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Thermodynamical admissibility of a set of constitutive equations coupling elasticity, isotropic damage and internal sliding

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ABSTRACT

The theoretical framework of irreversible processes thermodynamics is nowadays widely used for formulating constitutive laws. Both the physical and the thermodynamical consistency of a constitutive model can be ensured. A unique condition gathering the first and the second thermodynamics principles, known as the Clausius–Duhem–Truesdell inequality, allows checking the thermodynamical admissibility of a constitutive model. In this paper, the authors are focused on proposing a proof of the thermodynamical admissibility of a set of constitutive equations coupling elasticity, isotropic damage and internal sliding.

RÉSUMÉ

Le cadre théorique de la thermodynamique des processus irréversibles est de nos jours largement utilisé pour la formulation des lois de comportement. En effet, la cohérence physique et thermodynamique d'un modèle de comportement peut être vérifiée à travers ce cadre théorique. Une unique condition regroupant les premier et second principes thermodynamiques, connue sous le nom d'inégalité de Clausius–Duhem–Truesdell, permet si elle est vérifiée d'assurer l'admissibilité thermodynamique d'un modèle constitutif. Dans cette contribution, les auteurs proposent une preuve de l'admissibilité thermodynamique d'un ensemble d'équations constitutives couplant élasticité, endommagement isotrope et glissement interne.

1. Introduction

From experimental evidences, it appeared that some materials exhibit a constitutive behaviour involving several mechanisms. For instance, concrete-like materials are usually modelled by considering two mechanisms: elasticity and damage. The last decades have been very fruitful in the development of constitutive models coupling elasticity with isotropic damage. More recently, especially in seismic engineering, very sophisticated models have been proposed including local non-linear hysteretic effects. These phenomena are taken into account by considering an additional mechanism called internal sliding. The local friction occurring between crack lips is considered as being responsible for non-linear hysteretic effects [1,2]. Constitutive models based on these three mechanisms have been developed within the framework of irreversible processes

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thermodynamics. This ensures a physical consistency as well as a numerical robustness with respect to the numerical implementation. Nevertheless, developing a constitutive model by means of such a theoretical framework is not sufficient if the positivity of the so-called Clausius–Duhem–Truesdell inequality is not proved for all stress paths.

This Note has two objectives. The first one is to expose a general formulation of a set of constitutive equations coupling elasticity, isotropic damage and internal sliding. The second objective is to propose a proof of the thermodynamical admissibility of this set of constitutive equations. In order to achieve these two objectives, this Note is outlined as follows. Firstly, an introduction to a general expression of a thermodynamical state potential, expressed as the Helmholtz free energy is presented. A specific attention is paid to justify that such an expression fulfills all the mathematical requirements. In the third part of this paper, the state equations are derived from the state potential expression. They allow an efficient description of the reversible part of the mechanical behaviour at a constitutive level. Especially, the thermodynamical couplings between internal variables are exposed. The fourth part is dedicated to explain the flow rules used to manage the irreversible part of the mechanical behaviour. The last part of this paper aims to propose a proof of the positivity of the intrinsic dissipation, also known as the Clausius–Duhem inequality.

2. Thermodynamical state potential

The thermodynamical state potential can be expressed in various ways. In this Note, it has been chosen to express it in terms of Helmholtz free energy. By means of this single expression, the reversible part of any mechanical behaviour can be modelled. In this paper, three mechanisms are considered: elasticity, isotropic damage and internal sliding. The first mechanism is elasticity. It is commonly used to model the mechanical response of concrete-like materials when they are subject to a low loading level. As for the second mechanism, isotropic damage is considered to integrate all the non-linear effects due to micro cracking. A single scalar variable ranging from 0 (virgin material) to 1 (fractured material) is used. Its value is usually linked to positive extensions in order to create a variation of the elastic properties. The last mechanism is internal sliding, which allows accounting for non-linear hysteretic effects due to friction that may appear between the lips of the cracks. A suitable thermodynamical state potential considering all these mechanisms can be assumed. Nevertheless, several assumptions are made and must be specified before presenting its expression. Firstly, it is assumed that internal sliding only acts on the deviatoric part of the Helmholtz free energy. This is physically motivated by the fact that friction, related to sliding, results mainly from shearing mode (mode II). Secondly, a very important effect exhibited by concrete-like materials is the so-called unilateral effect [3,4]. Due to the scalar nature of the damage variable, a full unilateral effect cannot be taken into account. Nevertheless, by assuming that damage does not act on the negative part related to the hydrostatic part of the Helmholtz free energy, a quasi-unilateral effect can be obtained. The following expression can be used as a thermodynamical state potential.

