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Continuum damage model for thermo-mechanical coupling in quasi-brittle materials

Minh Ngo [a,*], Adnan Ibrahimbegovic [a], Delphine Brancherie [b]

[a] Ecole Normale Supérieure, LMT-Cachan, 61 Avenue du Président Wilson, 94235 Cachan, France
[b] Université de Technology de Compiegne, Laboratoire Roberval, 60205 Compiègne Cedex, France

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ABSTRACT

In this article we introduce a thermo-mechanical damage model, which is capable of representing the behavior of quasi-brittle materials subjected simultaneously to mechanical loading and heat transfer. Special care is taken of the quasi-brittle material behavior which can be represented by the continuum damage model, along with the solution procedures for fully coupled thermo mechanical loading conditions.

1. Introduction

In concrete structures exposed to high temperature conditions, such as constructions under fire disaster or concrete shells in the nuclear power plants, concrete structures have to bear not only the mechanical but also the temperature loading. In this case, thermo-mechanical coupling implies that the dissipation due to mechanical loading becomes an additional heat supply raising the temperature, while the temperature loading itself leads to mechanical deformation in the structure. In any such case, it is important to study the thermo-mechanical coupling effect in the structure. There are a number of previous studies focusing on different aspects of this problem [1–9]. However, the vast majority is limited to the elastic or elasto-plastic models, and thus they are more suitable to be applied to ductile materials such as steel rather than the quasi-brittle materials such as concrete. There are also more recent research works related to the behavior of concrete structures under thermo-mechanical coupling effect. We can mention the work of Baker and Borst [10] on damage model for concrete, which however, only proposed a thermo-dynamical theoretical framework for this problem without going into details of neither numerical implementation nor solution procedure. In this paper we present not only the new thermo-dynamical theoretical framework, which is more general than the previous ones, but alsoexamine the details of the numerical solution procedure considering full thermo-mechanical coupling. A detailed development is presented for the damage model suitable for quasi-brittle material such as concrete. Several numerical applications are also presented in order to show the ability of the proposed model to capture the salient features of the coupled thermo-mechanical response. The proposed model could be applied to estimate the behavior of the quasi-brittle material in continuum region, where the displacement is consider to be small and classical continuum mechanics can be applied. However, it is not capable of taking into account the localized failure of the material, which exceeds the boundary of classical continuum mechanics.

2. Continuum thermo-damage model for quasi-brittle materials

2.1. Thermodynamics framework

The starting point is the local form of the first principle of thermodynamics for the case of thermo-mechanical inelastic response [11]:

$$R - \nabla \cdot \mathbf{q} = -\boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} + \dot{\mathbf{e}}(\boldsymbol{\varepsilon}, \eta^e) \tag{1}$$

where R is the heat supply, $\mathbf{q}$ is the heat flow, $\boldsymbol{\sigma}$ is the stress field, $\boldsymbol{\varepsilon}$ is the strain field, $\mathbf{e}$ is the internal energy and η^e is the reversible part of entropy ("elastic" entropy).

By applying the Legendre transformation, we can introduce an alternative potential in terms of the free energy ψ, such that:

$$\mathbf{e} = \psi(\boldsymbol{\varepsilon}, \theta, \mathbf{D}, \xi) + \eta^e\theta$$

where θ is the temperature as dual variable to entropy. For such a potential, the state variables are the strain $\boldsymbol{\varepsilon}$, compliance tensor $\mathbf{D}$ and hardening variable ξ.

The first principle of thermodynamics (1) can be re-written in terms of this free energy potential:

* Corresponding author. Tel.: +33 634103775.
E-mail addresses: ngo@lmt.ens-cachan.fr (M. Ngo), adnan.ibrahimbegovic@ens-cachan.fr (A. Ibrahimbegovic), delphine.brancherie@utc.fr (D. Brancherie).

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$$R - \nabla \cdot \mathbf{q} = \left(\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} - \boldsymbol{\sigma}\right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(\frac{\partial \psi}{\partial \theta} + \eta^e\right)\dot{\theta} + \theta\dot{\eta}^e + \frac{\partial \psi}{\partial \mathbf{D}} \cdot \dot{\mathbf{D}} + \frac{\partial \psi}{\partial \xi}\dot{\xi} \quad (2)$$

In the case of an elastic process, where $\dot{\mathbf{D}} = 0$ and $\dot{\xi} = 0$, Eq. (2) provides the state equations for the stress and "elastic" entropy:

