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A thermodynamic approach to non-local damage modelling of concrete

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Abstract

This paper focuses on the development of a thermodynamic approach to constitutive modelling of concrete materials, with emphasis on the use of non-local damage models. Effort is put on the construction of a consistent and rigorous thermodynamic framework, which readily allows the incorporation of non-local features into the constitutive modelling. This is an important feature in developing non-local constitutive models based on thermodynamics. Examples of non-local constitutive models derived from this framework and numerical examples are given to demonstrate the promising features of the proposed approach.

Keywords: Constitutive modelling; Non-local; Thermodynamics; Damage; Concrete

1. Introduction

In the constitutive modelling for strain softening materials, localization due to softening is of great importance because strain softening and strength degradation are two of the important features of the material behaviour, especially when the post peak behaviour is of great interest (e.g. the crack initiation and propagation due to fatigue in metallic materials, and crack propagation in concrete structures). The use of damage mechanics, in combination with plasticity theory, enables us to derive appropriate models for the modelling of these materials. However, as the material exhibits significant post-peak softening, appropriate treatments, called regularization techniques, need to be applied to the constitutive modelling as well as the structural analysis.

This is because conventional continuum mechanics is inadequate to capture correctly the softening behaviour of the material. Mathematically speaking, quasi-static analysis of boundary value problems involving strain-softening material becomes ill-posed beyond a certain level of accumulated damage (Jirásek and

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Bazant, 2002). This is due to the local loss of ellipticity of the governing partial differential equations, if these are derived in the context of conventional continuum mechanics. From the numerical point of view, the strain in the damaged region tends to localize in a very narrow zone, called the fracture process zone (FPZ), which eventually leads to the formation of macro cracks. In the finite element analysis, this FPZ tends to narrow upon mesh refinement, resulting in mesh-dependent numerical solutions. The problem is however similar in many numerical methods (e.g. finite element, boundary element, and finite difference) employed for the solutions of the governing partial differential equations in continuum mechanics.

Non-local regularization techniques have been found to be appropriate for the modelling of softening materials (Pijaudier-Cabot and Bazant, 1987) and help to avoid pathological problems encountered in the constitutive modelling of these materials (Jirásek and Bazant, 2002). The key idea of non-local regularization is to introduce non-local integral or gradient terms with a length scale into the constitutive models. This length parameter, called characteristic length or internal length of the regularized continuum, is also used to control the size of the non-local interaction of material points. The type of the governing partial differential equations of the regularized continuum models then remain always unchanged (no loss of ellipticity in quasi-static analysis) and the boundary value problem therefore maintains the well-posedness during the deformation and damage processes. These techniques of regularization have been widely applied to the constitutive modelling in the context of both damage mechanics and softening plasticity (Pijaudier-Cabot and Bazant, 1987; Borino et al., 1999; Jirásek and Patzák, 2002; Grassl and Jirásek, 2006). Nevertheless, some of the existing non-local models (e.g. Addessi et al., 2002; Rodriguez-Ferran et al., 2004) are built without recourse to thermodynamics, resulting in difficulties in assessing their thermodynamic admissibility.

On the other hand, the thermodynamic aspects of constitutive modelling using non-local theories have been discussed by several researchers (Maugin, 1990; Santaoja, 2004; Nedjar, 2001; Polizzotto et al., 1998; Polizzotto and Borino, 1998; Borino et al., 1999; Benvenuti et al., 2002; Nilsson, 1997; Jirásek and Rolshoven, 2003; Peerlings et al., 2004; Voyiadjis and Dorgan, 2004; Makowski et al., 2006). In thermodynamic approaches, non-local or gradient terms can appear in the expressions of the first or second law of thermodynamics. However, none of the existing non-local thermodynamic approaches has exploited the transformation and interchanging between the dissipation function and the non-local yield/damage function. Instead, the dissipation expression, in the non-local form, is usually used as a means to verify the thermodynamic admissibility of the obtained non-local models. This process is complicated and sometimes leads to misinterpretation of the features of the non-local model. As an example, the non-local plasticity model of Nilsson (1997), formulated based on a thermodynamic approach, was found to produce results violating the condition of non-negative dissipation in some special cases (see Jirásek and Rolshoven, 2003).

In some thermodynamic approaches (Nedjar, 2001; Santaoja, 2004; Voyiadjis and Dorgan, 2004; Makowski et al., 2006), non-local or gradient terms of internal variables appear in the expressions of the energy potential, as independent internal variables. The corresponding associated thermodynamic forces are then defined on those gradient terms. However, inconsistencies in the definition of those thermodynamic forces between some approaches can be seen (e.g. in Santaoja, 2004 and Voyiadjis and Dorgan, 2004). In Santaoja (2004), a scalar damage variable and its gradient form are associated with two corresponding thermodynamic forces, both of which are of scalar form and subjected to a constraint. This is however different in Voyiadjis and Dorgan (2004) in which the thermodynamic force associated with a gradient quantity is arbitrarily assumed to be of gradient form.

The Italian researchers (Polizzotto et al., 1998; Polizzotto and Borino, 1998; Borino et al., 1999; Benvenuti et al., 2002) have also proposed a sound approach to thermodynamic non-local constitutive modelling. The energy exchange due to non-locality (Bazant, 1991, 1994) is exploited and realized through the global satisfaction of the first law of thermodynamics. A term called non-locality residual, which satisfies an insulation condition for its total vanishing over the body, is used to obtain a local expression of the first law (and the Clausius–Duhem inequality too). This concept of non-locality residual is in fact rooted from earlier work by Edelen and Laws (1971) and has been adapted in several papers (Polizzotto et al., 1998; Polizzotto and Borino, 1998; Borino et al., 1999; Benvenuti et al., 2002).

The motivation of this paper is to exploit the concept of non-locality residual, and the Legendre transformation of the loading functions and dissipation function (Houlsby and Puzrin, 2000, 2006), in the formulation of non-local model. Peerlings et al. (2004) argued that the insulation condition associated with the non-locality

residual in the "Italian approach" restricts the energy exchange only in the dissipation zone and therefore is too limiting. However, this argument in our opinion is not strong enough to restrict the use of the non-locality residual concept, as long range energy exchanges and interactions between representative volume elements (RVEs) inside and outside the dissipation zone can always take place at their boundaries, e.g. through equilibrium equations.

It should also be mentioned here that this study only aims at proposing a consistent thermo-mechanical approach for the formulation of non-local constitutive models. The formulation of a non-local model based on this approach therefore just requires the specification of two energy potentials and follows a set of consistently pre-established procedures. This simplifies the formulation and hence helps avoid potential violation of the laws of thermodynamics in formulating complicated non-local constitutive models. The regularization aspects of the derived non-local models in this study are therefore kept as simple as possible through some numerical examples to demonstrate the independence of the numerical results from the spatial discretization. It is desired to tackle those issues in future research.

The outline of this paper is as follows. In Section 2 two similar ways of introducing non-locality into an existing thermo-mechanical framework by Houlsby and Puzrin (2000, 2006), followed by the modification of this framework for the formulation of non-local models, are presented. The advantages of the modified framework in formulating non-local models are highlighted. In Section 3 two non-local damage models proposed and derived following procedures consistently established in the original framework and modified here for non-local models. Simple numerical examples are then given and conclusions are withdrawn.

2. A thermodynamic approach to non-local constitutive modelling

2.1. Choice of non-local variable

In the case of damage-induced softening in quasi-brittle materials, the damage variables or the associated damage energies should be treated as non-local quantities (Bazant, 1991). Of course, generally one can choose other variables, which are indirectly related to the strain softening behaviour of the materials (e.g. the elastic strain, which is in fact related to the damage energy) for non-local treatment. However, these treatments in some cases can lead to models producing high residual stresses even at the very late stages of the fracture/damage process (Jirásek, 1998). As the residual stresses at those late stages should be very small to represent the failure of the material prior to the appearance of macro cracks in a complete separation mode, these enhanced models are hence not capable of modelling realistic behaviour of the materials. Therefore the choice of non-local internal variables, and the corresponding non-local models, should be carefully considered and examined in order to avoid these pathologies. Among various non-local damage approaches using different non-local quantities, those that are based on the non-locality of the damage energy have been proved to be satisfactory and can give reasonably low residual stress when the damage measure is close to unity (Jirásek, 1998). In this study we will adopt this kind of damage energy non-locality.

2.2. Non-locality introduced to the first law of thermodynamics

Since our attempt in this study is to formulate models based on thermodynamics, the problem here is the possibility of adapting an existing 'local' thermodynamic framework to a non-local approach. The energy potential can be modified by introducing the damage gradient as a new internal variable (Maugin, 1990; Santaoja, 2004; Nedjar, 2001) in order to account for the energy exchange due to non-locality. An alternative and more physical way to introduce non-locality into an existing thermodynamic framework is to express the laws of thermodynamics in a more general form in order to account for the energy redistribution in a certain volume element, where damage occurs, due to the microcrack interactions. The size of this volume element, where the energy redistribution takes place, is proportional to the material characteristic length. Originally proposed by Edelen and Laws (1971) with the concept of the non-locality residual, this is the approach adopted by several Italian researchers (Polizzotto et al., 1998; Polizzotto and Borino, 1998; Borino et al., 1999; Benvenuti et al., 2002).

This approach is based on the assumption that there is energy exchange between points within a certain volume element, whose size is proportional to the material internal length scale. In this case, the non-locality

of damage, which can be explained through micromechanics analysis of microcrack interactions in a volume element (Bazant, 1991 and Bazant, 1994), is accounted for based on the thermodynamic analysis of that volume. The interactions of microcracks are represented through the energy exchange at points inside that volume element. Following the approach, the first law of thermodynamics, which is usually derived in its local form, is now stated in the non-local form over that volume of the material.

$$\int_{V_d} \dot{W} \mathrm{d}V + \int_{V_d} \dot{Q} \mathrm{d}V = \int_{V_d} \dot{u} \mathrm{d}V \tag{1}$$

where V_d is the representative region where the dissipation processes takes place; $\dot{W} = \sigma_{ij}\dot{\varepsilon}_{ij}$ is the rate of mechanical work input; $\dot{Q} = -q_{k,k}$ is the rate of heat supply to a volume element; and u is the specific internal energy. In contrast with local theory, the size V_d of the dissipation region here cannot be infinitesimal but is restricted by the material characteristic length (Polizzotto et al., 1998). As V_d is of finite size and cannot be arbitrarily small, the local form of energy balance can only be withdrawn from (1) by using a non-locality residual P accounting for the energy exchange in the region V_d.

$$\dot{W} + \dot{Q} + P = \dot{u} \tag{2}$$

In this case, the insulation condition (Polizzotto and Borino, 1998)

$$\int_{V_d} P \mathrm{d}V = 0 \tag{3}$$

must be satisfied, restricting the energy exchange only within the volume V_d. It should also be noted here that P is non-zero at points inside the volume V_d and equal to zero everywhere outside V_d, where there are no irreversible processes. The insulation condition therefore also holds in the whole material body.

The assumption on the non-locality of energy exchange seems reasonable as damage in this case produces effects not only where it occurs but also at neighbouring points within the defined volume element. As a result of this, the energy redistribution of points inside that volume results in the global satisfaction of the first law of thermodynamics in this volume element (Polizzotto et al., 1998).

The second law of thermodynamics in this case is still cast in its local form:

$$\dot{s} \geqslant -\left(\frac{q_k}{\theta}\right)_{,k} \tag{4}$$

with s being the entropy and q_k/θ denoting the entropy flux. Expansion of expression (4) then gives us

$$\theta\dot{s} + q_{k,k} - \frac{q_k \theta_{,k}}{\theta} \geqslant 0 \tag{5}$$

The dissipation here comprises two parts corresponding to the mechanical dissipation $\theta\dot{s} + q_{k,k}$ and thermal dissipation $-q_k\ \theta_{,k}/\theta$. As mentioned in the original framework (Houlsby and Puzrin, 2000), a more stringent law than the second law of thermodynamics can be assumed here by assuming that $\theta\dot{s} + q_{k,k} \geqslant 0$, using the fact that the thermal dissipation is always non-negative and small compared to the mechanical one for small thermal gradients. Therefore the dissipation function, which is actually the rate of dissipation, can be rewritten as:

$$d = \theta\dot{s} + q_{k,k} \geqslant 0 \tag{6}$$

from which and the modified form (2) of the first law of thermodynamics, it follows that

$$d = \theta\dot{s} + \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{u} + P \geqslant 0 \tag{7}$$

Using the Helmholtz specific free energy f, defined by $f = u - s\theta$, we then have:

$$d = \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{f} - s\dot{\theta} + P \geqslant 0 \tag{8a}$$

$$\text{or } \dot{f} = \sigma_{ij}\dot{\varepsilon}_{ij} - d - s\dot{\theta} + P \tag{8b}$$

It can be seen here that the dissipation (neglecting the thermal dissipation) turns out to be non-local due to the appearance of the non-locality residual P. In this case, the Clausius–Duhem inequality ($\sigma_{ij}\dot{\varepsilon}_{ij} - \dot{f} - s\dot{\theta} \geqslant 0$)

does not hold pointwise, as it does in the local approach. Instead, due to the insulation condition (3), the Clausius–Duhem inequality now takes the following non-local form

$$\int_{V_d} \left(\sigma_{ij}\dot{\varepsilon}_{ij} - \dot{f} - s\dot{\theta}\right) \mathrm{d}V \geqslant 0 \tag{9}$$

This means local violation of the inequality is allowed to occur during irreversible processes. Nevertheless, the local dissipation (Eq. (7) or (8)) is always non-negative, noting that in this case of non-locality it does not coincide with the local form of the Clausius–Duhem inequality.

2.3. Non-locality introduced to the second law of thermodynamics

In a similar way, one can also introduce non-locality into the existing thermodynamic approach by casting the second law in a non-local form, while retaining the local form of the first law of thermodynamics. We rewrite the first law in local form as

$$\dot{W} + \dot{Q} = \dot{u} \tag{10}$$

The non-local second law now reads

$$\int_{V_d} \left(\theta\dot{s} + q_{k,k} - \frac{q_k\theta_{,k}}{\theta}\right) dV \geqslant 0 \tag{11}$$

Using the non-locality residual P, we can transform the above law to a local form,

$$\theta\dot{s} + q_{k,k} - \frac{q_k\theta_{,k}}{\theta} + P \geqslant 0 \tag{12}$$

Neglecting the thermal term (see also Houlsby and Puzrin, 2000), the mechanical dissipation now becomes

$$d = \theta\dot{s} + q_{k,k} + P \geqslant 0 \tag{13}$$

which, after being substituted into the expression of the local first law of thermodynamics (10), coincides with (7) in the previous case. As a result, the Clausius–Duhem inequality in this case is also satisfied in a global sense (see Eq. (9)).

As can be seen from (11), the global satisfaction of the second law of thermodynamics can lead to processes in which (11) are satisfied as an equality at global level. These processes are therefore interpreted as reversible at global level. Since (11) does not guarantee the pointwise satisfaction of the second law, Polizzotto (2003) argued that these processes could be physically meaningless. However, in both cases of non-locality (non-locality introduced to the first and the second laws of thermodynamics), that mentioned problem also occurs with the Clausius–Duhem inequality (9), which is generally used as a condition for any thermodynamically admissible processes. The physical interpretation here could be the exchange of energies, which must have been dissipated by heat, at points in the defined representative volume element. In other words, in the irreversible processes, energy at point-wise level within each volume element can be either dissipated by heat or transferred to neighbouring points within that volume element. The latter case here represents the local violation of the second law of thermodynamics (or violation of the local Clausius–Duhem inequality), which can be directly predicted as a consequence of the global satisfaction of the second law.

2.4. Proposed approach

With the insulation condition (3), non-locality in either case, 2.2 or 2.3, is restricted to irreversible processes. Although the mathematical formulation is essentially the same, the physics behind that can be interpreted in different ways. In the first case, with non-locality introduced to the first law of thermodynamics, long distance transmission of energy (other than contact forces between material points) could be viewed as being responsible for the non-locality in the material behaviour. Nevertheless, this non-locality is only activated for irreversible processes, due to the insulation condition (3) which restricts energy exchange within the volume V_d of dissipative processes. In the second case (Section 2.3), non-locality could be viewed as a result of

the redistribution of energy which should have been totally dissipated to the outside (e.g. by heat). In other words, at the material point under consideration, part of this energy can be transmitted to surrounding material points, and the rest can be dissipated to the outside. In a similar way to the first case, this mechanism of long range transmission of energy is only active when irreversible processes occur. Therefore, in the author's view, the introductions of non-locality to the first and the second law of thermodynamics have equal physical meaning and can be treated as equivalent.

As can be seen in Sections 2.2 and 2.3, the difference here, compared with local approaches, is the appearance of the non-locality residual P. The problem therefore lies in the determination of the appropriate expression for the non-locality residual P, which can both preserve the non-negative condition of the dissipation d and satisfy the insulation condition (3). We adopt here the approach by Polizzotto and Borino (1998), in which the regularization operator L and its adjoint L^* were introduced. In this case, the non-local internal variable $\tilde{\alpha}_k$ is determined from its local counterpart α_k through the operator L. We leave aside the exact physical meaning of α_k and consider it here as an internal variable which can be in scalar, vector, tensorial form or possibly a set of internal variables. We have

$$\dot{\tilde{\alpha}}_k = L(\dot{\alpha}_k) \tag{14}$$

Generally the operator L can be of integral form (non-local theory) or gradient form (gradient theory). For non-local theory the operator can be defined as (Borino et al., 1999; Polizzotto et al., 1998):

$$\dot{\tilde{\alpha}}_k(\mathbf{x}) = L(\dot{\alpha}_k) = \frac{1}{G(\mathbf{x})}\int_{V_\mathrm{d}} g(\|\mathbf{y}-\mathbf{x}\|)\dot{\alpha}_k(\mathbf{y})\,\mathrm{d}V \tag{15}$$

in which $\mathbf{x}$ and $\mathbf{y}$ are coordinate vectors; $g(\|\mathbf{y}-\mathbf{x}\|) \geqslant 0$ is a certain weighting function and $G(\mathbf{x})$ is defined as a weight associated with the material point $\mathbf{x}$, aiming at normalizing the weighting scheme:

$$G(\mathbf{x}) = \int_{V_\mathrm{d}} g(\|\mathbf{y}-\mathbf{x}\|)\,\mathrm{d}V \tag{16}$$

Alternatively in the gradient theory, the operator is given explicitly by (Polizzotto et al., 1998)

$$L(\dot{\alpha}_k) = \dot{\alpha}_k + c^2\nabla^2\dot{\alpha}_k \tag{17}$$

where c is the gradient coefficient, related to the internal length of the non-local continuum.

With the appearance of non-local terms (see Eq. (8b)), the Helmholtz free energy f can be assumed to be a function of the total strain ε_{ij}, temperature θ, local internal variable β_i and non-local internal variable $\tilde{\alpha}_k$. Its time differentiation therefore reads

$$\dot{f} = \frac{\partial f}{\partial \varepsilon_{ij}}\dot{\varepsilon}_{ij} + \frac{\partial f}{\partial \theta}\dot{\theta} + \frac{\partial f}{\partial \beta_i}\dot{\beta}_i + \frac{\partial f}{\partial \tilde{\alpha}_k}\dot{\tilde{\alpha}}_k \tag{18}$$

Comparing Eq. (18) with Eq. (8b), we have the following state laws:

$$\sigma_{ij} = \frac{\partial f}{\partial \varepsilon_{ij}} \tag{19}$$

$$s = -\frac{\partial f}{\partial \theta} \tag{20}$$

The dissipation then becomes

$$d = \bar{\chi}_i^{\beta}\dot{\beta}_i + \bar{\chi}_k^{\alpha}\dot{\tilde{\alpha}}_k + P \tag{21}$$

where $\bar{\chi}_k^{\alpha} = -\partial f/\partial\tilde{\alpha}_k$ and $\bar{\chi}_i^{\beta} = -\partial f/\partial\beta_i$ are termed generalized stresses (Houlsby and Puzrin, 2000, 2006) associated with the non-local internal variable $\tilde{\alpha}_k$ and local internal variable β_i, respectively. For the second case of non-locality (Section 2.3), mathematically the same expression as (21) for the dissipation can be obtained, as Eqs. (18) and (8b) also hold in such a case.

On the other hand, for a rate-independent material, the dissipation must have a linear form (Borino et al., 1999; Houlsby and Puzrin, 2000):

$$d = \chi_k^\alpha \dot{\alpha}_k + \chi_i^\beta \dot{\beta}_i \tag{22}$$

where $\chi_k^\alpha = \partial d/\partial \dot{\alpha}_k$ and $\chi_i^\beta = \partial d/\partial \dot{\beta}_i$ are called dissipative generalized stresses in the thermodynamic framework by Houlsby and Puzrin (2000, 2006). For the non-local approach here, χ_k^α, which is associated with a non-local dissipation process, will be shown to be of non-local form. Comparing (21) and (22), we have

$$\bar{\chi}_i^\beta = \chi_i^\beta \tag{23}$$

$$\text{and } P = \chi_k^\alpha \dot{\alpha}_k - \bar{\chi}_k^\alpha L(\dot{\alpha}_k) \tag{24}$$

The former expression (23) is a form of the orthogonality condition for the generalized and dissipative generalized stresses χ_i^β and $\bar{\chi}_i^\beta$ (Houlsby and Puzrin, 2000, 2006). The latter expression (24) in this case acts as a special form of the orthogonality condition for χ_k^α and $\bar{\chi}_k^\alpha$, which will be shown to be of non-local form. In addition, the insulation condition on the non-locality residual P must be satisfied (Eq. (3)). In physical terms, this condition assures that energy exchange only takes place within a finite region V_d where the dissipation processes are. Hence

$$\int_{V_\mathrm{d}} \left[\chi_k^\alpha \dot{\alpha}_k - \bar{\chi}_k^\alpha L(\dot{\alpha}_k)\right] \mathrm{d}V = 0 \tag{25}$$

We introduce here the operator L^*, adjoint with L but applied to $\bar{\chi}_k^\alpha$ and defined by (see also Borino et al., 1999; Jirásek and Rolshoven, 2003):

$$L^*\left(\bar{\chi}_k^\alpha\right) = \tilde{\bar{\chi}}_k^\alpha(\mathbf{x}) = \int_{V_\mathrm{d}} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \bar{\chi}_k^\alpha(\mathbf{y}) \mathrm{d}V(\mathbf{y}) \tag{26}$$

where function $G(\mathbf{y})$ has been defined in (16). It is noted here that L^* is self-adjoint ($L^* = L$) only if function $G(\mathbf{x}) = \int_{V_\mathrm{d}} g(\|\mathbf{y}-\mathbf{x}\|)\mathrm{d}V$ is not dependent on the position of the point under consideration (Borino et al., 1999; Jirásek and Rolshoven, 2003). This is the case of infinite material bodies and results in symmetric non-local tangent stiffness matrix (Borino et al., 2003). For a structure of finite size, $L^* \neq L$ and the symmetry of the non-local tangent stiffness is lost. A modified weighting scheme was also proposed by Borino et al. (2003) to remedy the problems of a non-symmetric stiffness matrix. It is, however, not adopted in this study.

From the second term of (25), we have

$$\begin{aligned}\int_{V_\mathrm{d}} \bar{\chi}_k^\alpha(\mathbf{x}) L(\dot{\alpha}_k)\mathrm{d}V(\mathbf{x}) &= \int_{V_\mathrm{d}} \bar{\chi}_k^\alpha(\mathbf{y}) \left[\int_{V_\mathrm{d}} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \dot{\alpha}_k(\mathbf{x})\mathrm{d}V(\mathbf{x})\right]\mathrm{d}V(\mathbf{y}) \\ &= \int_{V_\mathrm{d}} \left[\int_{V_\mathrm{d}} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \bar{\chi}_k^\alpha(\mathbf{y})\mathrm{d}V(\mathbf{y})\right]\dot{\alpha}_k(\mathbf{x})\mathrm{d}V(\mathbf{x}) = \int_{V_\mathrm{d}} \tilde{\bar{\chi}}_k^\alpha(\mathbf{x})\dot{\alpha}_k(\mathbf{x})\mathrm{d}V(\mathbf{x})\end{aligned} \tag{27}$$

Therefore the following equality can be withdrawn using (26) and (27)

$$\int_{V_\mathrm{d}} \bar{\chi}_k^\alpha L(\dot{\alpha}_k)\mathrm{d}V = \int_{V_\mathrm{d}} L^*\left(\bar{\chi}_k^\alpha\right)\dot{\alpha}_k \mathrm{d}V \tag{28}$$

Substituting the above into (25), we obtain

$$\int_{V_\mathrm{d}} \left[\chi_k^\alpha - L^*\left(\bar{\chi}_k^\alpha\right)\right]\dot{\alpha}_k \mathrm{d}V = 0 \tag{29}$$

It can be seen from the above expression that for any dissipation mechanism, the bracketed terms must entirely vanish regardless of the relationship between it and $\dot{\alpha}_k$ (Borino et al., 1999). This then leads to the following non-local form of the orthogonality condition:

$$\chi_k^\alpha = L^*\left(\bar{\chi}_k^\alpha\right) = \int_{V_\mathrm{d}} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \bar{\chi}_k^\alpha(\mathbf{y})\mathrm{d}V(\mathbf{y}) \tag{30}$$

It can be seen from (30) that χ_k^α in (22) must be of non-local form. The above-presented approach has introduced a way for incorporating non-locality into an existing thermodynamic framework, based on the concept of non-locality residual. The idea can be adapted to any existing thermodynamic approach without any

difficulty. However, the use of the non-local form of the orthogonality condition in combination with the Legendre transformation of the dissipation function (Houlsby and Puzrin, 2000, 2006) in this thermodynamic framework furnishes a consistent and rigorous way for the derivation of non-local constitutive models.

2.5. Non-local loading function

The dissipation potential in (22) is assumed to be decomposed into two additive parts, both of which are homogeneous first order in the rate of corresponding internal variable. The requirement that every additive part of the dissipation potential be non-negative is in fact more stringent than the second law of thermodynamics. This assumption leads to the so-called weak coupling between internal variables, in contrast with the strong coupling cases in which the dissipation potential can no longer be decomposed into additive parts (see Einav et al., 2007). We rewrite the dissipation potential here, as:

$$d = d^{\alpha} + d^{\beta} = \chi_k^{\alpha}\dot{\alpha}_k + \chi_i^{\beta}\dot{\beta}_i \tag{31}$$

The loading functions in this case are direct results of the degenerate Legendre transformation of the dissipation potential d, with λ^{α} and λ^{β} being two corresponding non-negative multipliers:

$$\lambda^{\alpha} y^{\alpha} = \chi_k^{\alpha}\dot{\alpha}_k - d^{\alpha} = 0 \tag{32}$$

$$\lambda^{\beta} y^{\beta} = \chi_i^{\beta}\dot{\beta}_i - d^{\beta} = 0 \tag{33}$$

The flow rules can be obtained by differentiating both sides of (32) and (33):

$$\dot{\alpha}_k = \lambda^{\alpha}\frac{\partial y^{\alpha}}{\partial \chi_k^{\alpha}} \tag{34}$$

$$\dot{\beta}_i = \lambda^{\beta}\frac{\partial y^{\beta}}{\partial \chi_i^{\beta}} \tag{35}$$

In the model formulation, if d is explicitly specified, y^{α} and y^{β} can be worked out straightforwardly (Nguyen, 2005; Nguyen and Houlsby, 2007a,b). The enforcement of the orthogonality conditions, in both local (23) and non-local (30) forms, will then be made, resulting in two corresponding loading functions. Alternatively, the two loading functions y^{α} and y^{β} can also be specified based on experimental results, and the dissipation potential can then be obtained from these loading functions, also through the Legendre transformation. This dual process was described at length in Houlsby and Puzrin (2000) and illustrated in Nguyen (2005). The advantage of making an explicit link between dissipation potential and loading function here is that energy dissipation, e.g. due to fracturing processes in quasi-brittle materials, can be determined just by integrating the dissipation potential (in fact the rate of dissipation). Although in practice, yield/damage activation surfaces should be specified based on experimental tests, their evolutions and interaction can be more readily controlled in the constitutive model using the dissipation potential, especially in coupling cases with more than one dissipation mechanisms (Nguyen and Korsunsky, 2006).

