



# On the form of free energy and specific heat in coupled thermo-elasticity with isotropic damage

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## Abstract

This paper concerns the form of the free energy function in coupled thermo-mechanical problems with isotropic damage, particularly where damage accrues through both mechanical and thermal strains, and when the material is exposed to elevated temperatures. We show that with the normal assumption of a constant specific heat coefficient, mechanical dissipation is negative and so the second law of thermodynamics is violated. This is true even for a general isotropic damage model that allows independent damage on the Young's modulus and the bulk modulus. Our approach is to make specific heat damage dependent, and under these conditions, we show positive dissipation for a range of problems; for the case of concrete, at least, there is material evidence supporting this model. For elevated temperatures, we use the logarithmic form of thermal energy, again showing positive dissipation. Comparisons between the forms show a notable difference in the energy transformed to heat, which is significant when reintroduced into the computations. © 2000 Elsevier Science Ltd. All rights reserved.

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## 1. Introduction

The governing equations of (linearised) coupled thermo-elasticity are obtained from a quadratic free energy function, written in the form:

$$\psi = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{E} : \boldsymbol{\varepsilon} - \mathfrak{I} \mathbf{m} : \boldsymbol{\varepsilon} - \frac{1}{2} c \frac{\vartheta^2}{\theta_0} \quad (1)$$

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where  $\psi$  is the Helmholtz free energy,  $\boldsymbol{\sigma}$  and  $\boldsymbol{\varepsilon}$  are the local stress and strain tensors,  $\vartheta$  and  $\theta_0$  are the relative temperature and reference temperature, respectively, and  $\mathbf{m}$  is the thermo-elastic coupling tensor. Finally,  $c$  is the specific heat capacity, assumed to be constant and independent of strain (or stress) and temperature, which is defined by:

$$c = -\theta_0 \frac{\partial^2 \psi}{\partial \theta^2} \quad (2)$$

In fact, the tangent elasticity is obtained as the second derivative of  $\psi$ ,

$$\mathbf{E} = \frac{\partial^2 \psi}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\varepsilon}} \quad (3)$$

and so Eq. (1) can be recovered by integrating Eq. (3) twice with respect to strain and introducing Eq. (2).

The constitutive relations for stress,  $\boldsymbol{\sigma}$ , and entropy,  $\eta$ , in infinitesimal thermo-elasticity are given by:

$$\begin{aligned} \boldsymbol{\sigma} &= \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} = \mathbf{E}:\boldsymbol{\varepsilon} - \vartheta \mathbf{m} \\ \eta &= -\frac{\partial \psi}{\partial \theta} = \mathbf{m}:\boldsymbol{\varepsilon} + c \frac{\vartheta}{\theta_0} \end{aligned} \quad (4)$$

In this article, we are concerned with the free energy function for thermo-elasticity in the presence of damage at (possibly) very high and transient temperatures. For the analysis of concrete under stress and elevated temperatures in the range  $\theta = 25\text{--}800^\circ\text{C}$ , the authors have adapted Mazars' scalar damage model (Mazars and Pijaudier-Cabot, 1989) to include a temperature dependence. That is, both mechanical and thermal damage are included, based on the relevant eigenstrains in the material. That damage model assumed a free energy function given by:

$$\psi = \frac{1}{2} \boldsymbol{\varepsilon}:\mathbf{E}(d, g):\boldsymbol{\varepsilon} - \vartheta \mathbf{m}(d, g):\boldsymbol{\varepsilon} - \frac{1}{2} c \frac{\vartheta^2}{\theta_0} \quad (5)$$

where  $d$  is the stress induced (mechanical) damage parameter and  $g$  is the thermal damage parameter; the former is given in strain dependent functional form as in Mazars and Pijaudier-Cabot (1989), extended to include temperature reliance (Baker and Stabler, 1998), and the latter is given in a functional form determined from uniaxial test data. For completeness, we give the details of our model in Section 2, but the discussion focuses on the more fundamental thermodynamic framework.

We should also record that given a set of micro-structural damage variables,  $\mathbf{D} = (d, g)$ , the internal mechanical dissipation in the material is given by:

$$\phi_{\text{mech}} = -\frac{\partial \psi}{\partial \mathbf{D}}:\dot{\mathbf{D}} = -\left(\frac{\partial \psi}{\partial d} \dot{d} + \frac{\partial \psi}{\partial g} \dot{g}\right) \quad (6)$$

and the dissipation due to heat conduction is given by the standard relation:

$$\phi_{\text{con}} = -\frac{1}{\theta} \nabla \theta:\mathbf{q} \quad (7)$$

where  $\mathbf{q}$  is the heat flux tensor. We remark that this latter is just a condition which is automatically satisfied by the use of Fourier's Law of heat conduction.

The problem we address in this paper is that in using a free energy like Eq. (5), where elastic modulus reduces with temperature, it can be shown that the mechanical dissipation in Eq. (6) can be easily *negative*, and this, of course, entirely violates the second law of thermodynamics. Section 3 demonstrates the problem in both steady state and transient examples of heat conduction, without mechanical damage. We then generalise the isotropic damage model to include thermal damage parameters for elastic modulus and Poisson's ratio, but retain the original constant specific heat coefficient. The reason is that the differential effects might permit sufficient flexibility in the model to guarantee an overall positive dissipation even if mechanical dissipation associated with one of the damage parameters became negative. However, we again show analytically in a steady state problem that dissipation is negative, whatever is the relationship between the two parameters.

Our solution is to propose a damage dependent specific heat coefficient, which we show analytically and numerically to give positive mechanical dissipation in the same problems. The coefficient cannot be temperature dependent as the basic relationship between specific heat and free energy would be invalid. The experimental evidence suggests that specific heat in concrete increases with temperature (Schneider, 1988). However, in a damage model that adopts an effective continuum concept, it can be argued that the variation of specific heat is reflected through the corresponding damage parameters.

The quadratic form of thermal energy in Eq. (5) corresponds to the restriction to low temperatures. We extend the variable specific heat argument to a logarithmic form appropriate for elevated temperatures, and again show that dissipation is positive. In comparing the two forms, it is shown that the temperature profile in a specimen is virtually the same, but that the entropy and dissipation vary significantly; this latter is important in calculating and using the mechanical energy transformed to heat.

For completeness, we show the discrete form of the thermal evolution equations for a finite element code in Appendix A. While full details of suitable integration schemes are available for thermo-elasticity (Armero and Simo, 1992), thermo-plasticity (Simo and Miehe, 1992) and thermo-damage (Stabler and Baker, 2000), here we develop the algorithm to show the effect that the damage dependence of specific heat has on the discrete equations.

## 2. Isotropic thermo-damage model

The thermo-damage model developed in the current research project is a phenomenological model that considers concrete as a homogeneous material. The principal assumptions are that the material remains isotropic and that damage affects the Young's modulus and the bulk modulus equally i.e. Poisson's ratio is not affected by damage. Two internal variables are used to describe the damage in the material: a mechanically induced damage component  $d$ , and a thermally induced damage component  $g$ .

From the phenomenological point of view, two damage variables are used because there are different processes through which damage occurs. Mechanical damage represents damage that occurs when an external force system or a non-linear temperature profile induces stresses in the material. Thermal damage represents damage that occurs during thermal expansion of the material. Experimentally, it has been observed that a tensile strain of 1000  $\mu\epsilon$  resulting from an applied tensile load will cause almost total loss of material stiffness i.e.  $d \approx 1$  (Bažant and Pijaudier-Cabot, 1989). The same strain, when resulting from a temperature increase of approximately 80°C, results in only a 15% reduction in the stiffness of the material (Schneider, 1988).

Eq. (8) gives the reduction of Young's modulus which can be used to generate the stiffness and coupling tensors:

$$E = (1 - d)(1 - g)E_0 \quad (8)$$

In distinguishing between mechanical and thermal damage, it is necessary to decompose the strain tensor into the stress related part and the free thermal part. For a given temperature increase, the increase in the free thermal strain represents the thermal expansion in the stress free state. The relationship between the total strain, the stress related strain and the free thermal strain is given by:

$$\boldsymbol{\varepsilon}^{\text{stress}} = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{free}} = \boldsymbol{\varepsilon} - \beta \vartheta \mathbf{1} \quad (9)$$

In the above equation,  $\beta$  represents the coefficient of thermal expansion and  $\vartheta$  represents the temperature increase.

### 2.1. Model for mechanical damage

The mathematical model used to describe the mechanical damage is an extension of the non-local version of Mazars' scalar damage model. The evolution of damage is controlled by the definition of a damage surface which can be written as:

$$f_d = \bar{\varepsilon} - k(d, \theta) \quad (10)$$

In the above equation,  $\bar{\varepsilon}$  is the non-local equivalent strain and is calculated from the stress related strain. The symbol  $k(d, \theta)$  represents the hardening–softening parameter and controls the size of the damage surface. Initially, the size of the damage surface is given by a threshold strain  $k_0(\theta)$ . The temperature dependence implies that the size of the threshold damage surface expands with increasing temperature. Once damage has occurred,  $k$  takes the maximum value of either the temperature dependent threshold strain or the equivalent strain reached during the previous loading history.

The non-local equivalent strain is calculated from the weighted average of the local equivalent strain taken over a region about the point considered. This paper uses the Mazars' definition for the local equivalent strain which, for the thermo-damage model, is defined as follows:

$$\tilde{\varepsilon} = \sqrt{\sum_{i=1}^3 \left( \frac{|\varepsilon_i^{\text{stress}}| + \varepsilon_i^{\text{stress}}}{2} \right)^2} \quad (11)$$

where  $\varepsilon_i^{\text{stress}}$  refers to the principal values of the stress related strains. Note that it is also possible to use other definitions of equivalent strains, such as the modified von Mises definition (de Vree et al., 1995; Peerlings et al., 1998).