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} \quad (3)$$

$$\eta^e = -\frac{\partial \psi}{\partial \theta} \quad (4)$$

along with the final local conservation equation for energy, which can be written:

$$R - \nabla \cdot \mathbf{q} = \theta\dot{\eta}^e + \frac{\partial \psi}{\partial \mathbf{D}} \cdot \dot{\mathbf{D}} + \frac{\partial \psi}{\partial \xi}\dot{\xi} \quad (5)$$

By taking into account that the two state Eqs. (3) and (4) derive from the same free energy potential, we can confirm the Maxwell relation as the equality of mixed partial derivatives of such a potential and thus provide the definition of the thermal stress:

$$\boldsymbol{\beta} := -\frac{\partial \boldsymbol{\sigma}}{\partial \theta} = \frac{\partial \eta^e}{\partial \theta} - \frac{\partial^2 \psi}{\partial \theta \partial \boldsymbol{\varepsilon}} \quad (6)$$

We note that $\boldsymbol{\beta}$ is the second-order tensor that gives the relation between stress and temperature.

Moreover, the heat capacity coefficient (ρc), which controls the evolution of internal energy due to temperature, can be defined by the second derivative of free energy with respect to the temperature:

$$\rho c := \frac{\partial e}{\partial \theta} = \frac{\partial \psi}{\partial \theta} + \frac{\partial \eta^e}{\partial \theta}\theta + \eta^e = -\theta\frac{\partial^2 \psi}{\partial \theta^2} \quad (7)$$

Finally, the derivative of the free energy with respect to the strain tensor defines the tangent modulus:

$$\mathbf{C} := \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} = \frac{\partial^2 \psi}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\varepsilon}} \quad (8)$$

In this damage model, we note that the current value of tangent stiffness tensor is equal to the inverse value of compliance damage tensor $\mathbf{D}$:

$$\mathbf{C} := \frac{\partial^2 \psi}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\varepsilon}} = \mathbf{D}^{-1} \quad (9)$$

In building the formula of free energy potential, we assume that the free energy is a sum of mechanical energy (ψ_m) [13], thermal energy (ψ_t) and thermo-mechanical energy (ψ_{tm}). In our work, a quadratic form is chosen for mechanical and thermo-mechanical free energy, while the log-form in temperature is chosen for thermal free energy in order to re-establish the Fourier laws in heat transfer problem. More precisely, we write:

$$\psi_m = \frac{1}{2}\boldsymbol{\varepsilon} \cdot \mathbf{D}^{-1} \cdot \boldsymbol{\varepsilon} + \Xi(\xi)$$

$$\psi_t = \rho c\left[(\theta - \theta_0) - \theta \ln\frac{\theta}{\theta_0}\right]$$

$$\psi_{tm} = -\boldsymbol{\varepsilon} \cdot \boldsymbol{\beta}(\theta - \theta_0)$$

then

$$\psi = \frac{1}{2}\boldsymbol{\varepsilon} \cdot \mathbf{D}^{-1} \cdot \boldsymbol{\varepsilon} + \Xi(\xi) - \boldsymbol{\varepsilon} \cdot \boldsymbol{\beta}(\theta - \theta_0) + \rho c\left[(\theta - \theta_0) - \theta \ln\frac{\theta}{\theta_0}\right] \quad (10)$$

where is the reference temperature.

With the given formula of free energy, we can rewrite the state equations as:

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} = \mathbf{D}^{-1} \cdot \boldsymbol{\varepsilon} - \boldsymbol{\beta}(\theta - \theta_0) = \boldsymbol{\sigma}_\mathbf{m} - \boldsymbol{\sigma}_\mathbf{0} \quad (11)$$

$$\eta^e = -\frac{\partial \psi}{\partial \theta} = \varepsilon \cdot \beta + \rho c \ln\left(\frac{\theta}{\theta_0}\right) \quad (12)$$

The internal variable which controls the evolution of damage threshold () can also be computed as:

$$q = -\frac{\partial \psi}{\partial \xi} = -\frac{\partial \Xi}{\partial \xi} \quad (13)$$

The variable associated with compliance can also be defined:

$$\mathbf{Y} = -\frac{\partial \psi}{\partial \mathbf{D}} = -\frac{\partial \psi_m}{\partial \mathbf{D}} = \frac{1}{2}(\mathbf{D}^{-1}\boldsymbol{\varepsilon}) \otimes (\mathbf{D}^{-1}\boldsymbol{\varepsilon}) = \frac{1}{2}\boldsymbol{\sigma}_\mathbf{m} \otimes \boldsymbol{\sigma}_\mathbf{m} \quad (14)$$