$$\rho\Psi = \frac{\kappa}{6}\big((1-d)\langle\varepsilon_{kk}\rangle_+^2 + \langle\varepsilon_{kk}\rangle_-^2\big) + \mu(1-d)\varepsilon_{ij}^d\varepsilon_{ij}^d + \mu g(d)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big) + \frac{\gamma}{2}\alpha_{ij}\alpha_{ij} + H(z) \tag{1}$$

where ρ is the material density, Ψ is the Helmholtz free energy, $\langle(.)\rangle_+$ and $\langle(.)\rangle_-$ stand for the positive and negative parts related to $(.)$ respectively, κ and μ are the bulk coefficient and the shear modulus respectively, ε_{ij}^d is the second order deviatoric strain tensor, γ is the kinematic hardening modulus, H is the consolidation function related to the isotropic hardening (it is a differentiable and increasing scalar function from $[0,1]$ into $[0,1]$) and g is a continuous and differentiable scalar function defined from $[0,1]$ into $[0,1]$. The thermodynamic internal variables are the sliding strains tensor ε_{ij}^π, the damage variable d, the kinematic hardening tensor α_{ij} and the isotropic hardening variable z. From basic considerations, it can be stated that this thermodynamical state potential is clearly convex, null at the origin and totally differentiable with respect to each internal variable.

3. State equations

This section is devoted to present the state equations. Assuming that ρ is constant during the strain process, the state equations can be obtained by differentiating the thermodynamical state potential with respect to each internal variable. The first state equation allows defining the Cauchy stress tensor σ_{ij}:

$$\sigma_{ij} = \rho\frac{\partial\Psi}{\partial\varepsilon_{ij}} = \frac{\kappa}{3}\big((1-d)\langle\varepsilon_{kk}\rangle_+ + \langle\varepsilon_{kk}\rangle_-\big)\delta_{ij} + 2\mu(1-d)\varepsilon_{ij}^d + 2\mu g(d)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big) \tag{2}$$

The frictional stress tensor related to internal sliding mechanism can be defined according to:

$$\sigma_{ij}^\pi = 2\mu g(d)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big) \tag{3}$$

It can be noticed that the expression of the frictional stress tensor includes the damage variable. This thermodynamical state coupling allows making dependent the frictional stress to the damage level. The energy rate released due to the damage mechanism is:

$$Y = -\rho\frac{\partial\Psi}{\partial d} = \frac{\kappa}{6}\langle\varepsilon_{kk}\rangle_+^2 + \mu\varepsilon_{ij}^d\varepsilon_{ij}^d - \mu g'(d)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big) = Y_N^+ + Y_d - Y_\pi \tag{4}$$

The energy rate released related to damage Y can be split into three distinct parts. The first one is due to mode I (opening), the second one to mode II (shearing) and the last one to internal sliding. Since the last part is affected by a minus sign, it may lead to a negative dissipation. If such a case happens, the constitutive model does not fulfill the thermodynamical requirements and therefore is neither physically nor thermodynamically admissible. This point will be discussed in Section 5. The back stress tensor is associated to kinematic hardening and is defined by:

$$X_{ij} = \rho \frac{\partial \Psi}{\partial \alpha_{ij}} \tag{5}$$

Finally, the thermodynamical force related to isotropic hardening is:

$$Z = \rho \frac{\partial \Psi}{\partial z} = \frac{\partial H(z)}{\partial z} = H'(z) \tag{6}$$

where we assume that $H'(z) > 0 \ \forall z \in [0, 1]$.

4. Flow rules

In this section, the general form of the flow rules is presented. First, the damage mechanism is considered. The threshold surface should be a function of the energy rate released due to this dissipative mechanism. One choice can be:

$$f_d(\tilde{Y}; Z) = \tilde{Y} - (Y_0 + Z) \tag{7}$$

where $\tilde{Y}$ is the considered part of the energy rate released due to damage and Y_0 is an initial threshold whose the expression has to be identified from experience. The evolution laws result from the maximum dissipation principle [5]. They can be expressed as:

$$\dot{d} = \dot{\lambda}_d \frac{\partial f_d}{\partial \tilde{Y}} = \dot{\lambda}_d \tag{8}$$

$$\dot{z} = \dot{\lambda}_d \frac{\partial f_d}{\partial Z} = -\dot{\lambda}_d \tag{9}$$

where $\dot{\lambda}_d$ is the Lagrange multiplier associated to damage.

We can notice that the threshold surface related to damage is not a function of the energy rate released due to damage mechanism. Therefore, the convexity of the threshold surface is not a sufficient condition to ensure the positivity of the intrinsic dissipation. This specific point is studied in Section 5. The sliding mechanism has to be managed carefully. In accordance with the second assumption (3) presented in the previous section, the sliding tensor must be purely deviatoric. Nevertheless, it is well known that concrete-like materials may be sensitive to the confinement level. This feature can be taken into account by considering a non-associative framework. Hence, the threshold surface related to internal sliding is chosen as follows:

$$f_\pi\left(\sigma_{ij}^\pi; X_{ij}, \langle\sigma_{ij}\rangle_-\right) = \left\|\sigma_{ij}^\pi - X_{ij}\right\| + cI_1\left(\langle\sigma_{ij}\rangle_-\right) \tag{10}$$

where $\|.\|$ stands for any norm considering that the thermodynamical admissibility of the considered model is not affected (this norm will be specified in the next section), $I_1(.)$ is the first invariant of (.) and c is a material parameter to be identified managing the sensitivity of the constitutive response with respect to the confinement level. Obviously, it can be set to zero if the considered material is not sensitive at all to the hydrostatic pressure. According to the initial proposal made by [6], a pseudo-potential of dissipation necessary to the flow rules is considered as follows:

$$\phi_\pi\left(\sigma_{ij}^\pi; X_{ij}, a\right) = \left\|\sigma_{ij}^\pi - X_{ij}\right\| + \zeta_\pi(X_{ij}, a) \tag{11}$$

where a is a positive material parameter which has to be identified, $\zeta_\pi(.)$ is a norm which can be chosen according to conditions that have to be specified. Additional explanations will be given in the next section about the construction of this norm (25). The flow rules related to internal sliding and kinematic hardening are:

$$\dot{\varepsilon}_{ij}^\pi = \dot{\lambda}_\pi \frac{\partial \phi_\pi}{\partial \sigma_{ij}^\pi} \tag{12}$$

and

$$\dot{\alpha}_{ij} = -\dot{\lambda}_\pi \frac{\partial \phi_\pi}{\partial X_{ij}} \tag{13}$$

where $\dot{\lambda}_\pi$ is the Lagrange multiplier.

5. Thermodynamical admissibility

This section aims to expose a proof of the thermodynamical admissibility related to the constitutive set of equations previously described. A proof of the positivity of the intrinsic dissipation, for all strain paths is proposed. The Clausius–Duhem–Truesdell inequality can be expressed according to:

$$\varphi = \sigma_{ij}\dot{\varepsilon}_{ij} - \rho\dot{\Psi} \geqslant 0 \tag{14}$$

If Eq. (14) is satisfied, it means that the thermodynamical admissibility is ensured. Eq. (14) can be developed by considering the thermodynamical state potential expression:

$$\varphi = \left(\sigma_{ij} - \rho\frac{\partial\Psi}{\partial\varepsilon_{ij}}\right)\dot{\varepsilon}_{ij} - \rho\frac{\partial\Psi}{\partial\varepsilon^{\pi}_{ij}}\dot{\varepsilon}^{\pi}_{ij} - \rho\frac{\partial\Psi}{\partial\alpha_{ij}}\dot{\alpha}_{ij} - \rho\frac{\partial\Psi}{\partial d}\dot{d} - \rho\frac{\partial\Psi}{\partial z}\dot{z} \tag{15}$$

Considering the state equations (2)–(5), and (6), Eq. (15) can be rewritten as:

$$\varphi = \sigma^{\pi}_{ij}\dot{\varepsilon}^{\pi}_{ij} - X_{ij}\dot{\alpha}_{ij} + Y\dot{d} - Z\dot{z} \tag{16}$$

Substituting the relations (8), (9), (12) and (13) in Eq. (16), that allows writing the dissipation in the following form:

$$\varphi = \sigma^{\pi}_{ij}\dot{\lambda}_{\pi}\frac{\partial f_{\pi}}{\partial\sigma^{\pi}_{ij}} + X_{ij}\dot{\lambda}_{\pi}\frac{\partial\phi_{\pi}}{\partial X_{ij}} + \dot{\lambda}_d Y + \dot{\lambda}_d Z \tag{17}$$

Using Eqs. (10) and (11), we obtain:

$$\varphi = \dot{\lambda}_{\pi}\left[\left(\sigma^{\pi}_{ij} - X_{ij}\right)\frac{\partial f_{\pi}}{\partial\sigma^{\pi}_{ij}} + X_{ij}\frac{\partial\zeta_{\pi}}{\partial X_{ij}}\right] + \dot{\lambda}_d(Y + Z) \tag{18}$$

In order to show that the intrinsic dissipation φ is non-negative, it is sufficient to establish that both parts of its expression are non-negative:

$$\dot{\lambda}_{\pi}\left[\left(\sigma^{\pi}_{ij} - X_{ij}\right)\frac{\partial f_{\pi}}{\partial\sigma^{\pi}_{ij}} + X_{ij}\frac{\partial\zeta_{\pi}}{\partial X_{ij}}\right] > 0 \tag{19}$$

$$\dot{\lambda}_d(Y + Z) > 0 \tag{20}$$

Considering the left-hand side member related to Eq. (19), it can be noticed that the first term $\dot{\lambda}_{\pi}$ is non-negative from well-known loading/unloading conditions. Therefore, only the second term of this left-hand side member has to be demonstrated non-negative. Hence, it is sufficient to be shown that:

$$\left(\sigma^{\pi}_{ij} - X_{ij}\right)\frac{\partial f_{\pi}}{\partial\sigma^{\pi}_{ij}} > 0 \tag{21}$$

$$X_{ij}\frac{\partial\zeta_{\pi}}{\partial X_{ij}} > 0 \tag{22}$$

In order to ensure that Eq. (21) remains positive, the threshold surface f_{π} can be selected as follows:

$$f_{\pi}\left(\sigma^{\pi}_{ij}; X_{ij}\right) = J_2\left(\sigma^{\pi}_{ij} - X_{ij}\right) \tag{23}$$

where $J_2(.)$ is the Von Mises equivalent stress depending on the second invariant of the deviatoric part of $(.)$.

Eq. (21) becomes:

$$\left(\sigma^{\pi}_{ij} - X_{ij}\right)\frac{3}{2}\frac{1}{J_2(\sigma^{\pi}_{ij} - X_{ij})}\left(\sigma^{\pi}_{ij} - X_{ij}\right) > 0 \tag{24}$$

Hence, its positivity is straightforward. In the same manner, Eq. (22) can be forced to be positive by choosing ζ_{π} in quadratic forms:

$$\zeta_{\pi} = \frac{a}{2}X_{ij}X_{ij} \quad \text{or} \quad \zeta_{\pi} = aJ_2(X_{ij}) \tag{25}$$

If such choices are made, the positivity of Eq. (22) is ensured. Taking into account that $\dot{\lambda}_d$ is positive for the same reasons as those previously exposed, the positivity of $Y + Z$ has to be checked. By definition, the thermodynamical force related to isotropic hardening Z is positive, so, only the positivity of Y has to be shown. Indeed, by using the classical consistency conditions, the scalar damage variable can be explicitly integrated which improves the numerical robustness. Thus, the thermodynamic force Z associated to isotropic hardening can be expressed as [7,8]:

$$Z = \tilde{Y} - Y_0 \tag{26}$$

where $\tilde{Y} - Y_0$ is a difference in energy which must always be positive or null.

Since Y_N^+ is non-negative, proving the positivity of $Y_d - Y_\pi$ is sufficient which should imply that:

$$Y = Y_N^+ + Y_d - Y_\pi > Y_d - Y_\pi \tag{27}$$

In order to eliminate the damage variable in the expression of the energy rate, the properties related to the function g are used:

$$Y_d - Y_\pi = \mu\varepsilon_{ij}^d\varepsilon_{ij}^d - \mu g'(d)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big) > \mu\varepsilon_{ij}^d\varepsilon_{ij}^d - \mu\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big) \tag{28}$$

The last part of Eq. (28), $\mu\varepsilon_{ij}^d\varepsilon_{ij}^d - \mu(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi)(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi)$, can be rewritten in a different way by considering its incremental form over a pseudo-time step Δt. The following relation can be obtained:

$$\mu\varepsilon_{ij}^d\varepsilon_{ij}^d - \mu\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big) = 2\mu\int_{\Delta t}\big(\varepsilon_{ij}^d\dot{\varepsilon}_{ij}^d - \big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\dot{\varepsilon}_{ij}^d - \dot{\varepsilon}_{ij}^\pi\big)\big)\,\mathrm{d}t \tag{29}$$

From the saturation property linked to the kinematic hardening ($f_\pi = 0$ implies that $\sigma_{ij}^\pi = X_{ij}$, therefore, $\dot{\varepsilon}_{ij}^d \geqslant \dot{\varepsilon}_{ij}^\pi \geqslant 0$), it can be deduced that at each pseudo-time step, two cases can occur. In the first one, $\dot{\varepsilon}_{ij}^\pi \to 0$, then:

$$2\mu\varepsilon_{ij}^d\dot{\varepsilon}_{ij}^d - 2\mu\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\dot{\varepsilon}_{ij}^d - \dot{\varepsilon}_{ij}^\pi\big) \to 0 \tag{30}$$

And, in the second one, $\dot{\varepsilon}_{ij}^\pi \to \dot{\varepsilon}_{ij}^d$ leading to:

$$2\mu\varepsilon_{ij}^d\dot{\varepsilon}_{ij}^d - 2\mu\big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\dot{\varepsilon}_{ij}^d - \dot{\varepsilon}_{ij}^\pi\big) \to 2\mu\varepsilon_{ij}^d\dot{\varepsilon}_{ij}^d > 0 \tag{31}$$

Therefore, in both cases, $2\mu\varepsilon_{ij}^d\dot{\varepsilon}_{ij}^d - 2\mu(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi)(\dot{\varepsilon}_{ij}^d - \dot{\varepsilon}_{ij}^\pi) > 0$.

So, for any loading path, we get:

$$Y_d - Y_\pi = 2\mu\int_{\Delta t}\big(\varepsilon_{ij}^d\dot{\varepsilon}_{ij}^d - \big(\varepsilon_{ij}^d - \varepsilon_{ij}^\pi\big)\big(\dot{\varepsilon}_{ij}^d - \dot{\varepsilon}_{ij}^\pi\big)\big)\,\mathrm{d}t > 0 \tag{32}$$

Then, by considering Eq. (27), the energy rate released due to damage is positive for all strain paths. That allows concluding to the positivity of $Y + Z$. From this conclusion, the intrinsic dissipation can be stated as being positive, $\varphi > 0$. The thermodynamical admissibility of the set of constitutive equations coupling elasticity, isotropic damage and internal damage previously exposed is proved.

6. Conclusion

In this Note, a class of constitutive equations coupling elasticity, isotropic damage and internal sliding has been exposed. Several materials may be modelled within this framework such as concrete or the steel/concrete interface, for instance [7,8]. The irreversible processes thermodynamics framework is used in order to ensure a certain consistency and reliability with respect to well-known physics principles. A consistent thermodynamical state potential related to the constitutive framework satisfying the necessary mathematical requirements has been presented. State laws are derived naturally from its expression and a general form of the flow rules has been presented. Finally, a proof of the thermodynamical admissibility of this constitutive framework has been given. Moreover, specific choices related to the flow rules have been made in order to ensure the thermodynamical admissibility of the constitutive framework. Therefore, this framework allows to develop robust and reliable constitutive laws and should help better predicting the mechanical behaviour of quasi-brittle materials. Furthermore, the efficiency of this class of constitutive equations has been shown through numerical case-studies at structural scale in order to simulate the concrete behaviour [7] as well as the one of the steel/concrete interface [8]. A similar study should also be performed using an anisotropic damage model based on the same framework [9,10].

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