Using the gradients of temperature and internal parameters in Continuum Thermodynamics

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Abstract

In this paper, the possibility of using the gradients of the temperature and of the internal parameters as additional state variables in Continuum Thermodynamics is considered. The expressions of the two principles are discussed and Clausius–Duhem inequality is derived under an appropriate statement of the internal entropy production. Several formulations are proposed and compared to existing results in the literature. ***To cite this article: P. Ireman, Q.S. Nguyen, C. R. Mecanique 332 (2004).***
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Résumé

Introduction des gradients de température et de paramètres internes en Thermodynamique des Milieux Continus. On étudie dans cette note la possibilité d'introduire les gradients de la température et des paramètres internes comme des variables d'état supplémentaires en Thermodynamique des Milieux Continus. A partir d'une expression appropriée de la production interne d'entropie, on donne les énoncés des deux principes et l'expression associée de l'inégalité de Clausius–Duhem. Plusieurs formulations sont proposées et comparées aux résultats existants de la littérature. ***Pour citer cet article : P. Ireman, Q.S. Nguyen, C. R. Mecanique 332 (2004).***
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On s'intéresse principalement dans cette note au problème de l'utilisation du gradient de température comme une variable d'état additionnelle en thermodynamique des Milieux Continus. Dans ce cas, l'état local d'un élément de matière n'est pas en équilibre thermique et les relations de dualité classiques entre la température et l'entropie (1) ne sont pas justifiées a priori. Si l'énergie libre massique a pour expression $\psi(\varepsilon, T, \alpha, \nabla T)$, l'expression (2) de

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l'énergie interne est cependant admise. Les deux principes de la thermodynamique sont alors énoncés sous la forme (3), (4) dans laquelle une production d'entropie additionnelle $\mathcal{F}$ a été introduite pour tenir compte des irréversibilités thermiques intérieures. Cette production d'entropie additionnelle est représentée par une densité massique φ. Ainsi, on suit une approche due à Maugin [8] qui consiste à étendre l'énoncé du second principe en modifiant l'expression de la production interne d'entropie. Cependant, dans notre analyse, le terme additionnel de la production d'entropie ne provient pas nécessairement d'un flux externe d'entropie comme il a été proposé dans [8].

Trois modèles particuliers sont étudiés par le choix d'une expression appropriée de φ. Dans le modèle 1, on admet l'expression (11) de la production d'entropie additionnelle. Les deux principes nous permettent alors d'écrire l'équation locale de l'énergie et l'inégalité de Clausius–Duhem traduisant la non-négativité de la dissipation. On retrouve dans ce modèle la dualité température-entropie et l' expression usuelle de la dissipation (13) dans la description classique sans gradient thermique. L'expression de la dissipation permet d'appliquer comme avant, cf. [3] par exemple, le formalisme bien connu du potentiel de dissipation dans la recherche des lois complémentaires. Ce modèle permet de retrouver les résultats de Andrieux et al., cf. [12] car l'inégalité de Clausius–Duhem s'écrit aussi sous la forme (16). Le modèle 2 consiste à choisir φ sous la forme (17) qui traduit l'existence d'un flux de dissipation. Il conduit à l'expression classique de la dissipation et à une perte de dualité température-entropie. En effet, l'entropie est alors donnée par (19) et se compose d'une part classique s_{eq} et une part non classique s_{neq} due à la présence du gradient de température comme variable d'état. Dans le modèle 3, φ s'écrit sous la forme (20) et provient donc d'un flux d'entropie externe additionnel. On obtient alors un résultat analogue au modèle 2, une dissipation écrite sous la forme classique et une expression non classique de l'entropie. Le modèle 1 fournit donc l'extension la plus simple et la plus proche de la description thermodynamique classique. Par rapport aux résultats existants de la littérature, cf. Cardona et al. [13], notre analyse s'apparente à l'approche de Maugin [8], tandis que la discussion de Cardona et al. suit une approche développée par Frémond [7]. Cette dernière formulation est basée sur une expression étendue du principe des puissances virtuelles dans laquelle des forces généralisées associées à la température et à son gradient ont été introduites, [13,7].

En fait, la même discussion peut être menée pour le problème de l'utilisation du gradient de paramètres internes sur lequel on connait un nombre important de discussions, cf. par exemple [7–9,15]. Partant de l'hypothèse d'une production d'entropie additionnelle φ, trois modèles simples peuvent être de nouveau introduits dans le même esprit lorsque le matériau admet une énergie libre massique $\psi(\varepsilon, T, \alpha, \nabla\alpha)$. On montre que le deuxième choix (26) permet de retrouver la formulation de Frémond [7,15] et que le troisième choix (28) correspond à la formulation de Maugin [8,15]. Le premier choix (25) conduit par contre à une formulation plus simple et plus proche de la description classique sans gradient de paramètre interne.

1. Introduction

Continuum Thermodynamics have been much discussed in the modeling of materials (solids and fluids) in the last century, cf. [1–6]. In particular, the internal variable description consists of introducing a set of local state variables (ε, T, α) which represent respectively the strain, the temperature and internal parameters for any material element. The internal parameters represent additional physical parameters such as the plastic strain or the damage, etc. The element is classically assumed to be in thermal equilibrium. The notions of local entropy s and of internal energy e per unit mass are also accepted as functions of the state variables. Thermal equilibrium leads to the classical relations of thermostatics:

$$s = -\psi,_T, \qquad T = e,_s \tag{1}$$

$$e = \psi + Ts \tag{2}$$

where $\psi(\varepsilon, T, \alpha)$ and $e(\varepsilon, s, \alpha)$ denote respectively the free energy and internal energy per unit mass. The internal energy is a convex function with respect to the entropy. Eqs. (1) and (2) show that the energies $e(\varepsilon, s, \alpha)$ and

$-\psi(\varepsilon, T, \alpha)$ are two dual functions with respect to dual variables (s, T) in the sense of Legendre–Fenchel transform.

Some refined versions of this description have been also introduced in the literature. The possibility to add the strain gradient $\nabla \varepsilon$ as state variable has been discussed in the so called theory of second gradient and leads to the study of micropolar materials. More recently, the study of damage leads also to the introduction of the gradient of internal parameters $\nabla \alpha$ as additional state variable in order to prevent the localization phenomena and to avoid the difficulty of mesh-dependence in numerical simulations, cf. for example [7–11]. In most of these discussions, basic relations (1) and (2) still hold.

In this Note, the possibility of using the temperature gradient ∇T as an additional state variable is the principal subject of interest. Our objective is to look for a simple extension of the classical description of Continuum Thermodynamics including the case of the local states which are not in thermal equilibrium. The same analysis is then applied in a second section to the problem of introducing the gradient of the internal parameters. This analysis leads to some interesting formulations and to a better understanding on existing results in the literature.

2. Introducing the temperature gradient

It is assumed that $(\varepsilon, T, \alpha, \nabla T)$ are state variables and that the free energy per unit mass is a state function $\psi = \psi(\varepsilon, T, \alpha, \nabla T)$. It is clear that if $\nabla T \neq 0$, the material is not necessarily in thermal equilibrium and that the entropy s and the temperature T are not necessarily dual variables. Thus, (1) does not necessarily hold. The expression (2) of the internal energy is however accepted.

The case of a solid in dynamic thermo-mechanical evolution is now considered. For any material volume V in a reference configuration, the two principles of thermodynamics are postulated as

$$\dot{C} + \dot{E} = \mathcal{P}_e + \mathcal{P}_c \tag{3}$$

and

$$\dot{S} + \mathcal{F} \geqslant \mathcal{N} \tag{4}$$

where E is the internal energy, C the kinetic energy, $\mathcal{P}_e$ the power of the external forces and $\mathcal{P}_c$ is the heat supply per time unit, S is the entropy and $\mathcal{N}$ is the entropy supply per time unit for any material volume V. The entropy variation inside the volume is not reduced to $\dot{S}$ and an additional production of entropy due to thermal irreversibilities $\mathcal{F}$ is introduced:

$$\begin{cases} E = \int_V \rho e \, dV \\ \mathcal{P}_c = -\int_{\partial V} q \cdot n \, da \\ S = \int_V \rho s \, dV \\ \mathcal{N} = -\int_{\partial V} \frac{q}{T} \cdot n \, da \\ \mathcal{F} = \int_V \rho \varphi \, dV \end{cases}$$

where ρ is the mass density per unit reference volume, q is the heat flux, φ is the extra term of entropy production per unit mass. Thus, Maugin's idea [8] is followed with a slight difference since the extra term is an entropy production inside the volume and does not result necessarily from an entropy flux.

Taking account of the fundamental law of dynamics

$$\dot{C} + \int_V \sigma : \dot{\varepsilon} = \mathcal{P}_e \quad \forall V \tag{5}$$

where σ is the associated stress to the reference configuration (Kirchhoff stress in finite deformation or Cauchy stress in small deformation), the first principle leads to

$$\int_V (\rho \dot{e} - \sigma : \dot{\varepsilon} + \operatorname{div} q)\, dV = 0$$

and the local equation of energy is obtained:

$$\rho \dot{e} - \sigma : \dot{\varepsilon} + \operatorname{div} q = 0 \quad \forall x \in V \tag{6}$$

From the expression of the internal energy (2), this equation can also be written as

$$\rho T \dot{s} = \sigma : \dot{\varepsilon} - \rho s \dot{T} - \rho \dot{\psi} - \operatorname{div} q = 0 \tag{7}$$

The second principle gives

$$\int_V \left(\rho T \dot{s} + T \rho \varphi + \operatorname{div} q - q \cdot \frac{\nabla T}{T} \right) dV \geqslant 0$$

By combination of these results, one obtains Clausius–Duhem inequality which requires that the dissipation per unit volume d is nonnegative:

$$d = T \rho \varphi + \sigma : \dot{\varepsilon} - \rho \dot{\psi} - \rho s \dot{T} - q \cdot \frac{\nabla T}{T} \geqslant 0 \quad \forall x \in V \tag{8}$$

From the expression $\psi = \psi(\varepsilon, T, \alpha, \nabla T)$, it follows that

$$d = (\sigma - \rho \psi_{,\varepsilon}) : \dot{\varepsilon} - \rho(s + \psi_{,T})\dot{T} + T \rho \varphi - \rho \psi_{,\nabla T} \cdot \nabla \dot{T} - \rho \psi_{,\alpha} \cdot \dot{\alpha} - q \cdot \frac{\nabla T}{T} \geqslant 0$$

Thus, by defining

$$\sigma = \sigma^R + \sigma^{IR}, \quad \sigma^R = \rho \psi_{,\varepsilon}, \quad A = -\rho \psi_{,\alpha}, \quad G = -\rho \psi_{,\nabla T} \tag{9}$$

the following expression of the Clausius–Duhem inequality results:

$$d = \sigma^{IR} : \dot{\varepsilon} - \rho(s + \psi_{,T})\dot{T} + A \cdot \dot{\alpha} + T \rho \varphi + G \cdot \nabla \dot{T} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{10}$$

Our objective is to derive now some interesting thermodynamical descriptions by a proper choice of the expression of φ. Three straightforward particular choices are:

2.1. Model 1

By assuming the following expression for the extra term of entropy production

$$\rho \varphi = -\frac{1}{T} G \cdot \nabla \dot{T} \tag{11}$$

then Clausius–Duhem inequality is reduced to the following expression:

$$d = \sigma^{IR} : \dot{\varepsilon} + A \cdot \dot{\alpha} - \rho(s + \psi_{,T})\dot{T} - q \cdot \frac{\nabla T}{T} \geqslant 0$$

The duality relation (1) results when a variation of temperature at fixed deformation and internal parameters does not produce any intrinsic dissipation:

$$s = -\psi_{,T} \tag{12}$$

Thus, the classical expression of the dissipation per unit volume is recovered:

$$d = \sigma^{IR} : \dot{\varepsilon} + A \cdot \dot{\alpha} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{13}$$

The first term is the dissipation due to the irreversible stress, as classically obtained in visco-elasticity for example. The second term is the dissipation due to the irreversible nature of the physical mechanisms described by internal parameters, as classically observed in the modelling of metal plasticity. The last term is the thermal dissipation due to the existence of a thermal gradient. This expression of the dissipation enables us to apply again the formalism of dissipative potentials in the modeling of the constitutive equations for the irreversible stress, the internal parameters and for the thermal conduction, cf. [3]. The local equation of energy balance can also be arranged as

$$\operatorname{div} q + \rho T \dot{s} = \sigma^{IR} : \dot{\varepsilon} + A \cdot \dot{\alpha} + G \cdot \nabla \dot{T} \tag{14}$$

For example, Fourier laws of conduction, $q = -K \nabla T$ with $K > 0$ lead to the thermal equation

$$-K \Delta T + \rho T \dot{s} = \sigma^{IR} : \dot{\varepsilon} + A \cdot \dot{\alpha} + G \cdot \nabla \dot{T} \tag{15}$$

The choice (11) for the expression of φ is in agreement with some existing results in the literature on the subject, cf. Andrieux et al. [12]. In a discussion on the macroscopic behaviour of a thermo-elastic periodic composite, the dependence of the free energy of the composite on the temperature gradient has been introduced by these authors when the macroscopic thermal gradient is strong enough. Their result on the macroscopic expressions of entropy and of the Clausius–Duhem inequality are recovered in Model 1. This inequality can also be written as

$$d = \sigma : \dot{\varepsilon} - \rho \dot{\psi}|_{(T, \nabla T)} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{16}$$

where $\dot{\psi}|_{(T, \nabla T)}$ denotes the time variation of ψ at T and ∇T fixed.

2.2. Model 2

The following expression of the extra term of entropy production is now considered:

$$\rho \varphi = -\frac{1}{T} \operatorname{div}(G \dot{T}) \tag{17}$$

Here, the additional term $T \rho \varphi$ results from a dissipation flux since

$$\int_V \operatorname{div}(G \dot{T}) \, \mathrm{d}V = \int_{\partial V} G \cdot n \dot{T} \, \mathrm{d}a$$

From the fact that $\operatorname{div}(G \dot{T}) = G \cdot \nabla \dot{T} + \dot{T} \operatorname{div} G$, the Clausius–Duhem inequality reads:

$$d = \sigma^{IR} : \dot{\varepsilon} - (\rho s + \rho \psi,_T + \operatorname{div} G) \dot{T} + A \cdot \dot{\alpha} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{18}$$

The previous argument leads to the following expression of entropy:

$$s = -\psi,_T - \frac{1}{\rho} \operatorname{div} G \tag{19}$$

Thus, this choice leads to the classical expression of the dissipation (13) and to a nonclassical expression of the entropy. The entropy consists of an equilibrium part and a non-equilibrium part $s = s_{\text{eq}} + s_{\text{neq}}$ with $s_{\text{eq}} = -\psi,_T$ and $s_{\text{neq}} = -\frac{\operatorname{div} G}{\rho}$.

2.3. Model 3

The following expression of the extra term is now considered:

$$\rho\varphi = -\operatorname{div}\left(\frac{\dot{T}}{T}G\right) \tag{20}$$

It results from an entropy flux, cf. [8] since

$$\int_V \rho\varphi\,\mathrm{d}V = \int_{\partial V} \frac{\dot{T}}{T}G \cdot n\,\mathrm{d}a$$

From $T\operatorname{div}(\frac{G}{T}\dot{T}) = \operatorname{div}G\,\dot{T} + G \cdot \nabla\dot{T} - \dot{T}G \cdot \frac{\nabla T}{T}$, the Clausius–Duhem inequality (10) reads

$$d = \sigma^{IR} : \dot{\varepsilon} - \left(\rho s + \rho\psi,_T + \operatorname{div}G - G \cdot \frac{\nabla T}{T}\right)\dot{T} + A \cdot \dot{\alpha} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{21}$$

Coleman argument leads then to the following expression of entropy

$$s = -\psi,_T - \frac{1}{\rho}\operatorname{div}G + \frac{G}{\rho} \cdot \frac{\nabla T}{T} \tag{22}$$

while the dissipation is still given by (13). It should be underlined that in Models 2 and 3, the entropy and the temperature are not dual variables with respect to the energy.

2.4. General remarks

Compared to the existing results in the literature on the subject, cf. Cardonna et al. [13], our analysis results from an extended version of the entropy production in connection with Maugin's approach [8], while Cardonna et al. analysis is based upon an extended statement of the principle of virtual power using generalized internal forces, in connection with Frémond approach, cf. [7]. The last approach consists of modifying the energy balance instead of the entropy production and leads to the choice $a = \operatorname{div}b = -\operatorname{div}G$, i.e., to Model 2, and in a similar spirit, to Model 3. Thus, the same conclusions can be derived by two different approches basing respectively upon an appropriate modification of the energy balance or of the entropy production.

3. Introducing the gradient of the internal parameters

Our analysis suggests that the same discussion can also be applied to the problem of using the gradient of internal parameters as additional state variables, cf. [7,8,14,9,15]. This possibility is fully justified under the assumption that the variation of the gradient of internal parameters $\nabla\dot{\alpha}$ also induces an extra entropy production per unit mass φ.

If the state variables are $(\varepsilon, T, \alpha, \nabla\alpha)$ and the free energy is $\psi(\varepsilon, T, \alpha, \nabla\alpha)$, basic equations of thermostatics (1) and (2) hold. With the notation

$$B = -\rho\psi,_{\nabla\alpha} \tag{23}$$

the dissipation is

$$d = \sigma^{IR} : \dot{\varepsilon} + A \cdot \dot{\alpha} + \rho T\phi + B \cdot \nabla\dot{\alpha} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{24}$$

Again three simple formulations can be introduced. The first choice (Model 1) consists of assuming that

$$\rho\varphi = -\frac{1}{T}B \cdot \nabla\dot{\alpha} \tag{25}$$

and leads again to (13).

The second choice (Model 2) is

$$\rho\varphi = -\frac{1}{T}\operatorname{div}(B \cdot \dot{\alpha}) \tag{26}$$

and implies that

$$d = \sigma^{IR} : \dot{\varepsilon} + (A - \operatorname{div} B) \cdot \dot{\alpha} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{27}$$

This choice leads thus to Frémond's formulation, cf. [7,15].

The last choice (Model 3)

$$\rho\varphi = -\operatorname{div}\left(\frac{1}{T} B \cdot \dot{\alpha}\right) \tag{28}$$

implies that

$$d = \sigma^{IR} : \dot{\varepsilon} + \left(A - \operatorname{div} B + \frac{\nabla T}{T} \cdot B\right) \cdot \dot{\alpha} - q \cdot \frac{\nabla T}{T} \geqslant 0 \tag{29}$$

and leads to Maugin's formulation, cf. [8] and [15].

4. Conclusion

Our discussion contributes to the interesting question, cf. [12,13,7,14,8,9,15]: how to include the gradient of the temperature and of internal parameters as additional state variables in Continuum Thermodynamics? The discussion is based upon an extended expression of the internal entropy production according to the assumption that, for any material volume, the internal entropy production consists of three terms: the entropy variation, the external entropy supply and a nonclassical term due to the exchange of heat and energy inside the volume. Different formulations are then obtained and associated with some appropriate choices of the expression of this additional entropy production.

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