{\partial (\nabla_R \alpha)}, \\ S &= -\frac{\partial \bar{W}}{\partial \theta}, & W &= \bar{W}(\mathbf{F}, \theta, \alpha, \nabla_R \alpha) \end{aligned} \quad (4.28)$$

while there remains the following residual dissipation inequality:

$$\Phi := \mathbf{T}_{\text{irrev}} \cdot \dot{\mathbf{F}} - A_{\text{irrev}} \cdot \dot{\alpha} - \mathbf{B}_{\text{irrev}} \cdot \nabla_R \dot{\alpha} - \tilde{\mathbf{S}} \cdot \nabla_R \theta \geq 0. \quad (4.29)$$

In exploiting this inequality, one does as if the gradient of $\dot{\alpha}$ and $\dot{\alpha}$ itself were independent variables. This is a standard method reported and recommended in continuum mechanics books. Note that here the entropy flux satisfies the classical formula (4.25)₂. For instance, this is applied to liquid crystals (where α is a unit director) by Leslie [17] or to elastic dielectrics by Maugin [21,23] and elastic ferromagnets in Maugin [20] – also Maugin [19] where this was first applied to a sufficiently sophisticated case. We shall not pursue this exploitation of Eq. (4.29) here. It suffices to notice that, if the time parity of α as a tensor allows for it, there might be a direct linear coupling between the irreversible effect associated with α and heat conduction. On another occasion such a direct coupling could arise between heat conduction and the dissipative *process* associated with the gradient of α .

4.3 Canonical balance equations

Within the framework of the *Coleman–Noll continuum mechanics formulation* we let the reader check that the balances of canonical momentum and energy are given by the following two equations:

$$\left. \frac{\partial \bar{\mathbf{P}}}{\partial t} \right|_X - \text{div}_R \bar{\mathbf{b}} = S \nabla_R \theta + \mathbf{T}_{\text{irrev}} : (\nabla_R \mathbf{F})^T - A_{\text{irrev}} \nabla_R \alpha - \mathbf{B}_{\text{irrev}} \cdot \nabla_R (\nabla_R \alpha), \quad (4.30)$$

and

$$\frac{\partial(\theta S)}{\partial t} + \nabla_R \cdot \mathbf{Q} = S \dot{\theta} + \mathbf{T}_{\text{irrev}} : \dot{\mathbf{F}} - A_{\text{irrev}} \dot{\alpha} - \mathbf{B}_{\text{irrev}} \cdot \nabla_R \dot{\alpha} \quad (4.31)$$

wherein

$$\bar{\mathbf{P}} = -\rho_0(\mathbf{v} \cdot \mathbf{F} + \nabla_R \alpha \cdot \mathbf{I} \cdot \dot{\alpha}), \quad (4.32)$$

$$\bar{\mathbf{b}} = -\left[(K - W) \mathbf{1}_R + \mathbf{T}_{\text{rev}} \cdot \mathbf{F} - \mathbf{B}_{\text{rev}} \cdot (\nabla_R \alpha)^T \right], \quad (4.33)$$

$$K = \frac{1}{2} \rho_0(\mathbf{v}^2 + \dot{\alpha} \cdot \mathbf{I} \cdot \dot{\alpha}), \quad W = \bar{W}(\mathbf{F}, \alpha, \nabla_R \alpha). \quad (4.34)$$

Remark In the case when A presents no irreversible part, the field A does not appear at all in the reduced forms taken by Eqs. (4.30) and (4.33). As noticed before, the reason is that the reduced form of these equations only captures gradients of fields and A relates to α alone.

Hint Equation (4.30) is obtained by multiplying Eq. (4.10)₁ to the right by \mathbf{F} , and Eq. (4.11)₁ by $\nabla_R \alpha$, adding the two resulting co-vectorial material expressions and manipulating this on account of the already obtained constitutive equations for the reversible fields. We have assumed that the bulk data $\hat{\mathbf{f}}$ and \hat{A} vanished; otherwise they jointly add a source term in Eq. (5.5) in the form $-(\hat{\mathbf{f}} \cdot \mathbf{F} + \hat{A} \nabla_R \alpha)$.

4.3.1 The field-theoretic viewpoint

This is quite different in the sense that a scientist trained in analytical mechanics will not a priori assume that $\dot{\alpha}$ and $\nabla_R \dot{\alpha}$ are independent. He may prefer to keep the general expressions (4.8)₂ and (4.16) so that (4.29) will be replaced by the following expression in which $\tilde{\mathbf{S}}$ is given by (4.8)₂ while Eqs. (4.28) still hold true:

$$\Phi = \mathbf{T}_{\text{irrev}} \cdot \dot{\mathbf{F}} - A_{\text{irrev}} \cdot \dot{\alpha} - \mathbf{B}_{\text{irrev}} \cdot \nabla_R \dot{\alpha} + \nabla_R \cdot (\theta \mathbf{K}) - \tilde{\mathbf{S}} \cdot \nabla_R \theta \geq 0. \quad (4.35)$$

But we note that the very form of Eqn.(4.11)₁ suggests that we consider the grouping

$$\tilde{A} := A - \nabla_R \cdot \mathbf{B}. \quad (4.36)$$

According to Eqs. (4.28) the reversible part of this is given by

$$\tilde{A}_{\text{rev}} \equiv -\frac{\delta \bar{W}}{\delta \alpha} := -\left(\frac{\partial \bar{W}}{\partial \alpha} - \nabla_R \cdot \frac{\partial \bar{W}}{\partial (\nabla_R \alpha)} \right). \quad (4.37)$$

On the basis of (4.36) we also set

$$\tilde{A}_{\text{irrev}} := A_{\text{irrev}} - \nabla_R \cdot \mathbf{B}_{\text{irrev}}. \quad (4.38)$$

On selecting the extra entropy flux as

$$\mathbf{K} = \theta^{-1} \mathbf{B}_{\text{irrev}} \dot{\alpha}, \quad (4.39)$$

it is easily shown that the inequality (4.35) reduces to the following inequality

$$\Phi = \mathbf{T}_{\text{irrev}} \cdot \nabla_R \mathbf{v} - \tilde{A}_{\text{irrev}} \cdot \dot{\alpha} - \tilde{\mathbf{S}} \cdot \nabla_R \theta \geq 0, \quad (4.40)$$

where $\tilde{\mathbf{S}}$ is given by Eqs. (4.8)₂ and (4.39). The exploitation of this inequality would follow the usual formalism of irreversible thermodynamics.

Simultaneously, the heat propagation equation (4.17) is shown to take on the following form [cf. Eq. (4.22)]

$$\theta \frac{dS}{dt} + \nabla_R \cdot \tilde{\mathbf{Q}} = \mathbf{T}_{\text{irrev}} : \dot{\mathbf{F}} - \tilde{A}_{\text{irrev}} \dot{\alpha}, \quad \tilde{\mathbf{Q}} := \mathbf{Q} + \mathbf{B}_{\text{irrev}} \dot{\alpha}, \quad (4.41)$$

providing thus a completely coherent theory.

Comment Equation (4.34) is a sufficient condition for the nonexistence of a divergence term in the residual dissipation inequality.

4.4 Canonical balance equations

In this *field-theoretic formulation*, it is immediately shown that Eqs. (4.30) and (4.31) are replaced by

$$\left. \frac{\partial \tilde{\mathbf{P}}}{\partial t} \right|_X - \text{div}_R \tilde{\mathbf{b}} = S \nabla_R \theta + \mathbf{T}_{\text{irrev}} : (\nabla_R \mathbf{F})^T - \tilde{A}_{\text{irrev}} \nabla_R \alpha, \quad (4.42)$$

and

$$\frac{\partial (\theta S)}{\partial t} + \nabla_R \cdot \tilde{\mathbf{Q}} = S \dot{\theta} + \mathbf{T}_{\text{irrev}} : \dot{\mathbf{F}} - \tilde{A}_{\text{irrev}} \dot{\alpha}, \quad (4.43)$$

where $\tilde{\mathbf{Q}}$ is given by Eq. (4.41)₂ and $\tilde{\mathbf{b}}$ is defined by

$$\tilde{\mathbf{b}} = -[(K - W) \mathbf{1}_R + \mathbf{T}_{\text{rev}} \cdot \mathbf{F} - \mathbf{B} \cdot (\nabla_R \alpha)^T]. \quad (4.44)$$

5 Comparison with the diffusive internal-variable theory

It is clear that such a comparison must be carried out exactly in the conditions where the internal-variable theory holds and also while going from the more general to the particular. To that effect, α being not an internal degree of freedom, *it must have no inertia*, so that the left-hand side of Eq. (4.11)₁ vanishes identically. Furthermore, accepting Kestin's definition of internal variables of state as adopted in the book of Maugin [32], α should *not* be directly controllable by any means, thus requiring the vanishing of the data fields relative to α in the set (4.5). Accordingly, Eqs. (4.11) reduce to the following self-equilibrated form:

$$A - \nabla_R \cdot \mathbf{B} = 0 \quad \text{in } V_0, \quad \mathbf{N} \cdot \mathbf{B} = 0 \quad \text{at } \partial V_0. \quad (5.1)$$

Necessary and sufficient conditions for this to hold at all material points \mathbf{X} are the vanishing of A and that \mathbf{B} be divergence-free, separately at any point \mathbf{X} in the body. We can take \mathbf{B} identically zero without much loss in generality. It then follows from Eqs. (4.26) and (4.28) that the thermodynamically irreversible fields A_{irrev} and $\mathbf{B}_{\text{irrev}}$ are now defined in terms of the energy density W as

$$\begin{aligned} A_{\text{rev}} + A_{\text{irrev}} = 0 &\Rightarrow A_{\text{irrev}} = -A_{\text{rev}} = \frac{\partial \bar{W}}{\partial \alpha}, \\ \mathbf{B}_{\text{irrev}} = -\mathbf{B}_{\text{rev}} &= \frac{\partial \bar{W}}{\partial (\nabla_R \alpha)} \end{aligned} \quad (5.2)$$

Accordingly,

$$\tilde{A}_{\text{irrev}} = -\tilde{A}_{\text{rev}} \equiv \frac{\delta \bar{W}}{\delta \alpha} := \left(\frac{\partial \bar{W}}{\partial \alpha} - \nabla_R \cdot \frac{\partial \bar{W}}{\partial (\nabla_R \alpha)} \right) \quad (5.3)$$

and

$$\tilde{\mathbf{S}} = \theta^{-1} (\mathbf{Q} + \mathbf{B}_{\text{irrev}} \dot{\alpha}) = \theta^{-1} \left(\mathbf{Q} + \frac{\partial \bar{W}}{\partial (\nabla_R \alpha)} \dot{\alpha} \right). \quad (5.4)$$

On account of these results and in spite of apparent discrepancies in signs, we recover entirely the expressions of the diffusive internal-variable theory.

In so far as *canonical equations* are concerned, the reduction to the case of α being a diffusive internal variable of state treated in Sect. 3 is straightforward, since then $\mathbf{T} \equiv \mathbf{T}_{\text{rev}}$ as $\mathbf{T}_{\text{irrev}} \equiv \mathbf{0}$, and the reduction (5.2) and (5.3) applies.

6 Applications (all examples without body force)

6.1 Pure homogeneous elasticity

In that case $\rho_0 = \text{const.}$, and $W = \bar{W}(\mathbf{F})$ only. We have $h^{\text{int}} \equiv 0$, $\mathbf{f}^{\text{int}} \equiv \mathbf{0}$ since $\mathbf{T} = \partial \bar{W} / \partial \mathbf{F}$, and also $\mathbf{f}^{\text{inh}} = \mathbf{0}$, $\mathbf{Q} \equiv \mathbf{0}$. Equations (3.7) and (3.10) reduce to the following system ($\theta_0 = \text{const.}$):

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{0}, \quad \theta_0 \frac{dS}{dt} = 0. \quad (6.1)$$

It is easily checked that this system is Hamiltonian with canonical four-momentum given by $(\mathbf{P}, \theta_0 S)$.

6.2 Inhomogeneous thermoelasticity of conductors

In that case $\rho_0 = \bar{\rho}_0(\mathbf{X})$, and $W = \bar{W}(\mathbf{F}, \theta; \mathbf{X})$. We have the constitutive equations $\mathbf{T} = \partial \bar{W} / \partial \mathbf{F}$ and $S = -\partial \bar{W} / \partial \theta$ that follow from a standard exploitation of the Clausius–Duhem inequality. Accordingly, we obtain that $\mathbf{f}^{\text{int}} \equiv \mathbf{f}^{\text{th}}$ and $h^{\text{int}} \equiv h^{\text{th}} := S\dot{\theta}$, where $\mathbf{f}^{\text{th}} := S \nabla_R \theta$ is the material thermal force introduced by Bui [3] and Epstein and Maugin [5], so that (6.1) is replaced by the following canonical (*non*-Hamiltonian) system of balance of momentum and energy:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{\text{inh}} + \mathbf{f}^{\text{th}}, \quad \frac{d(S\theta)}{dt} + \nabla_R \cdot \mathbf{Q} = h^{\text{th}}, \tag{6.2}$$

as found by Maugin [29] up to the notation.

6.3 Homogeneous dissipative solid material described by means of a diffusive internal variable.

In general α is an internal variable of state whose tensorial nature is not specified. This may relate to damage, or inelasticity of some sort with a possible diffusion of the said variable so that its material gradient must be taken into account (e.g., in strain-gradient plasticity). Then W is specified as the general sufficiently regular function $W = \bar{W}(\mathbf{F}, \theta, \alpha, \nabla_R \alpha)$. Here we specify that α is a scalar variable c akin to a concentration. We keep the possibility that \mathbf{K} be not zero. The equations of state are given by the Gibbs equation as

$$\begin{aligned} \mathbf{T} &= \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}, \\ \mu &:= \frac{\partial \bar{W}}{\partial c}, \quad \mathbf{M} := \frac{\partial \bar{W}}{\partial (\nabla_R c)}. \end{aligned} \tag{6.3}$$

so that μ is a chemical potential. We find that

$$\mathbf{f}^{\text{int}} = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}}, \quad h^{\text{int}} = h^{\text{th}} + h^{\text{intr}}, \tag{6.4}$$

where the thermal sources have already been defined and the intrinsic sources are given by

$$\mathbf{f}^{\text{intr}} := -\mu(\nabla_R c)^T - \mathbf{M} \cdot \nabla_R (\nabla_R c)^T, \quad h^{\text{intr}} := -\mu \dot{c} - \mathbf{M} \cdot (\nabla_R \dot{c})^T, \tag{6.5}$$

so that we have the following consistent (*non*-Hamiltonian) system of canonical balance laws:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}}, \quad \frac{d(S\theta)}{dt} + \nabla_R \cdot \mathbf{Q} = h^{\text{th}} + h^{\text{intr}}, \tag{6.6}$$

while the dissipation reads

$$\Phi = h^{\text{intr}} - \mathbf{S} \cdot \nabla_R \theta \geq 0, \quad \mathbf{K} \equiv \mathbf{0}. \tag{6.7}$$

This approach favors the *continuum mechanics* (Coleman–Noll) standard viewpoint by accepting the classical relationship between heat and entropy flux, and assuming that c and its material gradient are essentially independent.

A more *field-theoretic* viewpoint is to envisage a non-zero $\mathbf{K} = \theta^{-1} \mathbf{M} \dot{c}$. We let the reader check that Eqs. (6.6) and (6.7) are then replaced by the following equations:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \tilde{\mathbf{b}} = \mathbf{f}^{\text{th}} + \tilde{\mathbf{f}}^{\text{intr}}, \quad \frac{d(S\theta)}{dt} + \nabla_R \cdot \tilde{\mathbf{Q}} = h^{\text{th}} + \tilde{h}^{\text{intr}}, \tag{6.8}$$

$$\tilde{\Phi} = \tilde{h}^{\text{intr}} - \tilde{\mathbf{S}} \cdot \nabla_R \theta \geq 0, \quad \tilde{h}^{\text{intr}} = -\tilde{\mu} \dot{c}, \tag{6.9}$$

where we have introduced the new definitions

$$\tilde{\mu} \equiv \frac{\delta \bar{W}}{\delta c} := \left(\frac{\partial \bar{W}}{\partial c} - \nabla_R \cdot \frac{\partial \bar{W}}{\partial (\nabla_R c)} \right) = \mu - \nabla_R \cdot \mathbf{M}, \quad \tilde{\mathbf{S}} := \tilde{\mathbf{Q}} / \theta, \quad \tilde{\mathbf{Q}} = \mathbf{Q} + \mathbf{M} \dot{c} \tag{6.10}$$

and

$$\tilde{\mathbf{b}} = -(L\mathbf{1}_R + \mathbf{T}\cdot\mathbf{F} + \mathbf{M} \otimes (\nabla_R c)), \tilde{\mathbf{f}}^{\text{intr}} := -\tilde{\mu} \nabla_R c. \quad (6.11)$$

This is in the spirit of the approach that we advocated before [26]. The two approaches are to be compared to the recent constructive comments of Ireman and Nguyen [15].

The closure of the thermodynamical system requires the setting of relationships between (μ, \mathbf{M}) and $(\dot{c}, \nabla_R \dot{c})$ on the one hand, or $\tilde{\mu}$ and \dot{c} on the other, and a relationship à la Fourier between $\tilde{\mathbf{S}}$ and $\nabla_R \theta$. We pursue the second line (the field-theoretic approach), considering as an example a free-energy function W of the type

$$\overline{W}(\mathbf{F}, \theta, c, \nabla_R c) = \frac{1}{2} \gamma (\nabla_R c) \cdot (\nabla_R c) + \hat{W}(\mathbf{F}, \theta, c), \quad (6.12)$$

where the positive scalar coefficient γ depends at most on the temperature θ . In agreement with (6.9) we select (sufficient conditions) the evolution equation and heat transport equation as

$$\dot{c} = -\tau^{-1} \tilde{\mu}, \quad \tilde{\mathbf{S}} = -\chi \nabla_R \theta, \quad (6.13)$$

with positive coefficients τ and χ (which could be temperature dependent). On account of these and Eqs. (6.12) and (6.10), we obtain a *nonlinear evolution–diffusion equation* for c in the following form:

$$\tau \dot{c} + f(c; \mathbf{F}, \theta) = \nabla_R \cdot (\gamma \nabla_R c), \quad (6.14)$$

where

$$f(c; \mathbf{F}, \theta) \equiv \frac{\partial \hat{W}}{\partial c} = \mu. \quad (6.15)$$

One could assume that \hat{W} behaves like c^2 for small c , but more generally it may be of a higher degree in c , or may even be non-convex in c , remaining nonetheless positive. To the same degree of approximation, the nonlinear evolution–diffusion equation for temperature is given by

$$\theta \dot{S} + (f - \nabla_R \cdot (\gamma \nabla_R c)) \dot{c} + \nabla_R \cdot (\theta \chi \nabla_R \theta) = 0, \quad (6.16)$$

where $S = -\partial W / \partial \theta$ is usually linear in θ , such that W is concave in this variable.

Finally, Eq. (6.8), considered with inertia neglected, yields the equation

$$\text{div}_R (W\mathbf{1}_R - \mathbf{T}\cdot\mathbf{F} - \lambda(\nabla_R c) \otimes (\nabla_R c)) + S \nabla_R \theta + \tilde{\mu} \nabla_R c = 0, \quad (6.17)$$

or equivalently

$$\text{div}_R \left(\tilde{G}\mathbf{1}_R - \mathbf{T}\cdot\mathbf{F} - \lambda(\nabla_R c) \otimes (\nabla_R c) \right) - \theta \nabla_R S - c \nabla_R \tilde{\mu} = 0, \quad (6.18)$$

where $\tilde{G} = W + S\theta + \tilde{\mu}c = E + \tilde{\mu}c$ is the Gibbs, energy density. (cf. Eq.(2.6)).

In the absence of temperature effects and for a nondiffusive variable c , this reduces to the simple equation

$$\text{div}_R (G\mathbf{1}_R - \mathbf{T}\cdot\mathbf{F}) - c \nabla_R \mu = 0, \quad (6.19)$$

where $G = W + \mu c$. In this case (6.14) reduces to a (generally) *nonlinear relaxation equation*: $\tau \dot{c} + f(c; \mathbf{F}) = 0$.

We let the reader construct more complicated or more physically motivated examples by following the general rules enunciated in this paper.

7 Conclusion

The developments described herein show that there is no unique thermomechanical description of continuous media exhibiting diffusion of some property. A first choice is between considering the additional variable required to describe this property either as a true additional degree of freedom (with an inertia and then safely following an application of the principle of virtual power) or as an internal variable of state. If the second possibility is selected (essentially when the new property is only dissipative) then the main question is whether this variable is diffusive and therefore controllable to some extent via a flux at a material boundary. Finally, it is shown that the field-theoretic viewpoint certainly prevails and is more economical from the point of view of thought even though both notions of entropy and Eshelby's material stress tensor must then be consistently revisited. The resulting formulation offers new perspectives of research in both biomechanics and the mechanics of biomaterials which are privileged domains of application.

As a final remark, we note that the reduction tentatively given in Sect. 5 is not completely satisfactory, for it is only schematic. The inertia associated with an internal degree of freedom accounts for some fast dynamics (or high frequency phenomena) at a small scale. The resulting internal variable may represent at the macroscale the print left by the internal degree of freedom. But in changing scales, the fast dynamics (e.g., spin waves, polaritons) is lost to the benefit of dissipation (e.g., hysteresis, hardening), and the internal variable, although noted with the same symbol, may be thought of as a kind of average (in a sense to be specified) of the former variable in agreement with the late Kroner's view. This happens in ferroelectric and ferromagnetic materials [32]. This transition should be thoroughly studied and the emergence of a nonconventional additional entropy flux may be justified in this transition.