The non-local equivalent strain is calculated by integrating the local equivalent strain over a region about the point being considered. This is done using the following equations:

$$\bar{\varepsilon} = \frac{1}{V_r} \int_{\Omega} \Psi(\mathbf{x} - \mathbf{s}) \tilde{\varepsilon} \, d\Omega \quad (12)$$

$$V_r = \int_{\Omega} \Psi(\mathbf{x} - \mathbf{s}) \, d\Omega \quad (13)$$

where  $\Omega$  is the volume of the structure. The weighting function  $\Psi(\mathbf{x} - \mathbf{s})$  is defined by the following function:

$$\Psi(\mathbf{x} - \mathbf{s}) = \exp\left(-\frac{4\|\mathbf{x} - \mathbf{s}\|^2}{l_c^2}\right) \quad (14)$$

where  $l_c$  is the internal length. The representative region over which  $\bar{\epsilon}$  is calculated is taken as a circle of radius  $1.2l_c$  about point  $s$ . Outside this region, the value of the weighting function is taken to be zero.

The growth of damage is governed by a set of flow rules. For an integrated damage model, these flow rules can be written as:  $d = d(\bar{\epsilon}, \theta)$  if  $f_d = 0$  and  $\dot{f}_d = 0$ , else  $\dot{d} = 0$ . In this model, the damage parameter  $d$  is taken as the weighted average of the damage function for uniaxial tension  $d_t$ , and the damage function for uniaxial compression  $d_c$ . This is given by

$$d = \alpha_t d_t + \alpha_c d_c \tag{15}$$

When the stress state is in biaxial compression, the weighting functions are given by  $\alpha_c = 1$  and  $\alpha_t = 0$ ; and when the stress state is in biaxial tension, the weighting functions are given by  $\alpha_c = 0$  and  $\alpha_t = 1$ . For the remaining case where one principal stress is tensile and the other is compressive, the weighting functions are calculated from the following equations:

$$\alpha_c = \frac{-\nu}{(\varpi - \nu)} \quad \text{and} \quad \alpha_t = \frac{\varpi}{(\varpi - \nu)} \tag{16}$$

In the above equations,  $\varpi = \sigma_j/\sigma_i$  and represents the ratio of the tensile principal stress  $\sigma_j$  to the compressive principal stress  $\sigma_i$ . This definition for the weighting function allows the use of both the Mazars' and the modified von Mises definition of the equivalent strain.

The uniaxial damage functions take the exponential form proposed by Mazars' and are written as:

$$d_i = 1 - \frac{(1 - A_i)k_0(\theta)}{\bar{\epsilon}} - \frac{A_i}{e^{[B_i F(\theta)(\bar{\epsilon} - k_0(\theta))]}}, \quad \text{where } i = c \text{ or } t \tag{17}$$

In the above equations,  $A_c$ ,  $A_t$ ,  $B_c$  and  $B_t$  are material damage parameters. A temperature dependence has been introduced via the function  $F(\theta)$  and the thermal dependence of the threshold strain  $k_0(\theta)$ . The function  $F(\theta)$  controls the decay of the peak stress with temperature and depends on the formulation of the thermal damage function which is given below.

### 2.2. Model for thermal damage

The thermal damage parameter  $g$  represents damage due to the differential thermal expansion of the constituents of the concrete and the thermal damage in the cement paste. Both of these damage mechanisms are functions of the temperature, and therefore, the thermal damage can be considered as a function of temperature. The growth of thermal damage is controlled by a one-dimensional thermal damage surface which is given by:

$$f_g = \theta - \bar{k}(g, \theta) \tag{18}$$

where  $\theta$  is the thermodynamic temperature and  $\bar{k}(g, \theta)$  represents a hardening parameter which controls the size of the damage surface. The initial size of the damage surface is given by the initial temperature of the system and the damage surface expands as thermal damage occurs with increasing temperature. The condition controlling the evolution of thermal damage can be written as:  $g = g(\theta)$  if  $f_g = 0$  and  $\dot{f}_g = 0$ , else  $\dot{g} = 0$ .

In this paper, the following expression has been used for the thermal damage function:

$$g = 1 - (Z_1 - Z_2\theta)F(\theta) \tag{19}$$

where the function  $F(\theta)$  is the same function used in Eq. (17) and is given by

Table 1  
Damage parameters used in the thermo-damage model

$A_c$	$B_c$	$A_t$	$B_t$	$Z_1$	$Z_2$ ( $^{\circ}\text{C}^{-1}$ )	$Z_3$ ( $^{\circ}\text{C}$ )	$Z_4$ ( $^{\circ}\text{C}$ )
1.4	1850	0.95	5300	1.296	$992 \times 10^{-6}$	312.5	14.5

$$F(\theta) = \frac{Z_3}{(\theta + Z_4)} \quad (20)$$

This model for the thermal damage requires four damage parameters  $Z_1$ – $Z_4$ . These parameters were determined by considering some of the experimental data for concrete tested in uniaxial compression at elevated temperatures. Values for these damage parameters, as well as the other material parameters required for the numerical examples, are given in Table 1 and 2.

### 3. The classical free energy function

The purpose of this section is to identify the problem associated with using an isotropic damage model in conjunction with the classical free energy function given by Eq. (5). This will be done both analytically and numerically. We point out that the analytical investigation is independent of the specific details of the thermo-damage model.

#### 3.1. Negative dissipation: the steady state case

Consider first a sample in which the temperature is raised uniformly throughout the material by an amount  $\vartheta$ . Because the temperature profile is uniform, the strain throughout the sample will be uniform and given by  $\boldsymbol{\varepsilon} = \beta\vartheta\mathbf{1}$ . Consequently, the sample will remain stress free and no mechanical damage will occur. Using  $\mathbf{E}_0$  and  $\mathbf{m}_0$  to represent the initial values of the elasticity and coupling tensors, the free energy function reduces to:

$$\psi = (1 - g)\frac{1}{2}\boldsymbol{\varepsilon}:\mathbf{E}_0:\boldsymbol{\varepsilon} - (1 - g)\vartheta\mathbf{m}_0:\boldsymbol{\varepsilon} - \frac{1}{2}c\frac{\vartheta^2}{\theta_0} \quad (21)$$

and so the thermodynamic force  $A$  becomes:

$$A = -\frac{\partial\psi}{\partial g} = \frac{1}{2}\boldsymbol{\varepsilon}:\mathbf{E}_0:\boldsymbol{\varepsilon} - \vartheta\mathbf{m}_0:\boldsymbol{\varepsilon} \quad (22)$$

Table 2  
Material properties used in the numerical examples

Young's modulus (MPa)	Poisson's ratio	Density ( $\text{kg}/\text{m}^3$ )	Coefficient thermal expansion ( $^{\circ}\text{C}^{-1}$ )	Specific heat ( $\text{J}/\text{m}^3\text{ }^{\circ}\text{C}$ )	Conduction coefficient ( $\text{J}/\text{s m }^{\circ}\text{C}$ )
31	0.2	2450	$12 \times 10^{-6}$	$2.06 \times 10^6$	3.0

or

$$A = \boldsymbol{\varepsilon} : \left( \frac{1}{2} \mathbf{E}_0 : \boldsymbol{\varepsilon} - \mathfrak{M}_0 \right) \tag{23}$$

The stress free condition requires that

$$\boldsymbol{\sigma} = (1 - g)(\mathbf{E}_0 : \boldsymbol{\varepsilon} - \mathfrak{M}_0) = 0 \tag{24}$$

which implies that the thermodynamic force must be negative.

In fact, we can determine the value of thermo-dynamic force for numerical comparisons later. For this problem, the strain field can be written as:

$$\boldsymbol{\varepsilon} = \beta \vartheta \mathbf{1} \tag{25}$$

where  $\beta$  is the linear coefficient of thermal expansion and  $\mathbf{1}$  is the second-order identity tensor.

Firstly, we evaluate the components of a tensor  $\mathbf{F} = \mathbf{E}_0 : \boldsymbol{\varepsilon}$ , in terms of the initial bulk modulus,  $K_0$ , giving:

$$\begin{aligned} F_{11} = F_{22} = F_{33} &= 3K_0\beta\vartheta \\ F_{12} = F_{21} = F_{23} = F_{32} = F_{13} = F_{31} &= 0 \end{aligned} \tag{26}$$

We then find  $\boldsymbol{\varepsilon} : \mathbf{E}_0 : \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon} : \mathbf{F}$  to be:

$$\boldsymbol{\varepsilon} : \mathbf{E}_0 : \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon} : \mathbf{F} = 9K_0\beta^2\vartheta^2 \tag{27}$$

and the product  $\mathfrak{M} : \boldsymbol{\varepsilon}$  to be:

$$\mathfrak{M} : \boldsymbol{\varepsilon} = \mathfrak{M} : \mathbf{1} = 9K_0\beta\mathbf{1} : \boldsymbol{\varepsilon} = 9K_0\beta^2\vartheta^2 \tag{28}$$

Substituting Eqs. (27) and (28) into Eq. (23) gives the thermodynamic force as:

$$A = -\frac{9}{2}K_0\beta^2\vartheta^2 \leq 0 \tag{29}$$

and so the dissipation inequality is violated.

### 3.2. Numerical simulation of the heating process

The next stage is to consider the variation of the temperature profile that exists during the heating of a specimen. The example shown in Fig. 1 was modelled numerically using the thermo-damage model

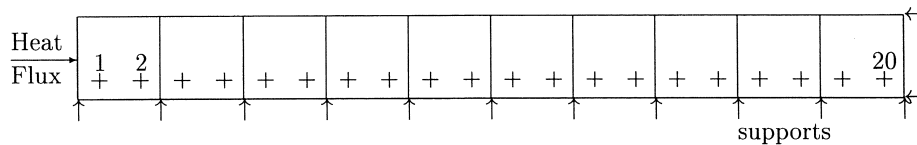


Fig. 1. Numerical heating problem.

described in Section 2 and the Helmholtz free energy function given by Eq. (5). The finite element integration was performed using a fractional step method described completely in Stabler and Baker (2000).

Fig. 1 shows that one face of the specimen is heated with a constant heat flux of  $500 \text{ W/m}^2$ . All other faces are insulated. The heat flux is applied for a period of 4000 s and then removed. The analysis continues for a further 6000 s to allow the temperature profile to equalise throughout. The thermal time step used was 5 s, and there were 200 mechanical time steps per thermal time step. For the purpose of this demonstration, thermal damage was allowed to proceed even if the calculated mechanical dissipation was negative.

Fig. 2 gives the variation of temperature, thermodynamic force and accumulated energy dissipated against time for each of the 20 Gauss points. For the purpose of this demonstration, we plot the accumulated energy dissipated at the individual Gauss points, which is just the integral over time of the mechanical dissipation. For this example, where there is no mechanical (stress based) damage, we have:

$$\mathcal{D} = - \int_t \frac{\partial \psi}{\partial \mathbf{g}} \dot{\mathbf{g}} dt \quad (30)$$

which is calculated using standard finite element quadrature rules. We remark again that the non-negativity of  $\phi_{\text{con}}$  is a condition which is automatically satisfied by the use of Fourier's Law of heat conduction, and its integral does not represent a physical quantity. Thus, the volume integral of  $\mathcal{D}$  represents the total amount of mechanical energy converted to heat.

It is clear from Fig. 1 that all Gauss points experience negative dissipation; moreover, the numerical value of the thermodynamic force at steady state conditions corresponds exactly to the value given by Eq. (29).

### 3.3. Generalised isotropic damage

The thermo-damage model presented in Section 2 assumes that both mechanical and thermal damage affect the Young's modulus and bulk modulus equally. Consequently, Poisson's ratio is not affected by damage. The more general form of an isotropic damage model allows the Young's modulus and the bulk modulus to be affected by damage differently. The following question must be asked: Is it possible to formulate an isotropic thermo-damage model with constant specific heat that satisfies the second law of thermodynamics?

Suppose that an isotropic thermo-damage model can be formulated with two damage parameters  $\alpha = (x, y)$ , where  $x$  is the thermo-damage parameter affecting the Young's modulus and  $y$  is the thermo-damage parameter affecting the bulk modulus. Suppose also that the parameters  $x, y$  include the effect of both mechanical and thermal damage. For a damage model of this form, the Helmholtz free energy function can be written as:

$$\psi = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{E}(x, y) : \boldsymbol{\varepsilon} - \mathfrak{m}(y) : \boldsymbol{\varepsilon} - \frac{1}{2} c \frac{\vartheta^2}{\theta_0} \quad (31)$$

The reduced Young's modulus and bulk modulus are given by the following equations:

$$E = (1 - x)E_0 \quad \text{and} \quad K = (1 - y)K_0 \quad (32)$$

In the damaged state, Poisson's ratio is given by



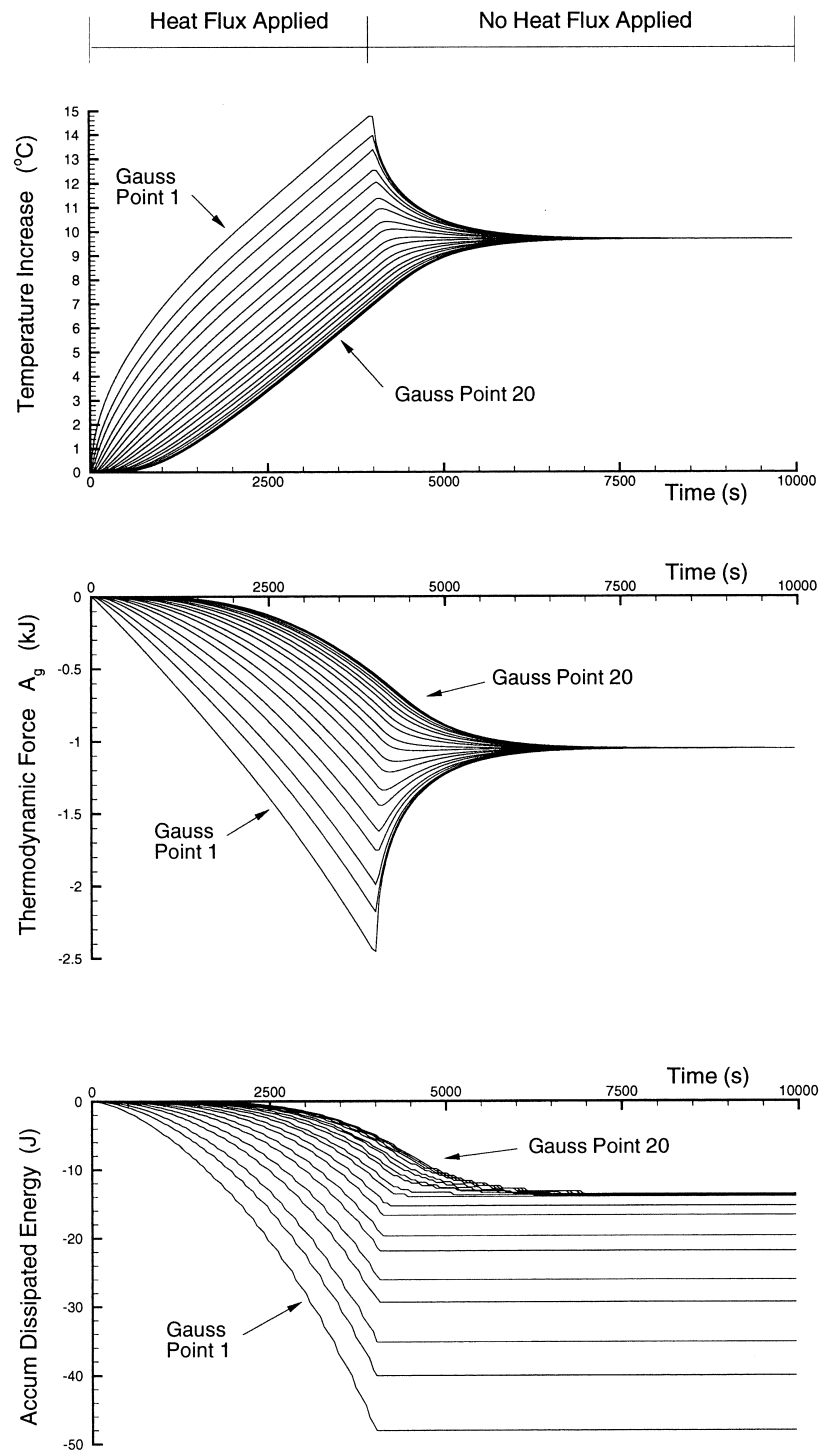


Fig. 2. Results for the original quadratic free energy function.

$$\nu = \frac{1}{2} - \frac{(1-x) E_0}{(1-y) 6K_0} \tag{33}$$

By considering allowable values of Poisson’s ratio, it is possible to map a region in the  $x, y$  space defining allowable values of  $x$  and  $y$  damage. This region is shown in Fig. 3 and is described by the relation:

$$\text{for } y = f(x) \quad 0 \leq x \leq 1 \quad 0 \leq y \leq 1 - (1-x) \frac{E_0}{3K_0} \tag{34}$$

The strain energy component  $\frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{E} : \boldsymbol{\varepsilon}$  of Eq. (31) can be written as:

$$\frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{E} : \boldsymbol{\varepsilon} = \frac{1}{2} C_1 [\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2] + C_2 [\varepsilon_{11} \varepsilon_{22} + \varepsilon_{22} \varepsilon_{33} + \varepsilon_{33} \varepsilon_{11}] + C_3 [\varepsilon_{12}^2 + \varepsilon_{23}^2 + \varepsilon_{13}^2] \tag{35}$$

and the thermo-elastic coupling  $\boldsymbol{\vartheta} \mathbf{m} : \boldsymbol{\varepsilon}$  is given by:

$$\boldsymbol{\vartheta} \mathbf{m} : \boldsymbol{\varepsilon} = 3\vartheta\beta(1-y)K_0[\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}] \tag{36}$$

In Eq. (35), the constitutive coefficients, obtained from Lamé’s constants, are:

$$C_1 = \lambda + 2\mu = \frac{3(1-y)K_0[3(1-y)K_0 + (1-x)E_0]}{[9(1-y)K_0 - (1-x)E_0]}$$

$$C_2 = \lambda = \frac{3(1-y)K_0[3(1-y)K_0 - (1-x)E_0]}{[9(1-y)K_0 - (1-x)E_0]}$$

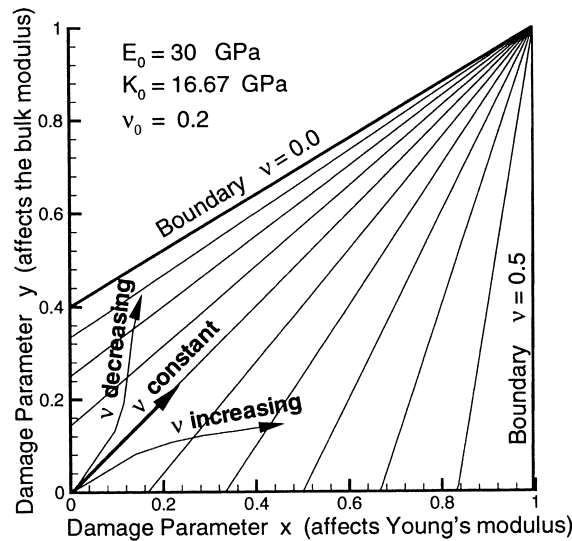


Fig. 3. Change of Poisson’s ratio with damage.

$$C_3 = 2\mu = \frac{6(1-y)K_0(1-x)E_0}{[9(1-y)K_0 - (1-x)E_0]} \quad (37)$$

The thermodynamic forces are evaluated as:

$$A_x = -\frac{\partial\psi}{\partial x} = -\frac{1}{2}\frac{\partial C_1}{\partial x}[\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2] - \frac{\partial C_2}{\partial x}[\varepsilon_{11}\varepsilon_{22} + \varepsilon_{22}\varepsilon_{33} + \varepsilon_{33}\varepsilon_{11}] - \frac{\partial C_3}{\partial x}[\varepsilon_{12}^2 + \varepsilon_{23}^2 + \varepsilon_{13}^2] \quad (38)$$

and

$$A_y = -\frac{\partial\psi}{\partial y} = -\frac{1}{2}\frac{\partial C_1}{\partial y}[\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2] - \frac{\partial C_2}{\partial y}[\varepsilon_{11}\varepsilon_{22} + \varepsilon_{22}\varepsilon_{33} + \varepsilon_{33}\varepsilon_{11}] - \frac{\partial C_3}{\partial y}[\varepsilon_{12}^2 + \varepsilon_{23}^2 + \varepsilon_{13}^2] - 3\vartheta\beta K_0[\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}] \quad (39)$$

where

$$\begin{aligned} \frac{\partial C_1}{\partial x} &= \frac{-36K^2 E_0}{(9K - E)^2} & \frac{\partial C_1}{\partial y} &= \frac{-3K_0(27K^2 - 6KE - E^2)}{(9K - E)^2} \\ \frac{\partial C_2}{\partial x} &= \frac{18K^2 E_0}{(9K - E)^2} & \frac{\partial C_2}{\partial y} &= \frac{-3K_0(27K^2 - 6KE + E^2)}{(9K - E)^2} \\ \frac{\partial C_3}{\partial x} &= \frac{-54K^2 E_0}{(9K - E)^2} & \frac{\partial C_3}{\partial y} &= \frac{6E^2 K_0}{(9K - E)^2} \end{aligned} \quad (40)$$

The mechanical dissipation is defined as

$$\phi_{\text{mech}} = A_x \dot{x} + A_y \dot{y} \quad (41)$$

and using Eqs. (38)–(40), the dissipation equation can be written as:

$$\begin{aligned} \phi_{\text{mech}} &= \left\{ \left[ 18K^2 E_0 \dot{x} + \frac{3K_0}{2}(27K^2 - 6KE - E^2)\dot{y} \right] [\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2] - \left[ 18K^2 E_0 \dot{x} - \frac{3K_0}{2}(54K^2 \right. \right. \\ &\quad \left. \left. - 12KE + 2E^2)\dot{y} \right] [\varepsilon_{11}\varepsilon_{22} + \varepsilon_{22}\varepsilon_{33} + \varepsilon_{33}\varepsilon_{11}] + \left[ 54K^2 E_0 \dot{x} - 6E^2 K_0 \dot{y} \right] [\varepsilon_{12}^2 + \varepsilon_{23}^2 + \varepsilon_{13}^2] \right\} \\ &\quad / (9K - E)^2 - 3\vartheta\beta K_0[\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}]\dot{y} \end{aligned} \quad (42)$$

Consider again the simple model problem described in Section 3.1 where the temperature of a specimen is raised uniformly throughout the material by a temperature  $\vartheta$ . The components of the strain tensor are

$$\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33} = \beta\vartheta \quad \text{and} \quad \varepsilon_{12} = \varepsilon_{23} = \varepsilon_{31} = 0 \quad (43)$$

Using these strains, Eq. (42) reduces to

$$\phi_{\text{mech}} = -\frac{9}{2}K_0\beta^2\vartheta^2\dot{y} \quad (44)$$

The above equation is true regardless of the relationship between  $x$  and  $y$  damage. Therefore, a two

parameter isotropic damage model with constant specific heat also violates the second law of thermodynamics.

#### 4. Modification to the free energy function solution

In this section, we propose a modification of the quadratic form of the free energy function and demonstrate that the second law of thermodynamics is now satisfied. In addition, we consider the logarithmic form of the free energy function as this is a more appropriate form for the case of large temperature changes. We conclude this section by considering some other loading cases and demonstrate that they also satisfy the second law of thermodynamics.

##### 4.1. Variable specific heat coefficient

Clearly, the free energy function must be modified to avoid violation of the dissipation inequality. Our approach is to allow the specific heat capacity to vary with damage, not temperature since otherwise the concept in Eq. (2) would no longer be valid. This results in the following general form for the free energy function:

$$\psi = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{E}(g, d) : \boldsymbol{\varepsilon} - \mathfrak{M}(g, d) : \boldsymbol{\varepsilon} - \frac{1}{2} c(g, d) \frac{g^2}{\theta_0} \quad (45)$$

In the above equation, the specific heat is a function of damage and should reflect the observed experimental behaviour. Furthermore, the relationship must obey the inequalities

$$\frac{\partial c(g, d)}{\partial g} > 0 \quad \text{and} \quad \frac{\partial c(g, d)}{\partial d} > 0 \quad (46)$$

so that it overcomes the negative term in the dissipation inequality. This allows the formulation to satisfy the second law of thermodynamics. The exact relationship between specific heat and damage depends on the formulation of the thermo-damage model. For the thermo-damage model presented in Section 2, the following exponential form can be used:

$$c(g, d) = \left[ x_1 + \frac{x_2}{(x_3 - g - d + dg)} \right] c_0 \quad (47)$$

##### 4.2. Thermal damage dependence

To evaluate the damage dependence of the specific heat, we first consider the unrestrained heating problem investigated in Section 3. In this problem, there is no mechanical damage and so the specific heat function becomes:

$$c(g) = \left[ x_1 + \frac{x_2}{(x_3 - g)} \right] c_0. \quad (48)$$

Substituting values of  $x_1 = 0.5707$ ,  $x_2 = 0.5623$  and  $x_3 = 1.31$  into the above equation results in a linear relationship between specific heat and temperature. This relationship is shown in Fig. 3. It should be said that the data for variation in specific heat is inconclusive (see Schneider, 1988), but a linear relationship between specific heat and temperature is quite justifiable.

*4.2.1. Positive dissipation: the steady state case*

Consider the steady state problem presented in Section 3.1. In this problem, the temperature throughout the sample was raised uniformly by an amount  $\vartheta$ . The thermodynamic force  $A_g$  associated with the modified free energy function is:

$$A_g = -\frac{\partial \psi}{\partial g} = \frac{1}{2} \left[ \frac{x_2 c_0}{(x_3 - g)^2 \theta_0} - 9\beta^2 k_0 \right] \vartheta^2 \tag{49}$$

If we consider properties corresponding to normal concrete, which are listed in Table 2, and substitute these values into Eq. (49), then conservatively setting  $g = 0$  yields the following equation for the thermodynamic force:

$$A(g) \geq A(0) = \frac{1}{2} [2265 - 0.0000216] \vartheta^2 \geq 0 \tag{50}$$

Note that not only is the thermodynamic force positive but also the positive term, which results from the variable specific heat, is much greater than the magnitude of the negative term. Therefore, it would be possible to adjust the model so that damage has a much smaller effect on the specific heat than that shown in Fig. 4 and still satisfy the second law of thermodynamics.

*4.2.2. Numerical simulation of the heating process*

We now consider the variation of the temperature profile that exists during the heating process. This is done by analysing the numerical example described in Section 3.2 using the modified Helmholtz free energy function. The results are presented in Figs. 5 and 6.

We note that dissipation is always positive as required. It appears from Fig. 6 that there is only a slight variation in temperature profile between the original and modified free energy functions. This is simply because we have small temperatures, and so the thermal damage is small and, hence, the change in specific heat is small. We consider elevated temperatures in the next section, where we note a

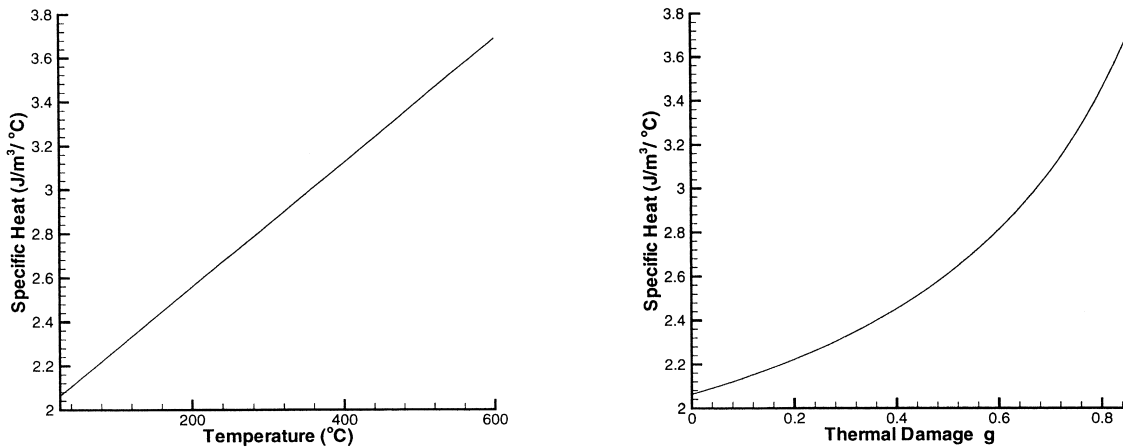


Fig. 4. Variation in specific heat.

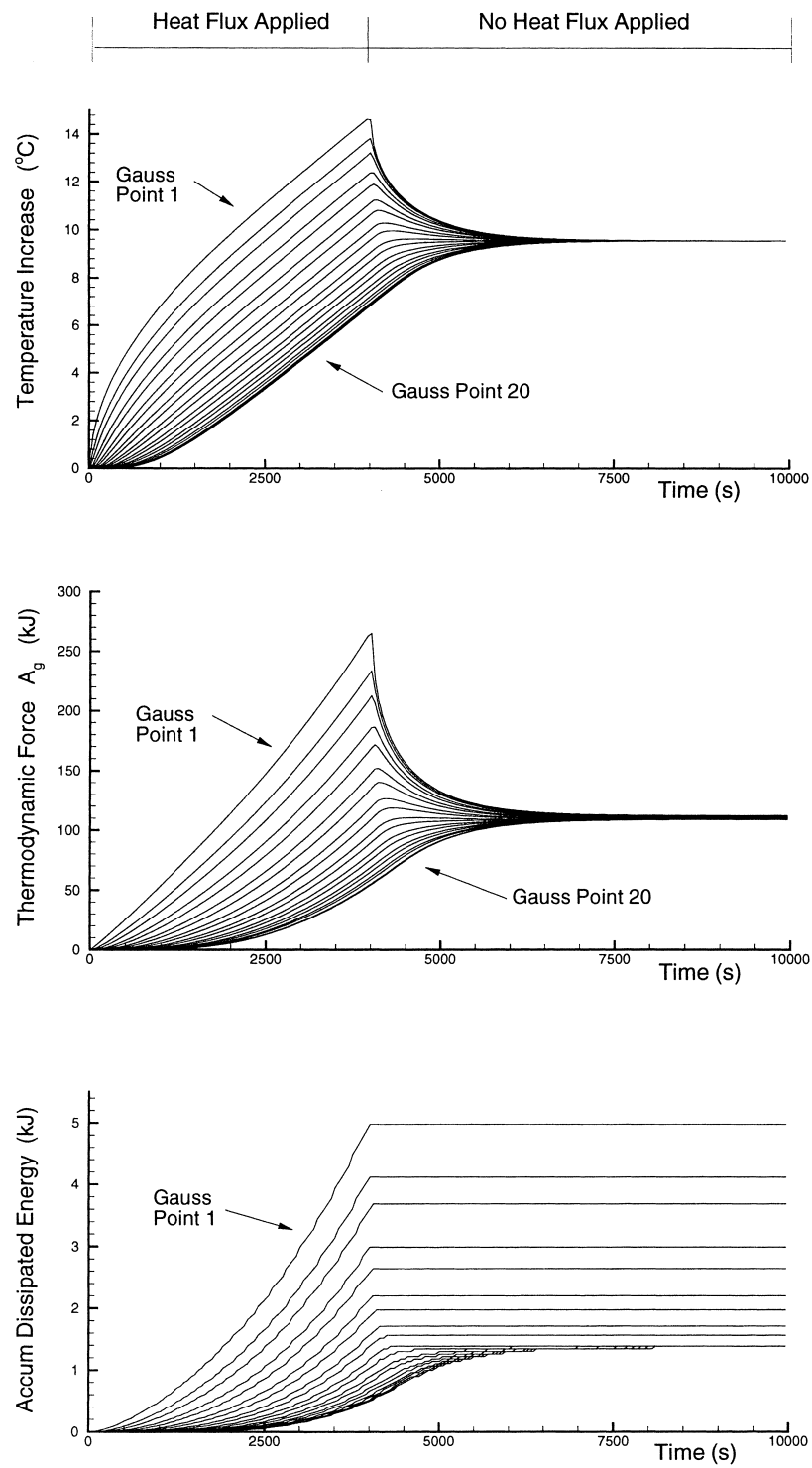


Fig. 5. Results for the modified quadratic free energy function.

considerable difference. Moreover, it is important to adopt a more appropriate prediction of dissipation, particularly in problems where the dissipation quantity may be reintroduced as heat input to the thermal equilibrium equations.

*4.3. Alternative form at elevated temperatures*

The definition of specific heat in Eq. (2) and the associated quadratic form of the free energy equation corresponds to the assumption that  $\theta\eta \approx \theta_0\eta$  in the formulation of the thermal equilibrium equation (Armero and Simo, 1992). This assumption is reasonable for small temperature increments, such as those resulting from mechanical effects, but is not applicable to transient elevated temperatures.

For higher temperatures, the specific heat should be written as:

$$c = -\theta \frac{\partial^2 \psi}{\partial \theta^2} \tag{51}$$

After double integration, the thermal term in the free energy function takes a logarithmic form (Simo and Miehe, 1992). This too would generate negative dissipation for the examples presented in Section 3. Therefore, we retain the damage dependent specific heat function  $c = c(g, d)$  and obtain the following equation for the free energy function:

$$\psi = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{E}(d, g) : \boldsymbol{\varepsilon} - (\theta - \theta_0) \mathbf{m}(d, g) : \boldsymbol{\varepsilon} + c(g, d) \left[ \theta - \theta_0 - \theta \ln \left( \frac{\theta}{\theta_0} \right) \right] \tag{52}$$

From this, the thermodynamic properties are:

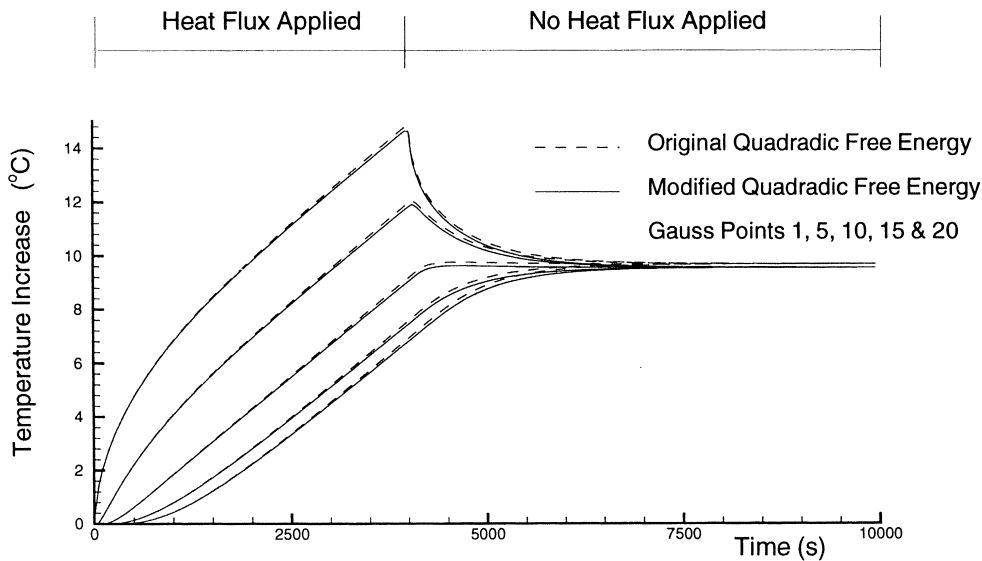


Fig. 6. Comparison of some Gauss point temperatures for the original and modified quadratic free energy functions.

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} = (1-d)(1-g)\mathbf{E}_0 : \boldsymbol{\varepsilon} - (1-d)(1-g)\mathbf{m}_0 \vartheta \quad (53)$$

$$\eta = \frac{-\partial \psi}{\partial \theta} = (1-d)(1-g)\mathbf{m}_0 : \boldsymbol{\varepsilon} + c(g, d) \ln\left(\frac{\theta}{\theta_0}\right) \quad (54)$$

$$A_d = \frac{-\partial \psi}{\partial d} = \frac{1}{2}\boldsymbol{\varepsilon} : (1-g)\mathbf{E}_0 : \boldsymbol{\varepsilon} - (1-g)\vartheta \mathbf{m}_0 : \boldsymbol{\varepsilon} - \frac{\partial c}{\partial d} \left[ \vartheta - \theta \ln\left(\frac{\theta}{\theta_0}\right) \right] \quad (55)$$

$$A_g = \frac{-\partial \psi}{\partial g} = \frac{1}{2}\boldsymbol{\varepsilon} : (1-d)\mathbf{E}_0 : \boldsymbol{\varepsilon} - (1-d)\vartheta \mathbf{m}_0 : \boldsymbol{\varepsilon} - \frac{\partial c}{\partial g} \left[ \vartheta - \theta \ln\left(\frac{\theta}{\theta_0}\right) \right] \quad (56)$$

As a second example, we repeat the heating problem described in Fig. 1 but this time raising the temperatures to  $\sim 250^\circ\text{C}$ . This was done by increasing the heat flux to  $10 \text{ kW/m}^2$ . All the other parameters remain unchanged. Fig. 7 shows a comparison of temperature profile, entropy and accumulated energy dissipated against time for both free energy forms. Importantly, dissipation is always positive as required. Furthermore, the temperature profile over time is virtually identical for both forms of thermal energy, and one might be tempted to believe that the thermal forms are alternatives, since the heat conduction problem seems unaffected. However, both entropy and dissipation differ significantly, although these are rarely examined. The more accurate logarithmic form exhibits lower entropy and conversion of energy to heat by about 25% at the heated end in the steady state condition. We repeat that this difference is very relevant in cases where dissipation is reintroduced as heat input into the thermal equilibrium phase.

For the same heating problem, we show the temperature profile using the quadratic form with both the constant specific heat (which gives negative dissipation) and the modified damage-dependent specific heat (which behaves correctly) in Fig. 8; recall that the temperature profile is the same for the logarithmic form. Evidently, there is now a significant influence on the temperature profile as well as on dissipation.

#### 4.4. Other loading situations

To conclude this investigation, we comment on the effect of combined mechanical and thermal damage. The expression for dissipation in Eq. (6) is expanded with Eqs. (55) and (56) to give:

$$\phi_{\text{mech}} = \left[ \boldsymbol{\varepsilon} : \left( \frac{1}{2}\mathbf{E}_0 : \boldsymbol{\varepsilon} - \vartheta \mathbf{m}_0 \right) \right] \left[ (1-g)\dot{d} + (1-d)\dot{g} \right] + \left[ \frac{\partial c}{\partial d}\dot{d} + \frac{\partial c}{\partial g}\dot{g} \right] \left[ \theta \ln\left(\frac{\theta}{\theta_0}\right) - \vartheta \right] \quad (57)$$

As previously discussed, the first term of Eq. (57) can be negative. Therefore, we require the second term to be non-negative and large enough to overcome any negative quantities generated in the first term.

Firstly, consider the case where there is only mechanical loading at room temperature (i.e.  $\vartheta \approx 0$ ;  $\dot{g} = 0$ ). It can be shown that the dissipation condition is automatically satisfied. This is because the temperature change due to structural heating and mechanical dissipation is very small and all the terms in Eq. (57) are positive.

To assess the combined damage effects, we construct a model problem quite like the physical experiment of Anderberg and Thelandersson (1976). Initially, a specimen is heated to a high temperature without load ( $\vartheta > 0$ ,  $g > 0$  and  $\dot{g} > 0$ ; but  $d = 0$ ) and then the temperature is held constant while load is



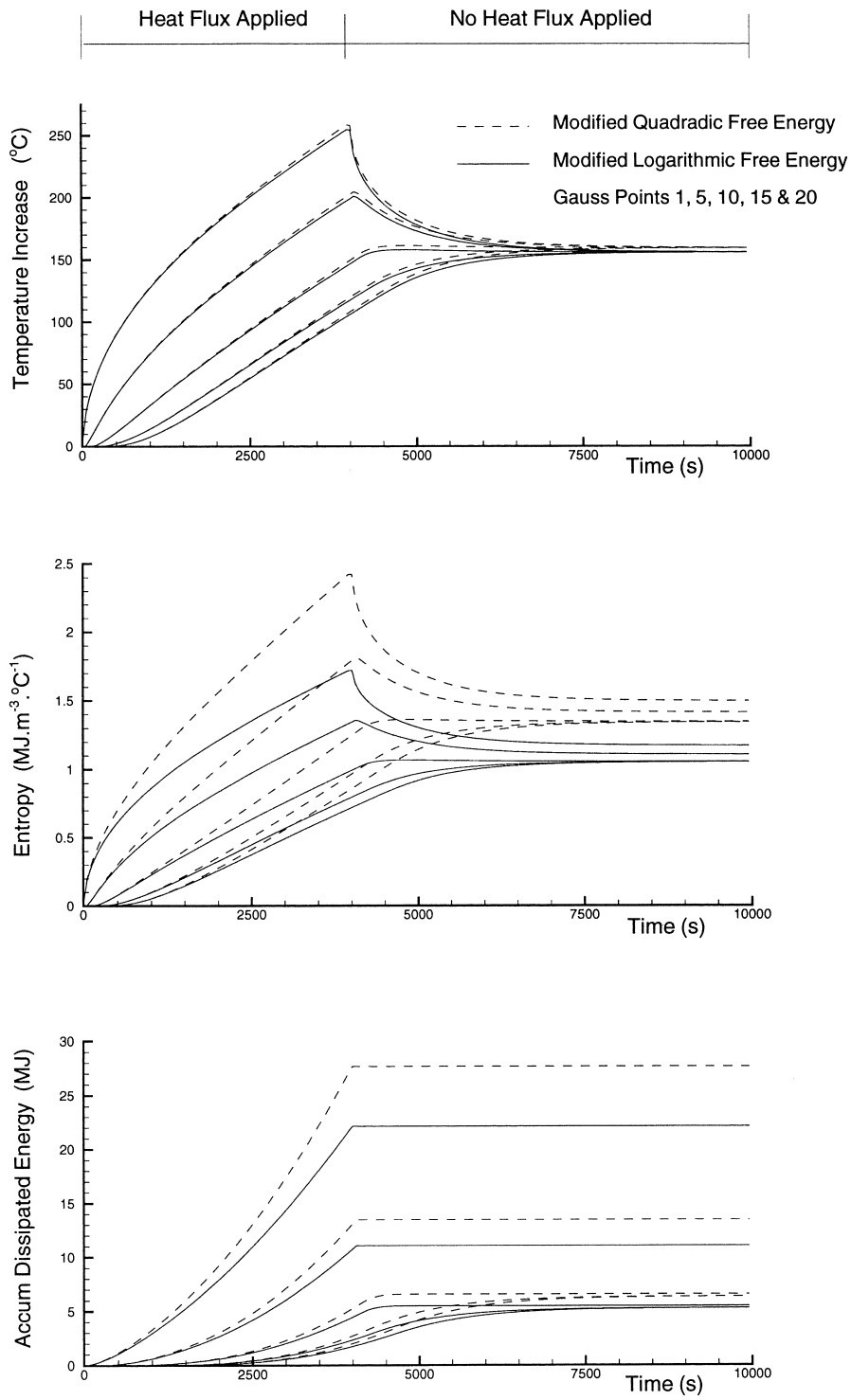


Fig. 7. Results for the modified quadratic and logarithmic free energy functions.

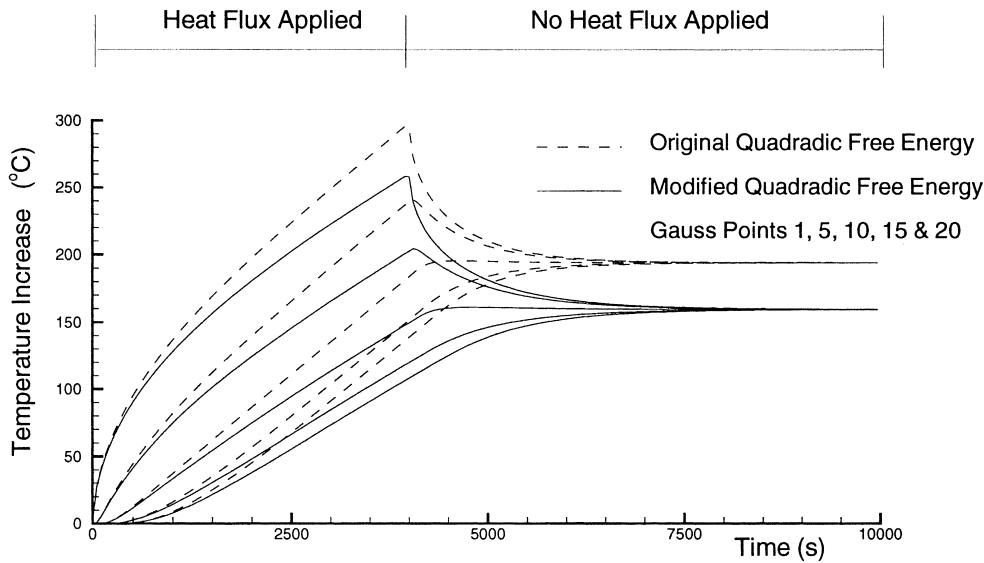


Fig. 8. Comparison of some Gauss point temperatures for the original and modified quadratic free energy functions.

applied ( $g > 0$  but  $\dot{g} = 0$ ;  $\dot{d} > 0$ ,  $d > 0$ ). The first phase of this experiment is covered in the discussion of Sections 4.2.1 and 4.2.2. For the second phase, the thermodynamic force reduces to

$$A_d = \left[ \boldsymbol{\varepsilon} : \left( \frac{1}{2} \mathbf{E}_0 : \boldsymbol{\varepsilon} - \mathfrak{J} \mathbf{m}_0 \right) \right] (1 - g) + \frac{\partial c}{\partial d} \left[ \theta \ln \left( \frac{\theta}{\theta_0} \right) - \mathfrak{J} \right]. \quad (58)$$

As discussed in Section 3, the first term in the square brackets can easily be negative and, therefore, the second term must be positive; and, moreover, the magnitude of the second term must be much greater than the magnitude of the first term. If we consider the thermo-damage model presented in Section 2 and the definition of specific heat given by Eq. (47), the thermodynamic force becomes

$$A_d = \left[ \boldsymbol{\varepsilon} : \left( \frac{1}{2} \mathbf{E}_0 : \boldsymbol{\varepsilon} - \mathfrak{J} \mathbf{m}_0 \right) + \frac{x_2 c_0}{(x_3 - z)^2} \left[ \theta \ln \left( \frac{\theta}{\theta_0} \right) - \mathfrak{J} \right] \right] (1 - g) \quad (59)$$

where

$$z = g + d - gd \quad \text{such that } z \in [0, 1]. \quad (60)$$

If one substitutes representative values into the above equation, it can be seen that the magnitude of the second term will be several orders of magnitude greater than the magnitude of the first term; see, for example, Eq. (50). Thus, the second law of thermodynamics will be satisfied. Again we point out that the influence that the damage parameters have on specific heat does not need to be as great as that used in this paper in order to obtain positive dissipation. The main point is that the damage parameters, when used in a thermo-mechanical setting, must have some influence on the specific heat such that the model satisfies the second law of thermodynamics. The nature of the relationship between the specific heat and the damage parameters depends on the specific details of the damage model used.

### 5. Concluding remarks

This paper concerns the form of the free energy function in coupled thermo-mechanical problems with isotropic damage, where both mechanical and thermal damage occurs, and when the material is exposed to elevated temperatures. It was shown that with the normal assumption of a constant specific heat coefficient, mechanical dissipation is negative and so the second law of thermodynamics is violated. This was confirmed by a numerical example in Section 3.2. In fact, the problem of negative dissipation is true for all isotropic damage models, even those that allow independent damage on the Young’s modulus and the bulk modulus.

The approach used to rectify this violation is to make specific heat dependent on damage, and under these conditions we show positive dissipation for a range of problems; for the case of concrete, at least, there is material evidence supporting this model. At low temperatures, it is not clear how significant this problem is for actual computations. Nevertheless, we show an error of at least 15% in the temperature profile in simple heat conduction along a bar, even without the presence of mechanical damage.

For elevated temperatures, we use the logarithmic form of thermal energy, again showing positive dissipation. A comparison between the logarithmic and quadratic forms reveals that temperature profile may not be adversely affected, thus giving a false sense of accuracy since dissipation can be in error by 25%. Since this represents energy transformation to heat, the correct form is vital when heat is reintroduced into the calculations. Finally, a more general example where there is a heating phase followed by a loading phase was considered. It was shown that for this problem, it is possible for the thermo-damage model to satisfy the second law of thermodynamics.

### Appendix A. Thermal equilibrium equation

In this appendix, we present algorithmic details for the evolution equations. Here, we wish to record the effects of introducing a damage dependent specific heat into the finite element discrete forms. For thermal evolution, we naturally begin with the local energy balance equation:

$$\theta \dot{\eta} = -\text{div } \mathbf{q} + r + \phi_{\text{mech}} \tag{A1}$$

where  $\mathbf{q}$  is again the heat flux, and  $r$  is a heat source. Our main interest is the logarithmic form, since it is more widely applicable, yet it is more complicated in the discrete form. That is, the logarithmic form binds discrete variables at different time steps, e.g.  $\theta_{n+1}$  and  $\theta_n$ , whereas with the quadratic form, the variables separate and lead to a more straightforward time marching scheme.

Applying the chain rule to Eq. (54), we can express the left-hand side of Eq. (A1) as:

$$\begin{aligned} \theta \dot{\eta} = & \theta(1-d)(1-g)\mathbf{m}_0:\dot{\boldsymbol{\varepsilon}} - [\theta(1-d)\mathbf{m}_0:\boldsymbol{\varepsilon}]\dot{g} - [\theta(1-g)\mathbf{m}_0:\boldsymbol{\varepsilon}]\dot{d} + \theta \frac{x_2}{(x_3-z)^2} c_0 \ln\left(\frac{\theta}{\theta_0}\right)\dot{z} + \left[ x_1 \right. \\ & \left. + \frac{x_2}{(x_3-z)} \right] c_0 \dot{\theta} \end{aligned} \tag{A2}$$

where

$$z = g + d - gd \quad \text{and} \quad \dot{z} = (1-d)\dot{g} + (1-g)\dot{d} \tag{A3}$$

Substituting Eq. (A2) into Eq. (A1) and discretising in time gives

$$\begin{aligned}
& \left[ x_1 + \frac{x_2}{\left(x_3 - z_{n+\frac{1}{2}}\right)} \right] c_0 \frac{(\theta_{n+1} - \theta_n)}{\Delta n} \\
&= -\frac{1}{2} \operatorname{div} \mathbf{q}_{n+1} - \frac{1}{2} \operatorname{div} \mathbf{q}_n - \frac{(\theta_{n+1} + \theta_n)}{2} \left[ \left(1 - d_{n+\frac{1}{2}}\right) \left(1 - g_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \dot{\boldsymbol{\varepsilon}} \right] + \frac{(\theta_{n+1} + \theta_n)}{2} \left[ \left(1 - d_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{g} + \frac{(\theta_{n+1} + \theta_n)}{2} \left[ \left(1 - g_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{d} \\
& - \frac{(\theta_{n+1} + \theta_n)}{2} \left[ \frac{x_2}{\left(x_3 - z_{n+\frac{1}{2}}\right)^2} c_0 \ln \left[ \frac{(\theta_{n+1} + \theta_n)}{2\theta_0} \right] \right] \dot{z} + r_{n+\frac{1}{2}} + \phi_{\text{mech}} \tag{A4}
\end{aligned}$$

Writing this equation in the weak form by premultiplying by a smooth continuous scalar function  $a$ , integrating over the volume and applying the divergence theorem gives:

$$\begin{aligned}
& \frac{1}{\Delta t} \int_{\Omega} a \left[ x_1 + \frac{x_2}{\left(x_3 - z_{n+\frac{1}{2}}\right)} \right] c_0 \theta_{n+1} \, d\Omega - \frac{1}{\Delta t} \int_{\Omega} a \left[ x_1 + \frac{x_2}{\left(x_3 - z_{n+\frac{1}{2}}\right)} \right] c_0 \theta_n \, d\Omega \\
&= -\frac{1}{2} \oint_s a \mathbf{q}_{n+1} \cdot \mathbf{n} \, ds - \frac{1}{2} \oint_s a \mathbf{q}_n \cdot \mathbf{n} \, ds + \frac{1}{2} \int_{\Omega} \nabla(a) \cdot \mathbf{q}_{n+1} \, d\Omega + \frac{1}{2} \int_{\Omega} \nabla(a) \cdot \mathbf{q}_n \, d\Omega - \frac{1}{2} \int_{\Omega} a \left[ \left(1 - d_{n+\frac{1}{2}}\right) \left(1 - g_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \dot{\boldsymbol{\varepsilon}} \right] \theta_{n+1} \, d\Omega - \frac{1}{2} \int_{\Omega} a \left[ \left(1 - d_{n+\frac{1}{2}}\right) \left(1 - g_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \dot{\boldsymbol{\varepsilon}} \right] \theta_n \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ \left(1 - d_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{g} \theta_{n+1} \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ \left(1 - d_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{g} \theta_n \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ \left(1 - g_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{d} \theta_{n+1} \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ \left(1 - g_{n+\frac{1}{2}}\right) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{d} \theta_n \, d\Omega \\
& - \frac{1}{2} \int_{\Omega} a \left[ \frac{x_2}{\left(x_3 - z_{n+\frac{1}{2}}\right)^2} c_0 \ln \left[ \frac{(\theta_{n+1} + \theta_n)}{2\theta_0} \right] \right] \dot{z} \theta_{n+1} \, d\Omega \\
& - \frac{1}{2} \int_{\Omega} a \left[ \frac{x_2}{\left(x_3 - z_{n+\frac{1}{2}}\right)^2} c_0 \ln \left[ \frac{(\theta_{n+1} + \theta_n)}{2\theta_0} \right] \right] \dot{z} \theta_n \, d\Omega + \int_{\Omega} a r_{n+\frac{1}{2}} \, d\Omega + \int_{\Omega} a \phi_{\text{mech}} \, d\Omega \tag{A5}
\end{aligned}$$

Using Fourier's Law of heat conduction, the above equation can be written as:

$$\begin{aligned}
 & \frac{1}{\Delta t} \int_{\Omega} a \left[ x_1 + \frac{x_2}{(x_3 - z_{n+\frac{1}{2}})} \right] c_0 \theta_{n+1} \, d\Omega + \frac{1}{2} \int_{\Omega} \nabla(a) \cdot \nabla(k\theta_{n+1}) \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ (1 - d_{n+\frac{1}{2}}) (1 \right. \\
 & \left. - g_{n+\frac{1}{2}}) \mathbf{m}_0 : \dot{\boldsymbol{\varepsilon}} \right] \theta_{n+1} \, d\Omega - \frac{1}{2} \int_{\Omega} a \left[ (1 - d_{n+\frac{1}{2}}) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{g} \theta_{n+1} \, d\Omega - \frac{1}{2} \int_{\Omega} a \left[ (1 \right. \\
 & \left. - g_{n+\frac{1}{2}}) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{d} \theta_{n+1} \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ \frac{x_2}{(x_3 - z_{n+\frac{1}{2}})^2} c_0 \ln \left[ \frac{(\theta_{n+1} + \theta_n)}{2\theta_0} \right] \dot{z} \right] \theta_{n+1} \, d\Omega \\
 & = -\frac{1}{2} \oint_s \mathbf{a} \mathbf{q}_{n+1} \cdot \mathbf{n} \, ds - \frac{1}{2} \oint_s \mathbf{a} \mathbf{q}_n \cdot \mathbf{n} \, ds + \frac{1}{\Delta t} \int_{\Omega} a \left[ x_1 + \frac{x_2}{(x_3 - z_{n+\frac{1}{2}})} \right] c_0 \theta_n \, d\Omega - \frac{1}{2} \int_{\Omega} \nabla(a) \\
 & \cdot \nabla(k\theta_n) \, d\Omega - \frac{1}{2} \int_{\Omega} a \left[ (1 - d_{n+\frac{1}{2}}) (1 - g_{n+\frac{1}{2}}) \mathbf{m}_0 : \dot{\boldsymbol{\varepsilon}} \right] \theta_n \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ (1 \right. \\
 & \left. - d_{n+\frac{1}{2}}) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{g} \theta_n \, d\Omega + \frac{1}{2} \int_{\Omega} a \left[ (1 - g_{n+\frac{1}{2}}) \mathbf{m}_0 : \boldsymbol{\varepsilon}_{n+\frac{1}{2}} \right] \dot{d} \theta_n \, d\Omega \\
 & \left. - \frac{1}{2} \int_{\Omega} a \left[ \frac{x_2}{(x_3 - z_{n+\frac{1}{2}})^2} c_0 \ln \left[ \frac{(\theta_{n+1} + \theta_n)}{2\theta_0} \right] \dot{z} \right] \theta_n \, d\Omega + \int_{\Omega} a r_{n+\frac{1}{2}} \, d\Omega + \int_{\Omega} a \phi_{\text{mech}} \, d\Omega \tag{A6}
 \end{aligned}$$

which can be implemented into a finite element code.

For either form of the free energy function, the discretised weak form of the momentum balance equation is given by:

$$\begin{aligned}
 & \frac{2}{(\Delta t)^2} \int_{\Omega} \hat{\mathbf{a}}^T \rho \hat{\mathbf{u}}_{j+1} \, d\Omega + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}) : [\mathbf{E}_{j+1} : \boldsymbol{\varepsilon} [\hat{\mathbf{u}}_{j+1}]]^T \, d\Omega \\
 & = \frac{1}{2} \oint_{\partial\Omega} \hat{\mathbf{a}}^T \boldsymbol{\sigma}_{j+1} \mathbf{n} \, ds + \frac{1}{2} \oint_{\partial\Omega} \hat{\mathbf{a}}^T \boldsymbol{\sigma}_j \mathbf{n} \, ds + \frac{2}{(\Delta t)^2} \int_{\Omega} \hat{\mathbf{a}}^T \rho \hat{\mathbf{u}}_j \, d\Omega - \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}) : [\mathbf{E}_j : \boldsymbol{\varepsilon} [\hat{\mathbf{u}}_j]]^T \, d\Omega \\
 & \left. + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}) : [\mathbf{m}_{j+1} \hat{\vartheta}_{j+1}]^T \, d\Omega + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}) : [\mathbf{m}_j \hat{\vartheta}_j]^T \, d\Omega + \frac{2}{\Delta t} \int_{\Omega} \hat{\mathbf{a}}^T \rho \hat{\mathbf{v}}_j \, d\Omega + \int_{\Omega} \hat{\mathbf{a}}^T \rho \mathbf{b} \, d\Omega \tag{A7}
 \end{aligned}$$

A number of integration schemes might be proposed for the coupled equations (A6) and (A7). In a simultaneous (load and heat) solution, or an isothermal phase of a fractional step algorithm (Stabler and Baker, 2000), Eq. (A7) can be used directly. However, for an isentropic phase, it is necessary to apply the isentropic condition between sub time steps  $j$  and  $j + 1$ . Recall that entropy is calculated from:

$$\eta = \mathbf{m} : \boldsymbol{\varepsilon} + c \ln \left( \frac{\theta}{\theta_0} \right) \tag{A8}$$

and so an isentropic sub time step would require

$$c_{j+1} \ln \left( \frac{\theta_{j+1}}{\theta_0} \right) + \mathbf{m}_{j+1} : \boldsymbol{\varepsilon}_{j+1} = c_j \ln \left( \frac{\theta_j}{\theta_0} \right) + \mathbf{m}_j : \boldsymbol{\varepsilon}_j \tag{A9}$$

Rearranging

$$\ln\left(\frac{\theta_{j+1}}{\theta_0}\right) = \frac{1}{c_{j+1}}[\mathbf{m}_j:\boldsymbol{\varepsilon}_j] - \frac{1}{c_{j+1}}[\mathbf{m}_{j+1}:\boldsymbol{\varepsilon}_{j+1}] + \frac{c_j}{c_{j+1}} \ln\left(\frac{\theta_j}{\theta_0}\right) \quad (\text{A10})$$

If we allow specific heat to evolve through the thermal phase only then  $c_{j+1} = c_j = c_n$ , i.e. specific heat is constant during the isentropic phase. Taking the exponential of both sides of Eq. (A10) gives:

$$\frac{\theta_{j+1}}{\theta_0} = \frac{\exp\left[\frac{1}{c_n}[\mathbf{m}_j:\boldsymbol{\varepsilon}_j]\right]}{\exp\left[\frac{1}{c_n}[\mathbf{m}_{j+1}:\boldsymbol{\varepsilon}_{j+1}]\right]} \frac{\theta_j}{\theta_0} \quad (\text{A11})$$

which we could then write as:

$$\vartheta_{j+1} = \theta_j \exp\left[\frac{1}{c_n}[\mathbf{m}_j:\boldsymbol{\varepsilon}_j - \mathbf{m}_{j+1}:\boldsymbol{\varepsilon}_{j+1}]\right] - \theta_0 \quad (\text{A12})$$

Unfortunately, if we substitute this equation into Eq. (A7), we cannot transfer  $\boldsymbol{\varepsilon}_{j+1}$  to the left-hand side of the equation. Therefore, the isentropic phase would require an iterative solution and as a result it will be computationally expensive.

To overcome this difficulty, it is necessary to realise that during the adiabatic phase the temperature change in the structure is quite small and so the following approximation can be established. Firstly, we find some constant  $\alpha_n$  such that:

$$\ln\left(\frac{\theta_n}{\theta_0}\right) = \alpha_n \frac{\vartheta_n}{\theta_0} \quad (\text{A13})$$

And so at the sub time step  $j + 1$ , the following approximation can be made:

$$\alpha_n \frac{(\vartheta_n + \Delta\vartheta_{j+1})}{\theta_0} \approx \ln\left(\frac{\theta_n + \Delta\vartheta_{j+1}}{\theta_0}\right) \quad \text{for small } \Delta\vartheta \quad (\text{A14})$$

And so the adiabatic condition can be approximated by:

$$\mathbf{m}_{j+1}:\boldsymbol{\varepsilon}_{j+1} + c_n \alpha_n \frac{\vartheta_{j+1}}{\theta_0} = \mathbf{m}_j:\boldsymbol{\varepsilon}_j + c_n \alpha_n \frac{\vartheta_j}{\theta_0} \quad (\text{A15})$$

and, hence, the relative temperature can be written as:

$$\vartheta_{j+1} = \frac{\theta_0}{\alpha_n c_n} \mathbf{m}_j:\boldsymbol{\varepsilon}_j - \frac{\theta_0}{\alpha_n c_n} \mathbf{m}_{j+1}:\boldsymbol{\varepsilon}_{j+1} + \vartheta_j \quad (\text{A16})$$

Substituting this into Eq. (A7) gives:

$$\begin{aligned}
 & \frac{2}{(\Delta t)^2} \int_{\Omega} \hat{\mathbf{a}}^T \rho \hat{\mathbf{u}}_{j+1} \, d\Omega + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}):[\mathbf{E}_{j+1}:\boldsymbol{\varepsilon}[\hat{\mathbf{u}}_{j+1}]]^T \, d\Omega + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}): \left[ \left[ \frac{\theta_0}{\alpha_n c_n} \mathbf{m}_{j+1} \otimes \mathbf{m}_{j+1} \right] : \boldsymbol{\varepsilon}[\hat{\mathbf{u}}_{j+1}] \right. \\
 & \left. \times \right]^T \, d\Omega \\
 & = \frac{1}{2} \oint_{\partial\Omega} \hat{\mathbf{a}}^T \boldsymbol{\sigma}_{j+1} \mathbf{n} \, ds + \frac{1}{2} \oint_{\partial\Omega} \hat{\mathbf{a}}^T \boldsymbol{\sigma}_j \mathbf{n} \, ds + \frac{2}{(\Delta t)^2} \int_{\Omega} \hat{\mathbf{a}}^T \rho \hat{\mathbf{u}}_j \, d\Omega - \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}):[\mathbf{E}_j:\boldsymbol{\varepsilon}[\hat{\mathbf{u}}_j]]^T \, d\Omega \\
 & + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}): \left[ \left[ \frac{\theta_0}{\alpha_n c_n} \mathbf{m}_{j+1} \otimes \mathbf{m}_j \right] : \boldsymbol{\varepsilon}[\hat{\mathbf{u}}_j] \right]^T \, d\Omega + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}):[\mathbf{m}_{j+1} \hat{\vartheta}_j]^T \, d\Omega \\
 & + \frac{1}{2} \int_{\Omega} \nabla(\hat{\mathbf{a}}):[\mathbf{m}_j \hat{\vartheta}_j]^T \, d\Omega + \frac{2}{\Delta t} \int_{\Omega} \hat{\mathbf{a}}^T \rho \hat{\mathbf{v}}_j \, d\Omega + \int_{\Omega} \hat{\mathbf{a}}^T \rho \mathbf{b} \, d\Omega \tag{A17}
 \end{aligned}$$

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