Denoting with η^d the irreversible part of entropy and with η the total entropy and accepting the additive split: $\eta = \eta^e + \eta^d$ [11], the local form of internal dissipation can be established as follows:

$$D_{\text{int}} = \theta\dot{\eta} + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} - \dot{\mathbf{e}} = \theta(\dot{\eta}^e + \dot{\eta}^d) + \boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} - \theta\dot{\eta}^e + \eta^e\dot{\theta} - \dot{\psi}$$

By taking into account that: $\dot{\psi} = \underbrace{\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}}_{\boldsymbol{\sigma}} \cdot \dot{\boldsymbol{\varepsilon}} + \underbrace{\frac{\partial \psi}{\partial \mathbf{D}}}_{-\mathbf{Y}} \cdot \dot{\mathbf{D}} + \underbrace{\frac{\partial \psi}{\partial \xi}}_{-q} \cdot \dot{\xi} + \underbrace{\frac{\partial \psi}{\partial \theta}}_{-\eta^e} \cdot \dot{\theta}$ we can further obtained:

$$D_{\text{int}} = \left(\boldsymbol{\sigma} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}\right) \cdot \dot{\boldsymbol{\varepsilon}} + \left(\eta^e - \frac{\partial \psi}{\partial \theta}\right)\dot{\theta} + \mathbf{Y} \cdot \dot{\mathbf{D}} + q\dot{\xi} + \theta\dot{\eta}^d$$

Finally, by exploiting the state Eqs. (11) and (12), we obtain the final expression of internal dissipation:

$$D_{\text{int}} = \underbrace{\mathbf{Y} \cdot \dot{\mathbf{D}} + q\dot{\xi}}_{D_{mech}} + \underbrace{\theta\dot{\eta}^d}_{D_t} \quad (15)$$

The particular result for $\mathbf{Y}$ in (14) finally gives the following expression for the internal dissipation:

$$D_{\text{int}} = \underbrace{\frac{1}{2}\boldsymbol{\sigma}_\mathbf{m} \cdot \dot{\mathbf{D}} \cdot \boldsymbol{\sigma}_\mathbf{m} + q\dot{\xi}}_{D_{mech}} + \underbrace{\theta\dot{\eta}^d}_{D_t} \quad (16)$$

We can also write the last result in an alternative form by taking into account the stress state equation in (11):

$$D_{\text{int}} = \underbrace{\frac{1}{2}(\boldsymbol{\sigma} + \boldsymbol{\beta}(\theta - \theta_0)) \cdot \dot{\mathbf{D}} \cdot (\boldsymbol{\sigma} + \boldsymbol{\beta}(\theta - \theta_0)) + q\dot{\xi}}_{D_{mech}} + \underbrace{\theta\dot{\eta}^d}_{D_t} \quad (17)$$

The damage threshold is chosen based upon the "mechanical" part of the stress state in the form:

$$0 \geqslant \Phi(\boldsymbol{\sigma}, q) = \underbrace{\sqrt{(\boldsymbol{\sigma} + \boldsymbol{\beta}(\theta - \theta_0)) \cdot \mathbf{D}^\mathbf{e} \cdot (\boldsymbol{\sigma} + \boldsymbol{\beta}(\theta - \theta_0))}}_{\|\boldsymbol{\sigma}_\mathbf{m}\|_{\mathbf{D}^\mathbf{e}}} - \frac{1}{\sqrt{E}}(\sigma_f - q) \quad (18)$$

where $\mathbf{D}^e$ denotes the undamaged elastic compliance ($\mathbf{D}^\mathbf{e} = \mathbf{C}^{\mathbf{e}^{-1}}$), σ_f denotes the damage limit stress and $q = -\frac{d\Xi}{d\xi}$ denotes the stress-like variable associated with hardening.

The evolution laws of internal variables ($\mathbf{D}$, ξ and η^d) are obtained by Kuhn Tucker optimality condition, in which the evolutions of internal variables have to guarantee the maximum value of dissipation, along with the stress admissibility ($\Phi \leqslant 0$). This could be formally defined as:

Find: maximum of D_{int} with the condition: $\Phi(\boldsymbol{\sigma}, q) \leqslant 0$

$$\iff \underbrace{\max}_{\gamma \geqslant 0} \min L = [-D_{\text{int}}(\boldsymbol{\sigma}, q) + \gamma\Phi(\boldsymbol{\sigma}, q)]$$

The corresponding Kuhn Tucker condition can be obtained as: