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Thermodynamic model formulation for viscoplastic solids as general equations for non-equilibrium reversible–irreversible coupling

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Abstract Thermodynamic models for viscoplastic solids are often formulated in the context of continuum thermodynamics and the dissipation principle. The purpose of the current work is to show that models for such material behavior can also be formulated in the form of a General Equation for Non-Equilibrium Reversible–Irreversible Coupling (GENERIC), see, e.g., Grmela and Öttinger (Phys Rev E, 56:6620–6632, 1997), Öttinger and Grmela (Phys Rev E, 56:6633–6655, 1997), Grmela (J Non-Newtonian Fluid Mech, 165:980–986, 2010). A GENERIC combines Hamiltonian-dynamics-based modeling of time-reversible processes with Onsager–Casimir-based modeling of time-irreversible processes. The result is a model for the approach of non-equilibrium systems to thermodynamic equilibrium. Originally developed to model complex fluids, it has recently been applied to anisotropic inelastic solids in Eulerian (Hütter and Tervoort, in J Non-Newtonian Fluid Mech, 152:45–52, 2008; Hütter and Tervoort, in J Non-Newtonian Fluid Mech, 152:53–65, 2008; Hütter and Tervoort, in Adv Appl Mech, 42:254–317, 2008) and Lagrangian (Hütter and Svendsen, in J Elast 104:357–368, 2011) settings, as well as to damage mechanics. For simplicity, attention is focused in the current work on the case of thermoelastic viscoplasticity. Central to this formulation is a GENERIC-based form for the viscoplastic flow rule. A detailed comparison with the formulation based on continuum thermodynamics and the dissipation principle is given.

Keywords GENERIC · Continuum thermodynamics · Viscoplastic solids

1 Introduction

Over the years, a number of approaches to the thermodynamic formulation of models for material behavior have been developed. Perhaps the most common of these in the modern era is that of continuum thermodynamics (e.g., [1]) as based on the Clausius–Duhem inequality and Coleman–Noll dissipation principle (e.g., [2,3]). Another is based on the entropy inequality of Müller–Liu (e.g., [4,5]), or on extended thermodynamics (e.g., [6]). Particularly challenging in this context is the formulation of constitutive relations for the behavior of history-dependent, and in particular inelastic, anisotropic solids. Besides the case of relaxation models in the context of extended linear irreversible thermodynamics (e.g., [7]), such models have generally been based on

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the concept of internal variables (e.g., [8]). This concept also lies at the heart of so-called generalized standard or standard dissipative materials [9,10]. The evolution-constitutive relations for such internal variables are often formulated with the help of inelastic potentials such as a dissipation potential [11–15].

From the point of view of irreversible thermodynamics, the goal here is to model the approach of non-equilibrium systems to thermodynamic equilibrium [16]. Perhaps the most prominent example of such models is offered by the Ginzburg–Landau equation as based on the free energy. More recently, an alternative approach has been developed in terms of the so-called General Equation for Non-Equilibrium Reversible–Irreversible Coupling (GENERIC), see e.g., [17–20], as based on the total energy and entropy. Originally developed for complex fluids, the GENERIC-based approach has recently been used [21,22] to formulate GENERIC-based models for anisotropic elastic and elastoplastic solids in a Eulerian setting. An alternative approach to the formulation of GENERIC-based models for inelastic solids was pursued in [23], who examined the case of thermoelastic solids with heat conduction and viscosity in a Lagrangian setting. Recently, a GENERIC-based formulation of models for inelastic materials (e.g., viscoelastic, elastoplastic) has been discussed in [24]. The purpose of the current work is to apply the approach of [23] to the formulation of a GENERIC-based model for thermoelastic, viscoplastic solids (which we understand to include heat conduction). In particular, this is based on a GENERIC-based form for the viscoplastic flow rule. For completeness, comparison is made with the formulation of models for thermoelastic viscoplasticity in the context of continuum thermodynamics (e.g., [1]). Similar to the continuum thermodynamic approach here is that of rational thermodynamics, which has also been compared to the GENERIC-based approach (e.g., [25]). The paper ends with a discussion.

Before we begin, a word on notation. For clarity and ease of understanding for continuum mechanicians and physicists alike, a number of results in this work will be expressed in both direct (i.e., symbolic) and (Cartesian) component notation. To this latter end, let lower latin indices $k, l, m, \dots = 1, 2, 3$, represent Cartesian components of spatial or Eulerian tensors, upper latin indices $K, L, M, \dots = 1, 2, 3$, represent Cartesian components of referential or Lagrangian tensors, and lower greek indices $\alpha, \beta, \gamma, \dots = 1, 2, 3$, represent Cartesian components of tensors in the intermediate local configuration. The summation convention on repeated such indices will be used throughout. Likewise, we use the notation $\nabla_L \varphi = \partial \varphi / \partial r_L$ for the components of the gradient of any field φ defined with respect to the reference configuration of the material in three-dimensional Euclidean space E^3 , i.e., functions of time $t \in \mathbb{R}^+$ and referential position $\mathbf{r} = r_K \mathbf{i}_K \in E^3$.

2 Form of the GENERIC used in this work

The GENERIC-based approach to models for non-equilibrium systems is by design universal in nature, i.e., applicable to all such systems. Hence, its general form is necessarily quite abstract and so adaptable. The purpose of this section is to establish the special form of the GENERIC to be used in the sequel.

Generally speaking, a GENERIC is formulated for closed systems without any interaction with its surrounding, neither thermally nor mechanically. In the case of solids, for example, the thermodynamic system in question is the material (body). Since the object of attention in this work is the material behavior of the system, the role of the environment is minimized for simplicity in that the formulation is restricted to supply-free processes, and any boundary effects are neglected. By moving the boundaries infinitely far away, their effect on the local behavior in the interior of the body can be neglected. As such, we approximate the reference configuration by E^3 for simplicity in what follows. Otherwise, as is common in solid mechanics for large deformation, all model relations to follow are represented in referential or Lagrangian form relative to the reference configuration.

Let A represent for example the total energy E or total entropy S of the system and its environment. In addition, let a be the density of A . As usual, A is a functional of the variables $\mathbf{x} = (\boldsymbol{\chi}, \dots)$ (e.g., deformation field $\boldsymbol{\chi}$) characterizing the system under consideration. Relevant to the current work is the class of models defined by the mathematical form

$$A(\mathbf{x}) = \int_{E^3} a(\mathbf{x}, \nabla \mathbf{x}) \, dv \quad (1)$$

of this functional in which a depends on both $\mathbf{x}$ and (one or more of) their spatial gradients $\nabla \mathbf{x}$. Since A is a functional of time-dependent fields $\mathbf{x}$,

$$\begin{aligned}
\dot{A} &= \int_{E^3} (\partial_{\mathbf{x}} a \cdot \dot{\mathbf{x}} + \partial_{\nabla \mathbf{x}} a \cdot \nabla \dot{\mathbf{x}}) dv \\
&= \int_{E^3} \delta_{\mathbf{x}} a \cdot \dot{\mathbf{x}} dv
\end{aligned} \tag{2}$$

follows for its time rate-of-change via the divergence theorem, where

$$\delta_{\mathbf{x}} a = \partial_{\mathbf{x}} a - \text{div } \partial_{\nabla \mathbf{x}} a \tag{3}$$

represents the first-order variational derivative of a .

In the field-theoretic context (see e.g., [19]), the GENERIC is in general formulated in terms of integro-differential operators and is spatially non-local in nature. Since attention is restricted in this work to local material behavior for simplicity, it suffices to work with a form of the GENERIC based on local (i.e., differential) operators. In addition, as implied by the case of thermoelasticity with heat conduction and viscosity [23], it is useful for the case of solids to work with a representation of the GENERIC in terms of the densities e and η , respectively, of the total energy E and total entropy S , respectively. On this basis, the form of the GENERIC utilized in this work is given by

$$\dot{\mathbf{x}} = \mathbf{L} \delta_{\mathbf{x}} e + \mathbf{M} \delta_{\mathbf{x}} \eta \tag{4}$$

in terms of the Poisson $\mathbf{L}$ and “friction” $\mathbf{M}$ operators. As with the case of the functional derivatives $\delta_{\mathbf{x}} e$ and $\delta_{\mathbf{x}} \eta$, which are given in the current context by (3), the specific forms of $\mathbf{L}$ and $\mathbf{M}$ are model-dependent.

The time-reversible part

$$\dot{\mathbf{x}}|_{\text{rev}} = \mathbf{L} \delta_{\mathbf{x}} e \tag{5}$$

of (4) represents the contribution of energy-conserving Hamiltonian dynamics to $\dot{\mathbf{x}}$. Embodying the symplecticity and time-reversal invariance of such dynamics, the Poisson operator $\mathbf{L}$ is required to be skew-symmetric

$$\mathbf{L}^T = -\mathbf{L}. \tag{6}$$

The corresponding Poisson bracket

$$\{A, B\} := \int_{E^3} \delta_{\mathbf{x}} a \cdot \mathbf{L} \delta_{\mathbf{x}} b dv \tag{7}$$

on all functionals A, B with densities a, b is then skew-symmetric, i.e.,

$$\{A, B\} = -\{B, A\}. \tag{8}$$

In addition, this bracket is required to satisfy the Jacobi identity

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0 \tag{9}$$

for all A, B, C .

The time-irreversible part

$$\dot{\mathbf{x}}|_{\text{irr}} = \mathbf{M} \delta_{\mathbf{x}} \eta \tag{10}$$

of (4) represents the contribution of relaxation and transport phenomena to $\dot{\mathbf{x}}$. To insure non-negative dissipation in any such process, $\mathbf{M}$ is required to be Onsager–Casimir symmetric

$$\mathbf{M}^T = \mathbf{M}. \tag{11}$$

The corresponding dissipation bracket

$$[A, B] := \int_{E^3} \delta_{\mathbf{x}} a \cdot \mathbf{M} \delta_{\mathbf{x}} b dv \tag{12}$$

induced by $\mathbf{M}$ on all A, B is then symmetric, i.e.,

$$[A, B] = [B, A]. \quad (13)$$

In addition, $\mathbf{M}$ is required to be non-negative definite, in which case

$$[A, A] \geq 0 \quad (14)$$

is non-negative for all A .

Lastly, $\mathbf{L}$ and $\mathbf{M}$ are required to satisfy the orthogonality conditions

$$\mathbf{L} \delta_{\mathbf{x}} \eta = \mathbf{0}, \quad \mathbf{M} \delta_{\mathbf{x}} e = \mathbf{0}, \quad (15)$$

implying

$$\{A, S\} = 0, \quad [A, E] = 0, \quad (16)$$

for all A . Together with the other properties of $\mathbf{L}$ and $\mathbf{M}$, these result in energy conservation

$$\dot{E} = \int_{E^3} \delta_{\mathbf{x}} e \cdot \dot{\mathbf{x}} \, dv = \int_{E^3} \delta_{\mathbf{x}} e \cdot \mathbf{L} \delta_{\mathbf{x}} e \, dv = \{E, E\} = 0 \quad (17)$$

as well as non-negative entropy production

$$\dot{S} = \int_{E^3} \delta_{\mathbf{x}} \eta \cdot \dot{\mathbf{x}} \, dv = \int_{E^3} \delta_{\mathbf{x}} \eta \cdot \mathbf{M} \delta_{\mathbf{x}} \eta \, dv = [S, S] \geq 0. \quad (18)$$

More generally, the evolution relation (2) of an arbitrary functional A becomes

$$\dot{A} = \{A, E\} + [A, S] \quad (19)$$

in terms of the brackets (7) and (12) as well as the total energy and entropy, which is closely related to the bracket formalism [26].

With this specialization of the general GENERIC in hand, we are now in a position to apply it to the case of thermoelastic viscoplasticity.

3 GENERIC for thermoelastic viscoplasticity

3.1 Choice of variables

For simplicity, attention is restricted here to single component, single phase systems. In this context, we work with the choice

$$\mathbf{x} = (\boldsymbol{\chi}, \mathbf{m}, \theta, \mathbf{F}_p). \quad (20)$$

Here, $\boldsymbol{\chi} = \chi_k \mathbf{i}_k$ represents the deformation field, $\mathbf{m}$ is the referential momentum density, θ is the absolute temperature, and $\mathbf{F}_p = F_{p\alpha K} \mathbf{i}_\alpha \otimes \mathbf{i}_K$ is the inelastic local deformation. This represents a direct generalization of the choice $\mathbf{x} = (\boldsymbol{\chi}, \mathbf{m}, \theta)$ made in [23] for the case of thermoelasticity with heat conduction and viscosity to the current case. Note that this choice is not unique. For example, Hütter and Tervoort [27] worked with $\mathbf{x} = (\mathbf{m}, \varepsilon, \mathbf{F}_E)$ in the spatial or Eulerian case in terms of the internal energy density ε and the local elastic deformation $\mathbf{F}_E = \mathbf{F} \mathbf{F}_p^{-1}$, with $\mathbf{F} = F_{kL} \mathbf{i}_k \otimes \mathbf{i}_L = \nabla \boldsymbol{\chi} = \nabla_L \chi_k \mathbf{i}_k \otimes \mathbf{i}_L$ the deformation gradient. Since $\mathbf{F}_E$ and $\mathbf{F}_p$ are related to each other by the deformation gradient, the formulation of a GENERIC based on the set (20) based on $\mathbf{F}_p$ can always be expressed with respect to the local elastic deformation $\mathbf{F}_E = F_{E k \alpha} \mathbf{i}_k \otimes \mathbf{i}_\alpha$ via $\dot{\mathbf{F}}_E \mathbf{F}_p = \dot{\mathbf{F}} - \mathbf{F}_E \dot{\mathbf{F}}_p$ as usual. In this sense, the choice to work with $\mathbf{F}_p$ is just a matter of convenience. Furthermore, the temperature θ is convenient from an engineering perspective, because it is an easily accessible thermodynamic state variable. Contrary, one could have chosen the internal energy density ε or the entropy

density η . However, in order to show the flexibility of the framework and to respect the freedom-of-choice of the modeler, we decide here specifically to use the temperature variable instead.

On the basis of (20), the forms

$$\begin{aligned} E(\mathbf{x}) &= \int_{E^3} e(\nabla \chi, \mathbf{m}, \theta, \mathbf{F}_p) \, dv \\ S(\mathbf{x}) &= \int_{E^3} \eta(\nabla \chi, \theta, \mathbf{F}_p) \, dv \end{aligned} \quad (21)$$

hold for the total energy E and total entropy S , respectively, in the case of thermoelastic viscoplasticity. Note that (21) are of the general form (1). Here,

$$e(\nabla \chi, \mathbf{m}, \theta, \mathbf{F}_p) = \varepsilon(\nabla \chi, \theta, \mathbf{F}_p) + \frac{1}{2\varrho} \mathbf{m} \cdot \mathbf{m} \quad (22)$$

represents the total energy density, with ϱ the (constant) referential mass density, and

$$\begin{aligned} \varepsilon &= \varepsilon(\nabla \chi, \theta, \mathbf{F}_p) \\ \eta &= \eta(\nabla \chi, \theta, \mathbf{F}_p) \end{aligned} \quad (23)$$

are the internal energy density and entropy density, respectively. In the context of (3), (22) and (23) yield the “components”¹

$$\begin{aligned} \delta_{\chi} e &= -\operatorname{div} \left(\partial_{\nabla \chi} \varepsilon \right), & \delta_{\chi_k} e &= -\nabla_L \left(\partial_{\nabla_L \chi_k} \varepsilon \right), \\ \delta_{\mathbf{m}} e &= \dot{\chi}, & \delta_{m_k} e &= \dot{\chi}_k \\ \delta_{\theta} e &= \partial_{\theta} \varepsilon, \\ \delta_{\mathbf{F}_p} e &= \partial_{\mathbf{F}_p} \varepsilon, & \delta_{F_{p\alpha K}} e &= \partial_{F_{p\alpha K}} \varepsilon, \end{aligned} \quad (24)$$

of $\delta_{\mathbf{x}} e$, with $\dot{\chi} = \dot{\chi}_k \mathbf{i}_k$ the material velocity, as well as those

$$\begin{aligned} \delta_{\chi} \eta &= -\operatorname{div} \left(\partial_{\nabla \chi} \eta \right), & \delta_{\chi_k} \eta &= -\nabla_L \left(\partial_{\nabla_L \chi_k} \eta \right), \\ \delta_{\mathbf{m}} \eta &= \mathbf{0}, & \delta_{m_k} \eta &= 0, \\ \delta_{\theta} \eta &= \partial_{\theta} \eta, \\ \delta_{\mathbf{F}_p} \eta &= \partial_{\mathbf{F}_p} \eta, & \delta_{F_{p\alpha K}} \eta &= \partial_{F_{p\alpha K}} \eta, \end{aligned} \quad (25)$$

of $\delta_{\mathbf{x}} \eta$, for the current case of thermoelastic viscoplasticity. For more details on the general issue of GENERIC-based functional derivatives, the reader is referred to [17], [18], or [19]. With the forms of $\delta_{\mathbf{x}} e$ and $\delta_{\mathbf{x}} \eta$ now determined for the current constitutive class, the next task is the formulation of $\mathbf{L}$ and $\mathbf{M}$.

3.2 Poisson operator and reversible part

The current GENERIC-based formulation of thermoelastic viscoplasticity is based in particular on the modeling of the evolution of both χ and $\mathbf{m}$ as purely symplectic or Hamiltonian and so time-reversible. On the other hand, the evolution of $\mathbf{F}_p$ is modeled as purely irreversible, and hence the $\mathbf{F}_p$ -related elements in the Poisson operator are set to zero. With the choice of variables (20), then, the reversible part (5) of the GENERIC (4) takes the form

$$\dot{\mathbf{x}}|_{\text{rev}} = \mathbf{L} \delta_{\mathbf{x}} e = \begin{bmatrix} \mathbf{0} & \mathbf{L}_{\chi \mathbf{m}} & \mathbf{L}_{\chi \theta} & \mathbf{0} \\ \mathbf{L}_{\mathbf{m} \chi} & \mathbf{0} & \mathbf{L}_{\mathbf{m} \theta} & \mathbf{0} \\ \mathbf{L}_{\theta \chi} & \mathbf{L}_{\theta \mathbf{m}} & \mathbf{L}_{\theta \theta} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \delta_{\chi} e \\ \delta_{\mathbf{m}} e \\ \delta_{\theta} e \\ \delta_{\mathbf{F}_p} e \end{bmatrix}. \quad (26)$$

¹ The second of these follows from $\dot{\chi} = \mathbf{m}/\varrho$.

The upper 2×2 suboperator in $\mathbf{L}$ determined by $\mathbf{L}_{\chi m}$ and $\mathbf{L}_{m\chi}$ represents the symplectic part of $\mathbf{L}$ for the evolution of χ and m . Given the skew-symmetry of $\mathbf{L}$ in the form (8), the suboperators $\mathbf{L}_{\chi m}$, $\mathbf{L}_{\chi\theta}$, $\mathbf{L}_{m\chi}$, $\mathbf{L}_{m\theta}$, $\mathbf{L}_{\theta\chi}$, $\mathbf{L}_{\theta m}$, and $\mathbf{L}_{\theta\theta}$ satisfy the skew-symmetry relations

$$\begin{aligned} \int_{E^3} \delta_{m_k} a L_{m_k \chi_l} \delta_{\chi_l} b \, dv &= - \int_{E^3} \delta_{\chi_k} b L_{\chi_k m_l} \delta_{m_l} a \, dv \\ \int_{E^3} \delta_{\theta} a L_{\theta m_k} \delta_{m_k} b \, dv &= - \int_{E^3} \delta_{m_k} b L_{m_k \theta} \delta_{\theta} a \, dv \\ \int_{E^3} \delta_{\theta} a L_{\theta \chi_k} \delta_{\chi_k} b \, dv &= - \int_{E^3} \delta_{\chi_k} b L_{\chi_k \theta} \delta_{\theta} a \, dv \\ \int_{E^3} \delta_{\theta} a L_{\theta \theta} \delta_{\theta} b \, dv &= - \int_{E^3} \delta_{\theta} b L_{\theta \theta} \delta_{\theta} a \, dv \end{aligned} \quad (27)$$

in component form for all densities a, b . Together with the corresponding component forms

$$\begin{aligned} L_{\chi_k \theta} \delta_{\theta} \eta &= 0 \\ L_{m_k \theta} \delta_{\theta} \eta &= -L_{m_k \chi_l} \delta_{\chi_l} \eta \\ L_{\theta \chi_k} \delta_{\chi_k} \eta &= -L_{\theta \theta} \delta_{\theta} \eta \end{aligned} \quad (28)$$

of the orthogonality condition (15)₁ via (25)₂ for the current case, these ensure energy conservation (17).

Since $\delta_{\theta} \eta$ as given by (25)₃ is generally non-zero, (28)₁ requires $L_{\chi_k \theta}$ to vanish². Since (27) is required to hold for all densities a and b , $\delta_{\theta} a$ and $\delta_{\chi_k} b$ are generally non-zero, (27)₃ and continuity of the integrand then requires $L_{\theta \chi_k}$ to vanish as well. In turn, $L_{\theta \theta}$ then vanishes via (28)₃. Alternatively, again since $\delta_{\theta} a$ and $\delta_{\theta} b$ are generally non-zero, (27)₄ and continuity of the integrand requires $L_{\theta \theta}$ to vanish directly. On this basis,

$$\dot{\chi}_k = L_{\chi_k m_l} \delta_{m_l} e = L_{\chi_k m_l} \dot{\chi}_l \quad (29)$$

is obtained from (24)₂, implying

$$L_{\chi_k m_l} = \delta_{kl}, \quad L_{m_k \chi_l} = -\delta_{kl}, \quad (30)$$

the latter following from the former via (27)₁. Substitution of the latter of these into (28)₂ and use of the relation

$$\theta = \partial_{\theta} \varepsilon / \partial_{\theta} \eta \quad (31)$$

for the absolute temperature yields the component form

$$L_{m_k \theta} = -\nabla_L \circ \left(\partial_{\nabla_L \chi_k} \eta \right) (\partial_{\theta} \eta)^{-1} \quad (32)$$

of the suboperator $\mathbf{L}_{m\theta}$ via (25)_{1,3}. The operator notation is defined here as

$$L_{m_k \theta} h = \left\{ -\nabla_L \circ \left(\partial_{\nabla_L \chi_k} \eta \right) (\partial_{\theta} \eta)^{-1} \right\} h := -\nabla_L \left\{ \left(\partial_{\nabla_L \chi_k} \eta \right) (\partial_{\theta} \eta)^{-1} h \right\} \quad (33)$$

on any function h . From this follow in particular

$$L_{m_k \theta} \delta_{\theta} \eta = -\nabla_L \left(\partial_{\nabla_L \chi_k} \eta \right), \quad L_{m_k \theta} \delta_{\theta} e = -\nabla_L \left(\theta \partial_{\nabla_L \chi_k} \eta \right) \quad (34)$$

² Mathematically speaking, terms proportional to $\nabla \circ (\delta_{\theta} \eta)^{-1}$ in $L_{\chi \theta}$ also satisfy (28)₁. Based on (26), however, $\dot{\chi}$ would then contain the term $\nabla \circ (\delta_{\theta} \eta)^{-1} (\delta_{\theta} e) = \nabla \theta$, which is clearly unphysical. An analogous argument holds for $L_{\theta \theta}$.

via (31). Given (32), (27)₂ reduces to

$$\begin{aligned}
 & \int_{E^3} \delta_\theta a \, L_{\theta m_k} \delta_{m_k} b \, dv \\
 &= - \int_{E^3} \delta_{m_k} b \, L_{m_k \theta} \delta_\theta a \, dv \\
 &= \int_{E^3} \left\{ \nabla_L \left\{ \delta_{m_k} b \left(\partial_{\nabla_L \chi_k} \eta \right) (\partial_\theta \eta)^{-1} \delta_\theta a \right\} - \delta_\theta a (\partial_\theta \eta)^{-1} \left(\partial_{\nabla_L \chi_k} \eta \right) \nabla_L \delta_{m_k} b \right\} dv \\
 &= - \int_{E^3} \delta_\theta a \left\{ (\partial_\theta \eta)^{-1} (\partial_{\nabla_L \chi_k} \eta) \circ \nabla_L \right\} \delta_{m_k} b \, dv
 \end{aligned} \tag{35}$$

since boundary terms and effects are being ignored in this work. Or expressed mathematically, this follows from the fact that E^3 has no boundary. Consequently,

$$L_{\theta m_k} = - (\partial_\theta \eta)^{-1} \left(\partial_{\nabla_L \chi_k} \eta \right) \circ \nabla_L \tag{36}$$

then follows for the component form of $\mathbf{L}_{\theta m}$.

To summarize, the results

$$\begin{aligned}
 L_{\chi_k m_l} &= \delta_{kl}, & L_{m_k \chi_l} &= -\delta_{kl}, \\
 L_{\chi_k \theta} &= 0, & L_{\theta \chi_k} &= 0, \\
 L_{m_k \theta} &= -\nabla_L \circ \left(\partial_{\nabla_L \chi_k} \eta \right) (\partial_\theta \eta)^{-1}, & L_{\theta m_k} &= -(\partial_\theta \eta)^{-1} \left(\partial_{\nabla_L \chi_k} \eta \right) \circ \nabla_L, \\
 L_{\theta \theta} &= 0,
 \end{aligned} \tag{37}$$

have been derived for the components of the Poisson operator $\mathbf{L}$ in (26) for the current model of thermoelastic viscoplasticity. The components (37) lead to the relation

$$\begin{aligned}
 \{A, B\} &= \int_{E^3} (\delta_\chi a \cdot \delta_m b - \delta_m a \cdot \delta_\chi b) \, dv \\
 &\quad + \int_{E^3} \frac{\partial_{\nabla \chi} \eta}{\partial_\theta \eta} \cdot \{(\nabla \delta_m a) \delta_\theta b - \delta_\theta a (\nabla \delta_m b)\} \, dv
 \end{aligned} \tag{38}$$

for the Poisson bracket (7) of the current model, again via neglect of boundary terms.

While the skew-symmetry (8) and the orthogonality condition (16)₁ are manifest in (38), the Jacobi identity (9) still needs to be verified. There are several procedures for checking the Jacobi identity (9), apart from tedious brute-force manual calculation. On the one hand, one can use a computer program that has been designed specifically for checking the Jacobi identity for field-theoretic models [28]. On the other hand, one can make use of the fact that the Jacobi identity is invariant with respect to a (invertible) transformation of variables from $\mathbf{x}$ to $\mathbf{x}'$ (see [19] for details). Choosing $\mathbf{x}' = (\chi, \mathbf{m}, \eta, \mathbf{F}_p)$ for the present case, the transformed Poisson operator assumes a simple form independent of $\mathbf{x}'$, for which case the Jacobi identity is automatically satisfied.

With all properties of the Poisson operator for the current model now in hand, substitution of (37) into (26) yields the forms

$$\begin{aligned}
 \dot{\chi}_k|_{\text{rev}} &= L_{\chi_k m_l} \delta_{m_l} e = m_k / \varrho, \\
 \dot{m}_k|_{\text{rev}} &= L_{m_k \chi_l} \delta_{\chi_l} e + L_{m_k \theta} \delta_\theta e = \nabla_L (\partial_{\nabla_L \chi_k} \varepsilon - \theta \partial_{\nabla_L \chi_k} \eta), \\
 \dot{\theta}|_{\text{rev}} &= L_{\theta m_k} \delta_{m_k} e = -c^{-1} \theta (\partial_{\nabla_L \chi_k} \eta) \nabla_L \dot{\chi}_k, \\
 \dot{F}_{p \alpha K}|_{\text{rev}} &= 0,
 \end{aligned} \tag{39}$$

for the components of the reversible part (5) of the GENERIC (4) in the current model. This completes the formulation of the time-reversible part of the model, i.e., of non-linear elasticity, the Hamiltonian structure of which has been examined earlier from different perspective [29]. Except for heat conduction, the reversible part of the GENERIC embodies the thermoelastic behavior. Indeed, heat conduction and viscoplasticity are modeled via the friction operator $\mathbf{M}$ and the irreversible part (10) of the GENERIC (4), to which we now turn.

3.3 Friction operator and irreversible part

Recall that the current formulation is based on the modeling of the evolution of χ and m as purely reversible. Consequently, the choice of variables (20) implies that the irreversible part (10) of the GENERIC (4) is given by

$$\dot{\mathbf{x}}|_{\text{irr}} = \mathbf{M} \delta_{\mathbf{x}} \eta = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{M}_{\theta\theta} & \mathbf{M}_{\theta F_P} \\ \mathbf{0} & \mathbf{0} & \mathbf{M}_{F_P\theta} & \mathbf{M}_{F_P F_P} \end{bmatrix} \begin{bmatrix} \delta_{\chi} \eta \\ \delta_m \eta \\ \delta_{\theta} \eta \\ \delta_{F_P} \eta \end{bmatrix}. \quad (40)$$

In this case, the symmetry condition (13) reduces to

$$\begin{aligned} \int_{E^3} \delta_{\theta} a \, M_{\theta\theta} \, \delta_{\theta} b \, dv &= \int_{E^3} \delta_{\theta} b \, M_{\theta\theta} \, \delta_{\theta} a \, dv \\ \int_{E^3} \delta_{\theta} a \, M_{\theta F_P \alpha K} \, \delta_{F_P \alpha K} b \, dv &= \int_{E^3} \delta_{F_P \alpha K} b \, M_{F_P \alpha K \theta} \, \delta_{\theta} a \, dv, \\ \int_{E^3} \delta_{F_P \alpha K} a \, M_{F_P \alpha K F_P \beta L} \, \delta_{F_P \beta L} b \, dv &= \int_{E^3} \delta_{F_P \alpha K} b \, M_{F_P \alpha K F_P \beta L} \, \delta_{F_P \beta L} a \, dv, \end{aligned} \quad (41)$$

in component form for all densities a, b . To these we add the relations

$$\begin{aligned} M_{\theta\theta} \, \delta_{\theta} e &= -M_{\theta F_P \alpha K} \, \delta_{F_P \alpha K} e \\ M_{F_P \alpha K \theta} \, \delta_{\theta} e &= -M_{F_P \alpha K F_P \beta L} \, \delta_{F_P \beta L} e \end{aligned} \quad (42)$$

between the suboperators of $\mathbf{M}$ from the orthogonality condition (15)₂. The dissipation bracket (12) then reduces to

$$\begin{aligned} [A, B] &= \int_{E^3} \{ \delta_{\theta} a \, M_{\theta\theta} \, \delta_{\theta} b + \delta_{F_P \alpha K} a \, M_{F_P \alpha K F_P \beta L} \, \delta_{F_P \beta L} b \} \, dv \\ &\quad + \int_{E^3} \{ \delta_{\theta} a \, M_{\theta F_P \alpha K} \, \delta_{F_P \alpha K} b + \delta_{F_P \alpha K} a \, M_{F_P \alpha K \theta} \, \delta_{\theta} b \} \, dv \end{aligned} \quad (43)$$

in components for the current model. In particular, this yields directly the model form of the non-negativity condition (14).

For simplicity, the temperature gradient $\nabla\theta$ is assumed to influence only the evolution of the temperature θ through heat conduction, while it does not drive plastic flow and hence does not affect the inelastic local deformation F_P . On the other hand, inelastic flow is assumed to affect that of both θ and F_P , the former through the conservation of the total energy. In this case, the thermal suboperator

$$M_{\theta\theta} = M_{P\theta\theta} + M_{C\theta\theta} \quad (44)$$

splits into inelastic $M_{P\theta\theta}$ and conductive $M_{C\theta\theta}$ parts. The latter is given by

$$M_{C\theta\theta} = -c^{-1} \nabla_M \circ \theta^2 K_{MN} \nabla_N \circ c^{-1} \quad (45)$$

(see e.g., [23]) in terms of the heat capacity

$$c = \partial_\theta \varepsilon = \theta \partial_\theta \eta \quad (46)$$

at constant deformation and the thermal conductivity $\mathbf{K} = K_{MN} \mathbf{i}_M \otimes \mathbf{i}_N$, with

$$\begin{aligned} M_{C\theta\theta} h &= \{-c^{-1} \nabla_M \circ \theta^2 K_{MN} \nabla_N \circ c^{-1}\} h \\ &:= -c^{-1} \nabla_M \{\theta^2 K_{MN} \nabla_N (c^{-1} h)\} \end{aligned} \quad (47)$$

for all functions h . A necessary condition for $\mathbf{M}$ to be (Onsager–Casimir) symmetric and non-negative definite is for $\mathbf{K}$ to have these properties, i.e.,

$$\mathbf{K}^T = \mathbf{K}, \quad K_{NM} = K_{MN}, \quad (48)$$

and

$$\mathbf{g} \cdot \mathbf{K} \mathbf{g} = g_M K_{MN} g_N \geq 0 \quad (49)$$

for all vectors $\mathbf{g} = g_K \mathbf{i}_K$, respectively. On this basis, one can define the heat conduction bracket

$$\begin{aligned} [A, B]_C &:= \int_{E^3} \delta_\theta a \, M_{C\theta\theta} \, \delta_\theta b \, dv \\ &= - \int_{E^3} \delta_\theta a \, \{c^{-1} \nabla_M \circ \theta^2 K_{MN} \nabla_N \circ c^{-1}\} \, \delta_\theta b \, dv \\ &= \int_{E^3} \nabla_M (c^{-1} \delta_\theta a) \, \theta^2 K_{MN} \nabla_N (c^{-1} \delta_\theta b) \, dv \end{aligned} \quad (50)$$

where the second form follows via partial integration and neglect of boundary terms. Given then symmetry (48) and non-negative definiteness (49) of $\mathbf{K}$, the corresponding properties $[A, B]_C = [B, A]_C$ and $[A, A]_C \geq 0$, respectively, hold for the bracket.

Turning next to viscoplasticity, the current GENERIC-based model for this takes the constitutive form

$$\mathbf{M}_{F_P F_P} = \theta \mathbf{N}, \quad M_{F_P \alpha K F_P \beta L} = \theta N_{\alpha K \beta L}, \quad (51)$$

in terms of the fourth-order inelastic flow tensor $\mathbf{N}$. As with the case of the thermal conductivity tensor, $\mathbf{N}$ is modeled as symmetric and non-negative definite in order for $\mathbf{M}$ to have these properties, as shown further below. In this case,

$$\mathbf{N}^T = \mathbf{N}, \quad N_{\beta L \alpha K} = N_{\alpha K \beta L}, \quad (52)$$

and

$$\boldsymbol{\Sigma} \cdot \mathbf{N} \boldsymbol{\Sigma} = \Sigma_{\alpha K} N_{\alpha K \beta L} \Sigma_{\beta L} \geq 0 \quad (53)$$

hold, the latter for all second-order tensors $\boldsymbol{\Sigma} = \Sigma_{\alpha K} \mathbf{i}_\alpha \otimes \mathbf{i}_K$. This is formally analogous to the case of the viscosity tensor in a GENERIC-based formulation of a model for thermoelastic solids with heat conduction and viscosity (see e.g., [23]). On this basis, the symmetry condition (41)₃ is satisfied identically. Further, the constitutive relation (51) and the orthogonality condition (42)₂ imply

$$M_{F_P \alpha K \theta} = -\theta N_{\alpha K \beta L} (\partial_{F_P \beta L} \varepsilon) c^{-1} \quad (54)$$

via (46). Substituting this into the symmetry condition (41)₂, we obtain

$$\begin{aligned} \int_{E^3} \delta_\theta a \, M_{\theta F_{\alpha K}} \delta_{F_{\alpha K}} b \, dv &= - \int_{E^3} \delta_{F_{\alpha K}} b \, \theta N_{\alpha K \beta L} (\partial_{F_{\beta L}} \varepsilon) c^{-1} \delta_\theta a \, dv \\ &= - \int_{E^3} \delta_\theta a \, c^{-1} (\partial_{F_{\beta L}} \varepsilon) \theta N_{\beta L \alpha K} \delta_{F_{\alpha K}} b \, dv \end{aligned} \quad (55)$$

via the symmetry of N , and so

$$M_{\theta F_{\alpha K}} = -c^{-1} (\partial_{F_{\beta L}} \varepsilon) \theta N_{\beta L \alpha K}. \quad (56)$$

Combining this with the orthogonality condition (42)₁,

$$M_{P\theta\theta} = c^{-1} (\partial_{F_{\alpha K}} \varepsilon) \theta N_{\alpha K \beta L} (\partial_{F_{\beta L}} \varepsilon) c^{-1} \quad (57)$$

follows for the inelastic flow part $M_{P\theta\theta}$ of $M_{\theta\theta}$ from (44) since $M_{C\theta\theta}$ from (45) annihilates $\delta_\theta e$ via (46).

In summary, then, we have the non-zero components

$$\begin{aligned} M_{\theta\theta} &= c^{-1} \left\{ (\partial_{F_{\alpha K}} \varepsilon) \theta N_{\alpha K \beta L} (\partial_{F_{\beta L}} \varepsilon) - \nabla_M \circ \theta^2 K_{MN} \nabla_N \circ \right\} c^{-1} \\ M_{\theta F_{\alpha K}} &= -c^{-1} (\partial_{F_{\beta L}} \varepsilon) \theta N_{\beta L \alpha K} \\ M_{F_{\alpha K} \theta} &= -\theta N_{\alpha K \beta L} (\partial_{F_{\beta L}} \varepsilon) c^{-1} \\ M_{F_{\alpha K} F_{\beta L}} &= \theta N_{\alpha K \beta L} \end{aligned} \quad (58)$$

of $\mathbf{M}$ in the current model for thermoelastic viscoplasticity from (45), (54), (56), and (57). In turn, (43) and (58) yield the reduced form

$$\begin{aligned} [A, B] &= \int_{E^3} \nabla \left(\frac{\delta_\theta a}{\partial_\theta \varepsilon} \right) \cdot \theta^2 \mathbf{K} \nabla \left(\frac{\delta_\theta b}{\partial_\theta \varepsilon} \right) \\ &\quad + \int_{E^3} \left(\frac{\delta_\theta a}{\partial_\theta \varepsilon} \partial_{F_P} \varepsilon - \delta_{F_P} a \right) \cdot \theta N \left(\frac{\delta_\theta b}{\partial_\theta \varepsilon} \partial_{F_P} \varepsilon - \delta_{F_P} b \right) \end{aligned} \quad (59)$$

of (43) for the dissipation bracket of the current model via (46). Again due to the symmetry and non-negative definiteness of N and $\mathbf{K}$ together with the fact that $\theta \geq 0$, this bracket is also symmetric and non-negative definite, i.e., $[A, B] = [B, A]$ and $[A, A] \geq 0$. The orthogonality condition (16)₂ is also manifest in (59), i.e., $[A, E] = 0$ for all A . Lastly, with all properties of the friction operator $\mathbf{M}$ required by the GENERIC now in hand, (58) yield the components relations

$$\begin{aligned} \dot{\chi}_k|_{\text{irr}} &= 0 \\ \dot{m}_k|_{\text{irr}} &= 0 \\ \dot{\theta}|_{\text{irr}} &= M_{\theta\theta} \delta_\theta \eta + M_{\theta F_{\alpha K}} \delta_{F_{\alpha K}} \eta \\ &= c^{-1} (\partial_{F_{\alpha K}} \varepsilon) N_{\alpha K \beta L} (\partial_{F_{\beta L}} \varepsilon - \theta \partial_{F_{\beta L}} \eta) \\ &\quad + c^{-1} \nabla_M (K_{MN} \nabla_N \theta) \\ \dot{F}_{P\alpha K}|_{\text{irr}} &= M_{F_{\alpha K} \theta} \delta_\theta \eta + M_{F_{\alpha K} F_{\beta L}} \delta_{F_{\beta L}} \eta \\ &= -N_{\alpha K \beta L} (\partial_{F_{\beta L}} \varepsilon - \theta \partial_{F_{\beta L}} \eta) \end{aligned} \quad (60)$$

for the irreversible part (10) of the GENERIC (4) in the current model.

3.4 Summary of complete model

Combining the reversible (39) and irreversible (60) parts of the GENERIC results then in the complete system

$$\begin{aligned}
 \dot{\chi} &= \partial_m e \\
 \dot{m} &= \operatorname{div} \left(\partial_{\nabla \chi} \varepsilon - \theta \partial_{\nabla \chi} \eta \right) \\
 \dot{\theta} &= -c^{-1} \theta \left(\partial_{\nabla \chi} \eta \right) \cdot \nabla \dot{\chi} \\
 &\quad + c^{-1} \left(\partial_{F_p} \varepsilon \right) \cdot N \left(\partial_{F_p} \varepsilon - \theta \partial_{F_p} \eta \right) + c^{-1} \operatorname{div} \left(\mathbf{K} \nabla \theta \right) \\
 \dot{F}_p &= -N \left(\partial_{F_p} \varepsilon - \theta \partial_{F_p} \eta \right)
 \end{aligned} \tag{61}$$

in symbolic form for the current model. Or in more familiar terms,

$$\begin{aligned}
 \dot{\chi} &= \mathbf{m} / \varrho \\
 \dot{m} &= \operatorname{div} \mathbf{P} \\
 c \dot{\theta} &= \mathbf{P}_\eta \cdot \nabla \dot{\chi} - \partial_{F_p} \varepsilon \cdot N \Sigma - \operatorname{div} \mathbf{q} \\
 \dot{F}_p &= N \Sigma.
 \end{aligned} \tag{62}$$

Here,

$$\begin{aligned}
 \mathbf{P} &= \partial_{\nabla \chi} \varepsilon - \theta \partial_{\nabla \chi} \eta \\
 \mathbf{P}_\eta &= -\theta \partial_{\nabla \chi} \eta \\
 \Sigma &= -\partial_{F_p} \varepsilon + \theta \partial_{F_p} \eta \\
 \mathbf{q} &= -\mathbf{K} \nabla \theta
 \end{aligned} \tag{63}$$

represent the first Piola-Kirchhoff stress $\mathbf{P} = P_{kL} \mathbf{i}_k \otimes \mathbf{i}_L$, its entropic part $\mathbf{P}_\eta$, the stress-like quantity conjugate to F_p , $\Sigma = \Sigma_{\alpha K} \mathbf{i}_\alpha \otimes \mathbf{i}_K$, and the referential heat flux $\mathbf{q} = q_L \mathbf{i}_L$, respectively. The stress-like quantity Σ also determines the model relation

$$\dot{S} = [S, S] = \int_{E^3} \left\{ \theta^{-2} (\nabla \theta) \cdot \mathbf{K} (\nabla \theta) + \theta^{-1} \Sigma \cdot N \Sigma \right\} dv \geq 0 \tag{64}$$

for the entropy production-rate obtained from (59) via (31).

Although the densities of internal energy and entropy are the principle thermodynamic potentials in the context of the GENERIC, it is interesting to see that the free-energy-like combination $\varepsilon - \theta \eta$ appears in both the reversible (39) and irreversible (60) parts of the GENERIC (see also [24]), as well as in the entropy production-rate (64). This is a result of the orthogonality conditions (15). Indeed, (15)₁ induces for example the dependence of $\mathbf{L}$ on η in (37), and so that of $\dot{\chi}|_{\text{rev}}$ on $\varepsilon - \theta \eta$ in (39). Likewise, (15)₂ induces the dependence of $\mathbf{M}$ on ε in (58), and so that of $\dot{\chi}|_{\text{irr}}$ on $\varepsilon - \theta \eta$ in (60). Besides by ε in this fashion, $\mathbf{M}$ is determined constitutively by the thermal conductivity $\mathbf{K}$ and the inelastic flow N . Consequently, the GENERIC (61) for thermoelastic viscoplasticity is constitutively complete once the particular model forms of ε , η , $\mathbf{K}$, and N have been specified.

Like ε and η from (23), note that $\mathbf{K}$ and N may depend constitutively on $\nabla \chi$, θ , and F_p . In addition, $\mathbf{K}$ and N may depend in general on the thermodynamic forces $\nabla \theta$ and Σ , i.e., in any fashion preserving their symmetry and non-negative definiteness. To examine this in more detail, consider the simplest possible case relevant to “standard” viscoplasticity. In this case, $\mathbf{K}$ is assumed independent of $\nabla \theta$ and Σ , and N is assumed independent of $\nabla \theta$. Then, $N(\dots, \Sigma)$ depends in particular on Σ . Next, on the basis of (63)₃, note that Σ represents in particular a (linear) function of $\delta_{F_p} \eta$, i.e., $\Sigma(\dots, \delta_{F_p} \eta)$. Consequently, a dependence of N on Σ induces one of $\mathbf{M}$ on $\delta_{F_p} \eta$ via (58), i.e.,

$$\begin{aligned}
M_{\theta\theta}(\dots, \delta_{F_P} \eta) &= \frac{\partial_{F_P} \varepsilon}{\partial_\theta \varepsilon} \cdot \theta N(\dots, \Sigma(\dots, \delta_{F_P} \eta)) \frac{\partial_{F_P} \varepsilon}{\partial_\theta \varepsilon} + M_{C\theta\theta}(\dots) \\
\mathbf{M}_{\theta F_P}(\dots, \delta_{F_P} \eta) &= -\theta N^T(\dots, \Sigma(\dots, \delta_{F_P} \eta)) \frac{\partial_{F_P} \varepsilon}{\partial_\theta \varepsilon} \\
\mathbf{M}_{F_P \theta}(\dots, \delta_{F_P} \eta) &= -\theta N(\dots, \Sigma(\dots, \delta_{F_P} \eta)) \frac{\partial_{F_P} \varepsilon}{\partial_\theta \varepsilon} \\
\mathbf{M}_{F_P F_P}(\dots, \delta_{F_P} \eta) &= \theta N(\dots, \Sigma(\dots, \delta_{F_P} \eta))
\end{aligned} \tag{65}$$

via (46). In turn,

$$\begin{aligned}
\dot{\theta}|_{\text{irr}}(\dots, \delta_\theta \eta, \delta_{F_P} \eta) &= M_{\theta\theta}(\dots, \delta_{F_P} \eta) \delta_\theta \eta + \mathbf{M}_{\theta F_P}(\dots, \delta_{F_P} \eta) \delta_{F_P} \eta \\
\dot{F}_P(\dots, \delta_\theta \eta, \delta_{F_P} \eta) &= \mathbf{M}_{F_P \theta}(\dots, \delta_{F_P} \eta) \delta_\theta \eta + \mathbf{M}_{F_P F_P}(\dots, \delta_{F_P} \eta) \delta_{F_P} \eta
\end{aligned} \tag{66}$$

then follow for (60)_{3,4} linear in $\delta_\theta \eta$ and quasi-linear in $\delta_{F_P} \eta$. So, in this case, the irreversible part (10) of the GENERIC is in fact quasi-linear in $\delta_{\mathbf{x}} \eta$, i.e.,

$$\dot{\mathbf{x}}|_{\text{irr}}(\dots, \delta_{\mathbf{x}} \eta) = \mathbf{M}(\dots, \delta_{\mathbf{x}} \eta) \delta_{\mathbf{x}} \eta. \tag{67}$$

Among other things, this has ramifications for the question of whether or not there exists a potential representation for $\mathbf{M}$, something that is apparently simply assumed “axiomatically” in some formulations (e.g., [20,24,30]) of the GENERIC. We come back to this issue below.

4 Continuum thermodynamic formulation and comparison

For comparison with the results from the previous section, and for completeness, the formulation of thermoelastic viscoplasticity in the context of continuum thermodynamics [1] is briefly summarized in this section. To this end, as done for the GENERIC-based formulation in the previous section, attention is restricted for simplicity here to supply-free processes. In this case, we have the standard referential forms

$$\begin{aligned}
\dot{\mathbf{m}} &= \text{div } \mathbf{P} \\
\dot{\varepsilon} &= \mathbf{P} \cdot \nabla \dot{\chi} - \text{div } \mathbf{q}
\end{aligned} \tag{68}$$

for the balances of linear momentum and (internal) energy, respectively. In addition to (68), the Clausius–Duhem form

$$\theta \dot{\eta} = \delta + \mathbf{q} / \theta \cdot \nabla \theta - \text{div } \mathbf{q} \tag{69}$$

of the referential entropy balance is also relevant. From the constitutive point of view, this basically represents the definition of the referential dissipation-rate density δ lying at the heart of the (local form of the) dissipation principle. As usual (see, e.g., [1], Ch. 9), this requires $\delta \geq 0$ for all thermodynamically-admissible processes.

The thermoelastic part of the model is based on the dynamic free energy density

$$f(\theta, \nabla \chi, F_P, \mathbf{m}) = \psi(\theta, \nabla \chi, F_P) + \frac{1}{2Q} \mathbf{m} \cdot \mathbf{m} \tag{70}$$

analogous to (22). Its “static” part $\psi(\theta, \nabla \chi, F_P)$ determines as usual the thermoelastic relations

$$-\eta = \partial_\theta \psi, \quad \varepsilon = \psi - \theta \partial_\theta \psi, \quad c = -\theta \partial_\theta \partial_\theta \psi, \quad \mathbf{P} = \partial_{\nabla \chi} \psi \tag{71}$$

for the entropy density, internal energy density, heat capacity at constant deformation, and first Piola-Kirchhoff stress, respectively. These result in the residual form

$$\delta = -\partial_{F_P} \psi \cdot \dot{F}_P - \mathbf{q} / \theta \cdot \nabla \theta \tag{72}$$

for the dissipation-rate density δ from (69).

In the GENERIC-based formulation above, the processes of heat conduction and inelastic flow are accounted for via the transport-theory-based constitutive relations (45) and (51), respectively. In the continuum thermodynamic context as manifest in particular by the form (72) of the residual dissipation-rate density, we have the analogous forms

$$\begin{aligned}\mathbf{q} &= -\mathbf{K} \nabla \theta \\ \dot{\mathbf{F}}_P &= -N \partial_{\mathbf{F}_P} \psi\end{aligned}\quad (73)$$

for the heat flux and the viscoplastic flow rule, respectively. From these follow for example the non-negative form

$$\delta = \partial_{\mathbf{F}_P} \psi \cdot N \partial_{\mathbf{F}_P} \psi + \theta^{-1} (\nabla \theta) \cdot \mathbf{K} (\nabla \theta) \quad (74)$$

for the dissipation-rate density analogous to entropy production-rate density in (64) in the context of the GENERIC. On this basis, the dissipation-rate density δ will be non-trivially non-negative when N and $\mathbf{K}$ are symmetric and non-negative definite. Combination then of (71)_{1,4} with (68) and (73) results in the system

$$\begin{aligned}\dot{\chi} &= \partial_m f \\ \dot{\mathbf{m}} &= \text{div } \partial_{\nabla \chi} \psi \\ \dot{\theta} &= c^{-1} \partial_{\nabla \chi} (\theta \partial_{\theta} \psi) \cdot \nabla \dot{\chi} \\ &\quad + c^{-1} \partial_{\mathbf{F}_P} (\psi - \theta \partial_{\theta} \psi) \cdot N \partial_{\mathbf{F}_P} \psi + c^{-1} \text{div } (\mathbf{K} \nabla \theta) \\ \dot{\mathbf{F}}_P &= -N \partial_{\mathbf{F}_P} \psi\end{aligned}\quad (75)$$

of evolution-field relations for $\mathbf{x} = (\chi, \mathbf{m}, \theta, \mathbf{F}_P)$.

Comparing now the GENERIC-based system (61) with that (75) from continuum thermodynamics, we see that the connection between these two basically boils down to the “standard” relation

$$\psi = \varepsilon - \theta \eta \quad (76)$$

between the densities of free energy, internal energy, and entropy. As evident in the formulation of this section as based on the form (72) for the dissipation-rate density and the corresponding dissipation principle, the free energy is primal in the continuum thermodynamics of solids. Indeed, together with transport relations like (73), it determines all other model quantities, e.g., the entropy and internal energy via (71)_{1,2}. This is in contrast to the formulation from the last section, as well as from the basic form of the GENERIC (4) itself, in which energy and entropy are primal. Together with $\mathbf{L}$ and $\mathbf{M}$, they determine constitutively all other quantities in the model, e.g., the free energy via (76). This is basically in keeping with its roots in non-equilibrium thermodynamics and statistical mechanics.

5 The issue of dissipation potentials

Being based on physical considerations in the context of transport theory and irreversible thermodynamics, the GENERIC-based constitutive relations (45) and (51), or their continuum thermodynamic counterparts (73)_{1,2}, for heat flux and inelastic flow, respectively, account by definition for the physics of these processes relevant to the current model. In other words, from a physical point of view, nothing further is needed. Mathematically, however, this is not necessarily the end of the story. Indeed, the properties of $\mathbf{M}$ may facilitate the mathematical representation of the time-irreversible part (10) of the GENERIC (4) in the form

$$\dot{\mathbf{x}}|_{\text{irr}}(\dots, \delta_{\mathbf{x}} \eta) = \partial_{\delta_{\mathbf{x}} \eta} \varphi(\dots, \delta_{\mathbf{x}} \eta) = \mathbf{M}(\dots, \delta_{\mathbf{x}} \eta) \delta_{\mathbf{x}} \eta \quad (77)$$

from (67) with respect to a potential $\varphi(\dots, \delta_{\mathbf{x}} \eta)$. To use the terminology of (see Ch. 1, Definition 7.10, in [31]), if φ in fact exists, then $\mathbf{M}$ represents a potential operator. Again, although this is of no physical consequence, a potential representation for $\mathbf{M}$, if it exists, would be very useful for example for the formulation of the corresponding initial boundary-value problem in variational form. In this regard, the question arises as to under what conditions such a representation may exist.

The symmetry and non-negative definiteness of $\mathbf{M}$ are necessary, but generally not sufficient, for φ to exist. In the special case that $\mathbf{M}$ is independent of $\delta_{\mathbf{x}} \eta$, these are also sufficient. In the current case, the dependence of

$\mathbf{M}$ on $\delta_{\mathbf{x}}\eta$ is induced by that of N on Σ via (65). Necessary then for the existence of a potential representation for $\mathbf{M}(\dots, \delta_{\mathbf{x}}\eta)$ is that one exist for $N(\dots, \Sigma)$. To discuss this in more detail, consider the corresponding form

$$\dot{\mathbf{F}}_{\mathbf{P}}(\dots, \Sigma) = N(\dots, \Sigma) \Sigma \quad (78)$$

for the viscoplastic flow rule (73)₂ quasi-linear in

$$\Sigma = -\partial_{F_{\mathbf{P}}} \psi \quad (79)$$

from (63)₃ and (76). On this basis, a necessary condition for $N(\dots, \Sigma)$ to have a potential representation is the (major) symmetry of

$$\partial_{\Sigma} \dot{\mathbf{F}}_{\mathbf{P}}(\dots, \Sigma) = (\partial_{\Sigma} N)^S(\dots, \Sigma) \Sigma + N(\dots, \Sigma) \quad (80)$$

in terms of the notation

$$((\partial_{\Sigma} N)^S Y) Z := ((\partial_{\Sigma} N) Z) Y \quad (81)$$

for all second-order tensors Y and Z . Given the symmetry of N , this implies that $\partial_{\Sigma} \dot{\mathbf{F}}_{\mathbf{P}}$ will be symmetric iff $(\partial_{\Sigma} N)^S \Sigma$ is as well. In other words, iff the restriction

$$Y \cdot ((\partial_{\Sigma} N) Z) \Sigma = Z \cdot ((\partial_{\Sigma} N) Y) \Sigma$$

$$Y_{\alpha L} \left(\partial_{\Sigma_{\gamma M}} N_{\alpha L \beta K} \right) Z_{\gamma M} \Sigma_{\beta K} = Z_{\gamma M} \left(\partial_{\Sigma_{\alpha L}} N_{\gamma M \beta K} \right) Y_{\alpha L} \Sigma_{\beta K} \quad (82)$$

on the functional form of $N(\dots, \Sigma)$ holds for all Y and Z via (81). Again, note that (82) represents an additional constitutive restriction on the form of $N(\dots, \Sigma)$ going beyond those of Onsager–Casimir symmetry and non-negative definiteness.

This state of affairs carries over to the GENERIC context directly via (66). In particular, we have

$$\begin{aligned} \partial_{\delta_{F_{\mathbf{P}}}\eta} \dot{\mathbf{F}}_{\mathbf{P}} &= \left(\partial_{\delta_{F_{\mathbf{P}}}\eta} \mathbf{M}_{F_{\mathbf{P}}\theta} \right) \delta_{\theta} \eta + \left(\partial_{\delta_{F_{\mathbf{P}}}\eta} \mathbf{M}_{F_{\mathbf{P}}F_{\mathbf{P}}} \right)^S \delta_{F_{\mathbf{P}}}\eta + \mathbf{M}_{F_{\mathbf{P}}F_{\mathbf{P}}} \\ &= \theta^2 (\partial_{\Sigma} N)^S \left(\delta_{F_{\mathbf{P}}}\eta - \frac{\partial_{F_{\mathbf{P}}}\varepsilon}{\partial_{\theta}\varepsilon} \delta_{\theta}\eta \right) + \theta N \\ &= \theta \partial_{\Sigma} \dot{\mathbf{F}}_{\mathbf{P}} \end{aligned} \quad (83)$$

via (65), (79) and (80). Consequently, $\partial_{\delta_{F_{\mathbf{P}}}\eta} \dot{\mathbf{F}}_{\mathbf{P}}$ will be symmetric iff (82) holds. So again, the existence of a potential representation for N and (78) is necessary, but not sufficient, for one to exist for $\mathbf{M}$ and (10), i.e., (77). But if it does in fact exist, note that the representation (77) results in the form

$$\dot{S} = [S, S] = \int_{E^3} \delta_{\mathbf{x}}\eta \cdot \partial_{\delta_{\mathbf{x}}\eta} \varphi \, dv \quad (84)$$

of the entropy production-rate from (18). In this case, a sufficient condition for non-negative entropy production is the convexity and non-negativity of $\varphi(\dots, \delta_{\mathbf{x}}\eta)$, i.e.,

$$\int_{E^3} \delta_{\mathbf{x}}\eta \cdot \partial_{\delta_{\mathbf{x}}\eta} \varphi \, dv \geq \int_{E^3} \varphi \, dv \geq 0. \quad (85)$$

A conjugate form $\partial_{\dot{\mathbf{x}}|_{\text{irr}}} \chi = \delta_{\mathbf{x}}\eta$ of this in terms of the potential χ dual to φ could also be formulated. These and other aspects of a potential-based representation for the irreversible part of the GENERIC represent work in progress to be reported in the future.

In the above treatment we have accounted for the dependence of transport coefficient N on the driving force Σ . Doing so is physically reasonable for viscoplastic solids. From a purely mathematical perspective, one could use the constitutive relation $\Sigma = \Sigma(\nabla \chi, \theta, F_{\mathbf{P}})$ in order to represent N in a form independent of the driving

force Σ , which would result in a dissipation potential being quadratic in the forces. However, the transport coefficients N , as well as K , retain their physical meaning only when interpreted in terms of the driving forces. In this section, we are interested in the case where the physically-based flux-force structure with force-dependent transport coefficient can be represented in potential form. This amounts to dissipation potentials that are non-quadratic in the forces, as has been underlined also by Grmela [30]. This being said, a separate study is warranted about the connection between dissipation-potential-based and quasi-linear constitutive relations, in particular about which class of constitutive relations is the more general one [32].

6 Discussion

In the realm of continuum thermodynamic phenomenology (e.g., [10–15]), one often simply assumes in a constitutive fashion that a potential representation for evolution-constitutive relations like $\dot{F}_P(\dots, \Sigma)$ exists. For example, the residual form (72) of the dissipation-rate density motivates the generalized Ginzburg–Landau form

$$\dot{F}_P(\dots, -\partial_{F_P} \psi) = \partial_{-\partial_{F_P} \psi} \varphi_P(\dots, -\partial_{F_P} \psi) \quad (86)$$

in terms of $\varphi_P(\dots, \Sigma)$ which is convex and non-negative in order to satisfy the dissipation principle sufficiently. For example, we could have the simple activation form

$$\varphi_P(\dots, \Sigma) = \left\langle \sqrt{\Sigma \cdot A(\dots) \Sigma} - \sigma_A(\dots) \right\rangle \quad (87)$$

for φ_P determined by the fourth-order flow anisotropy tensor A , the activation (“yield”) stress σ_A , and the ramp function $\langle x \rangle = \frac{1}{2}(x + |x|)$. Then

$$N(\dots, \Sigma) = \frac{\left\langle \sqrt{\Sigma \cdot A(\dots) \Sigma} - \sigma_A(\dots) \right\rangle'}{\sqrt{\Sigma \cdot A(\dots) \Sigma}} A(\dots) \quad (88)$$

and

$$(\partial_\Sigma N)^S(\dots, \Sigma) \Sigma \propto A(\dots) \Sigma \otimes A(\dots) \Sigma \quad (89)$$

follow with $\langle x \rangle' = \frac{1}{2}(1 + x/|x|)$. Clearly, the latter relation satisfies (82) as expected. Note that this latter condition is non-trivial. For example, a form like $N(\dots, \Sigma) = s(\mathbf{I} \cdot \Sigma) / l$ in terms of some scalar non-negative function $s(\mathbf{I} \cdot \Sigma)$ of the trace $\mathbf{I} \cdot \Sigma$ of Σ and the fourth-order identity l does not satisfy (82). In general, then, such a potential and the corresponding representation (86) may not exist for all transport-theory-based models of quasi-linear form such as (78).

Focusing next on metals, one often works with the assumption that inelastic processes such as dislocation motion do not affect the elastic behavior of the crystal lattice at the single-crystal level, nor that of a polycrystalline material. In this case, F_P represents an elastic material isomorphism (e.g., [33,34]), and we have the split

$$\begin{aligned} \varepsilon(\theta, \nabla \chi, F_P) &= \varepsilon_E(\theta, F_E) + \varepsilon_H(\theta, F_P) \\ \eta(\theta, \nabla \chi, F_P) &= \eta_E(\theta, F_E) + \eta_H(\theta, F_P) \end{aligned} \quad (90)$$

into contributions due to elastic (i.e., lattice) distortion ψ_E as well as to energetic hardening ψ_H , the former in terms of the elastic local deformation. In this case,

$$\begin{aligned} \Sigma_{\alpha K} F_{P\beta K} &= F_{E\alpha K} (\partial_{F_{E\beta K}} \psi_E) - (\partial_{F_{P\alpha K}} \psi_H) F_{P\beta K} \\ &= M_{\alpha\beta} - X_{\alpha\beta} \\ \Sigma F_P^T &= F_E^T (\partial_{F_E} \psi_E) - (\partial_{F_P} \psi_H) F_P^T \\ &= M - X \end{aligned} \quad (91)$$

holds, where $M = F_E^T (\partial_{F_E} \psi_E)$ is the Mandel stress, and $X = (\partial_{F_P} \psi_H) F_P^T$ is the back stress.

More common than the form of the viscoplastic flow rule which has been considered in this work, i.e., (62)₄, is that

$$\begin{aligned}\dot{F}_{P\alpha K} &= L_{P\alpha\beta} F_{P\beta K}, \\ \dot{F}_P &= L_P F_P,\end{aligned}\quad (92)$$

in terms of the plastic “velocity gradient” L_P . Assuming for example that an inelastic flow potential

$$\varphi_P(\dots, \Sigma) = \phi_P(\dots, M - X), \quad (93)$$

exists, the corresponding potential form

$$\begin{aligned}L_{P\alpha\beta} &= \partial_{M_{\alpha\beta} - X_{\alpha\beta}} \phi_P \\ L_P &= \partial_{M - X} \phi_P\end{aligned}\quad (94)$$

for L_P follows. More generally,

$$\begin{aligned}L_{P\alpha\beta} &= N_{\alpha K \gamma L} F_{P L \nu}^{-1} F_{P K \beta}^{-1} (M_{\gamma \nu} - X_{\gamma \nu}) \\ L_P &= \left(I \square F_P^{-1} \right) N \left(I \square F_P^{-T} \right) [M - X]\end{aligned}\quad (95)$$

follows from (62)₄ of the GENERIC, the second via the tensor production notation $(A \square B) C := A C B$. In (95), the first term $N_{\alpha K \gamma L} F_{P L \nu}^{-1} F_{P K \beta}^{-1}$ is the kinetic “pre-factor”, while the second term $M_{\gamma \nu} - X_{\gamma \nu}$ is the driving force for viscoplastic deformation. We point out that the structure of $L_{P\alpha\beta}$ is analogous to what has been examined from a completely different perspective in [27]. There, systematic coarse-graining has been employed to arrive at constitutive relation for L_P in the evolution equation for the local elastic deformation

$$\dot{F}_E|_{\text{irr}} = -F_E L_P \quad (96)$$

in an Eulerian formulation. As a key result of that work, the kinetic prefactor in L_P was expressed in terms of the time-correlation of the fluctuations in the deformation gradient, in the spirit of a fluctuation-dissipation theorem (for more details, see [27]). Hence, we infer that correspondingly the first term on the right-hand side of (95) is a measure of fluctuations.

More general than the approach taken in this work is the derivation of constitutive relations by systematic coarse-graining using nonequilibrium statistical mechanics. It is a cornerstone of coarse-graining that the variables on the coarse-grained level can be expressed in terms of instantaneous configurations on the microscopic level. As for the local elastic deformation F_E , this seems feasible by comparing actual snapshots of particle configurations to configurations of the corresponding unstressed state or inherent structure. In contrast, if the local inelastic deformation F_P is a dynamic variable, it is less clear to the authors at present how to express it in terms of instantaneous snapshots of particle arrangements. This complication originates from the fact that F_P by definition serves the purpose of quantifying unrecoverable deformation.

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