References

1. Bowen, R.M.: Towards a thermodynamics and mechanics of mixtures. *Arch. Rat. Mech. Anal.* **24**, 370–403 (1967)
2. Bowen, R.M.: Theory of Mixtures, in: Eringen A.C., *Continuum Physics*, Vol. III, pp.1–127. Academic, New York (1976)
3. Bui, H.D.: *Mécanique de la Rupture Fragile*, Masson, Paris (1978)
4. de Groot, S.R., Mazur P.: *Non-equilibrium Thermodynamics*. North-Holland, Amsterdam (1962)
5. Epstein, M. Maugin, G.A.: Thermoelastic material forces: definition and geometric aspects. *C. R. Acad. Sci. Paris* **II-320**, 63–68 (1995)
6. Epstein, M. Maugin, G.A.: Thermomechanics of volumetric growth in uniform bodies. *Int. J. Plasticity* **16**, 951–978 (2000)
7. Forest, S., Cordona, J.-M.: Thermoelasticity of second-grade materials, In: Maugin, G.A., Drouot, R. Sidoroff F., (eds.) 163–176, *Kluwer, Continuum Thermoelasticity: The Art and Science of Modeling Materials' Behaviour* Dordrecht (2000)
8. Forest, S. Sievert, R.: Elastoviscoplastic constitutive frameworks for generalized continua. *Acta Mech.* **160**, 71–111 (2003)
9. Frémond, M., Nedjar, B., Endommagement et principe des puissances virtuelles. *C. R. Acad. Sci. Paris.* **317-II**, 857–864 (1993)
10. Frémond, M., Nedjar, B.: Damage, Gradient of damage and principle of virtual power. *Int. J. Solids Struct.* **33**, 1083–1103 (1996)
11. Germain, P.: La méthode des puissances virtuelles en mécanique des milieux continus- I: Théorie du second gradient. *J. Mécanique (Paris)* **12**, 135–274 (1973a)
12. Germain, P.: The method of virtual power in continuum mechanics-II: microstructure. *SIAM J. Appl. Math.* **25**, 556–575 (1973b)
13. Goldstein, H.: *Classical Mechanics*. Addison–Wesley, Reading, (1950)
14. Grinfeld, M.A.: *Thermodynamic Methods in the Theory of Heterogeneous Systems*. Longman, Harlow, (1991)
15. Ireman P., Nguyen, Q.-S.: Using the gradients of the temperature and internal parameters in continuum thermodynamics. *C. R. Mécanique* **333**, 249–255 (2004)
16. Kats, E.I., Lebedev, V.V.: *Dynamics of liquid crystals (in Russian)* Nauka, Moscow (1988)
17. Leslie, F.M.: Constitutive equations for liquid crystals. *Arch. Rat. Mech. Anal.* **28**, 265–283 (1968)
18. Lorentz, E., Andrieux, S.: A variational formulation of nonlocal damage models. *Int. J. Plasticity* **15**, 119–198 (1999)
19. Maugin, G.A.: Remarks on dissipative processes in the continuum theory of micromagnetics. *J. Phys. (UK)* **A5**, 1550–1562 (1972)
20. Maugin, G.A.: Sur la dynamique des milieux déformables avec spin magnétique – Théorie classique *J. Mécanique (Paris)*, **13**, 75–96 (1974a)
21. Maugin, G.A.: Quasi-electrostatics of electrically polarized continua. *Lett. Appl. Eng. Sci.* **2**, 293–306 (1974b)
22. Maugin, G.A.: On the foundations of the electrodynamics of deformable media with interactions. *Lett. Appl. Eng. Sci.* **4**, 3–17 (1976)
23. Maugin, G.A.: Deformable dielectrics II – Voigt's intramolecular force balance in elastic dielectrics. *Arch. Mech.* **29**, 143–159 (1977)
24. Maugin, G.A.: Nonlocal theories or gradient-type theories: a matter of convenience? *Arch. Mech.* **31**, 1–26 (1979)
25. Maugin, G.A.: The method of virtual power in continuum mechanics: application to coupled fields. *Acta Mech.* **35**, 1–80 (1980)
26. Maugin, G.A.: Internal variables and dissipative structures. *J. Non-Eq. Thermodyn.* **15**, 173–192 (1990)
27. Maugin, G.A.: *Material Inhomogeneities in Elasticity*. Chapman and Hall, London (1993)

-
28. Maugin, G.A.: Material forces: concepts and applications. *ASME Appl. Mech. Rev.* **48**, 213–245 (1995)
 29. Maugin, G.A.: Canonical momentum and energy in elastic systems with additional state variables. *C. R. Acad. Sci. Paris* **IIb-323**, 407–412 (1996)
 30. Maugin, G.A.: Thermomechanics of inhomogeneous-heterogeneous systems: application to the irreversible progress of two- and three-dimensional defects. *ARI* **50**, 41–56 (1997)
 31. Maugin, G.A.: Remarks on the thermomechanics of weakly nonlocal theories In: Brillard, A., Ganghoffer, J.-F., *Nonlocal Aspects in Solid Mechanics (Proc. Euromech Coll.378)* pp. 2–9. Univ. Mulhouse, France (1998)
 32. Maugin, G.A.: *The Thermomechanics of Nonlinear Irreversible Behaviors*. World Scientific, Singapore (1999)
 33. Maugin, G.A.: On the universality of the thermomechanics of forces driving singular sets. *Arch. Appl. Mech.* **70**, 31–45 (2000)
 34. Maugin, G.A.: Pseudo-plasticity and pseudo-inhomogeneity effects in materials mechanics. *J. Elast. (Special issue in Memory of C. A. Truesdell)* **71**, 81–103 (2003)
 35. Truesdell, C.A.: *Rational Thermodynamics*, 2nd enlarged edition, Springer, Berlin Heidelberg New York (1984)
 36. Truskinovskii, L.M.: The chemical tensor. *Geokhimiya* **12**, 1730–1744 (1983)