In summary, any models formulated based on the proposed approach just need the specification of two potentials: the energy and the dissipation potentials. The dissipation potential here acts as a real potential governing the evolutions of internal variables, which is in contrast with the use of the dissipation as a pseudo potential in other thermodynamic frameworks (e.g. in Lemaitre, 1992; Lemaitre and Chaboche, 1990). In other words, χ_k^{α} and χ_i^{β} need to be specified here to have an explicitly defined dissipation potential for the formulation of constitutive models. In combination with the Legendre transformation of the dissipation function, the enforcement of the orthogonality condition in both local (23) and non-local (30) forms during the model formulation creates ways for the natural occurrence of the loading functions with desired features. The proposed approach is hence distinguishable from other existing ones thanks to this feature of the thermodynamic framework. Illustrations on formulation of non-local models in the context of damage mechanics will be presented in the following sections.

It should also be noted that although in the above approach two dissipation mechanisms with corresponding internal variables α_i and β_i are used, their interaction (or coupling) in a non-local thermodynamic framework is not yet considered here. Use of two different sets of local and non-local internal variables in the

presented approach here is just to illustrate the difference in the arising forms of the orthogonality conditions. Coupling between local and non-local internal variables is to be tackled in a separate study in which the weak and strong coupling between different internal variables (see Einav et al., 2007) will also be accounted for.

3. Application of the proposed approach to non-local constitutive modelling of concrete

In the original approach (Polizzotto et al., 1998; Polizzotto and Borino, 1998; Borino et al., 1999; Benvenuti et al., 2002) the Italian researchers just used the property (13), to specify a non-local form of a loading function (e.g. a non-local yield function in Borino et al. (1999)), which is in line with the principle of maximum dissipation. In other words, due to Eqs. (22) and (30), the non-local form of χ_k^α must appear in the loading function. This is in contrast with the non-local approach by Nilsson (1997), in which the thermodynamic admissibility of the non-local model is only partly assured (see Jirásek and Rolshoven, 2003). Neither approach specifies a non-local form of the dissipation function and uses it to derive the corresponding non-local loading function. In this section, we will make use of the Legendre transformation illustrated in the case of non-local modelling, and show that a non-local form of the loading function can be directly derived from two specified energy potentials: non-local dissipation potential and energy potential, following procedures consistently established beforehand. The flexibility of the proposed approach here lies in the so-called non-local form (30) of the orthogonality condition. Any expression for the dissipative generalized stress χ_k^α can be specified to obtain a non-local damage model with desired damage criterion and softening behaviour.

The proposed approach is applied here for the formulation of non-local damage models for concrete. However, only pure damage models are considered here. Coupling between damage and plasticity within this non-local thermodynamic approach is not accounted for and should be an issue for further study.

3.1. A strain-based non-local damage model

The formulation of a simple non-local damage model is used here as an illustration. For a strain-based formulation, the following Helmholtz free energy function is specified for isothermal processes.

$$f = \frac{(1-\tilde{\alpha}_{\mathrm{d}})E}{2(1+\nu)}\left[\varepsilon_{ij}\varepsilon_{ij} + \frac{\nu}{(1-2\nu)}\varepsilon_{kk}\varepsilon_{ll}\right] \tag{36}$$

or in a more convenient form

$$f = \frac{1}{2}(1-\tilde{\alpha}_{\mathrm{d}})a_{ijkl}\varepsilon_{ij}\varepsilon_{kl} \tag{37}$$

in which $\tilde{\alpha}_{\mathrm{d}}$ is a non-local internal variable characterizing the damage processes; a_{ijkl} is the elasticity stiffness tensor expressed in terms of elasticity modulus E and Poisson's ratio ν

$$a_{ijkl} = \frac{E}{2(1+\nu)}\left[\frac{2\nu}{1-2\nu}\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right]$$

The evolution laws of internal variables, following several thermo-mechanical frameworks (Lemaitre and Chaboche, 1990; Maugin, 1992; Lemaitre, 1992), are derived by differentiating a pseudo-dissipation potential, which is postulated to exist. The whole problem of specifying a constitutive law is then reduced to specifying two potentials: the free energy and the dissipation potential. However, things are different here. Instead of postulating the existence of a pseudo dissipation potential, the dissipation in the framework used here is assumed to be a function of the thermodynamics state of the material and the rate of change of state. In addition, use of loading functions (yield and/or damage functions) or dissipation function is interchangeable in the framework. Here, a dissipation function, which is in fact worked out from an energy-based damage function, is used and takes the form

$$d = F_1^*(\tilde{\alpha}_{\mathrm{d}}, \varepsilon_{ij})\dot{\alpha}_{\mathrm{d}} \tag{38}$$

where $F_1^*(\tilde{\alpha}_{\mathrm{d}}, \varepsilon_{ij})$ is a positive and increasing function associated with the damage process; this function in fact controls the rate of damage dissipation.

A note should be given here to the forms of damage variable in the energy potential and dissipation potential. For formal purposes (see Houlsby and Puzrin, 2000), the generalized stress $\bar{\chi}$ and dissipative generalized stress χ should be kept separate (see Section 2.3). The enforcement of the orthogonality condition in the form $\bar{\chi} = \chi$ is then made during the model formulation. In combination with the Legendre transformation of the dissipation function, it furnishes a way for the natural occurrence of the loading function. For a local formulation (e.g. Nguyen, 2005; Nguyen and Houlsby, 2007a) based on the framework used, as the orthogonality condition is enforced in a local form the same local internal variable is associated with $\bar{\chi}$ and χ. However, for a non-local form of the orthogonality condition in this study (see Eq. (30)), different forms of the same internal variable are correspondingly associated with the generalized stress $\bar{\chi}$ and dissipative generalized stress χ (see Eqs. (21) and (22)). Therefore, the rate of local damage variable must be used in the dissipation potential (38), while its non-local counterpart is used in the Helmholtz free energy function f in (36) and component function F_1^* in (38).

The derivation of a constitutive model here follows standard procedures established beforehand in the original framework (Houlsby and Puzrin, 2000, 2006), and partly illustrated in the preceding sections. The stress and generalized stresses are derived from the energy function:

$$\sigma_{ij} = \frac{\partial f}{\partial \varepsilon_{ij}} = (1 - \tilde{\alpha}_\mathrm{d}) a_{ijkl} \varepsilon_{kl} \tag{39}$$

$$\bar{\chi}_\mathrm{d} = -\frac{\partial f}{\partial \tilde{\alpha}_\mathrm{d}} = \frac{1}{2} a_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \tag{40}$$

In (40), the thermodynamic force $\bar{\chi}_\mathrm{d}$ conjugate to the non-local damage indicator $\tilde{\alpha}_\mathrm{d}$ is of local form and can be identified as the strain energy release rate with respect to $\tilde{\alpha}_\mathrm{d}$ under constant stress (Lemaitre, 1992). The dissipative generalized stresses in this case can be obtained from the dissipation function in a way similar to the above derivation of the stress and generalized stresses:

$$\chi_\mathrm{d} = \frac{\partial d}{\partial \dot{\alpha}_\mathrm{d}} = F_1^*(\tilde{\alpha}_\mathrm{d}, \varepsilon_{ij}) \tag{41}$$

The damage criterion is then derived by eliminating $\dot{\alpha}_\mathrm{d}$ from Eq. (41). It is a result of the degenerate Legendre transformation of the dissipation function, in which the strain ε_{ij} appearing in (41) is considered as a passive variable in the transformation (see Collins and Houlsby, 1997). In the case of scalar damage variable here, (41) directly results in a damage loading function of the form

$$y_\mathrm{d} = \chi_\mathrm{d} - F_1^*(\tilde{\alpha}_\mathrm{d}, \varepsilon_{ij}) = 0 \tag{42}$$

Since α_d is only a scalar variable, there is actually no "flow rule" for the damage process, and the damage multiplier, which resembles that in plasticity, coincides with the scalar damage increment $\dot{\alpha}_\mathrm{d}$

$$\dot{\alpha}_\mathrm{d} = \lambda_\mathrm{d} \frac{\partial y_\mathrm{d}^*}{\partial \chi_\mathrm{d}} = \lambda_\mathrm{d} \tag{43}$$

Following the non-local thermodynamic formulation in Section 2.4, the non-local form $\chi_\mathrm{d} = L^*(\bar{\chi}_\mathrm{d})$ of the orthogonality condition must hold, turning the above damage loading function to

$$y_\mathrm{d} = L^*(\bar{\chi}_\mathrm{d}) - F_1^*(\tilde{\alpha}_\mathrm{d}, \varepsilon_{ij}) = 0 \tag{44}$$

The choice of function $F_1^*(\tilde{\alpha}_\mathrm{d}, \varepsilon_{ij})$ is flexible and can be made on the basis of desired features of the damage surface and the evolution law of damage. In the simplest case we may have $F_1^* = F_1(\tilde{\alpha}_\mathrm{d})$, as a function of the non-local damage variable $\tilde{\alpha}_\mathrm{d}$ only. For pure damage behaviour, $F_1(\tilde{\alpha}_\mathrm{d})$ can assume the following form (Nguyen, 2005):

$$F_1(\tilde{\alpha}_\mathrm{d}) = \frac{f_\mathrm{t}'^2}{2E} \left[\frac{E + E_\mathrm{pt}(1 - \tilde{\alpha}_\mathrm{d})^{n_\mathrm{t}}}{E(1 - \tilde{\alpha}_\mathrm{d}) + E_\mathrm{pt}(1 - \tilde{\alpha}_\mathrm{d})^{n_\mathrm{t}}} \right]^2 \tag{45}$$

in which f_t' is the uniaxial tensile strength; E_pt and n_t are two parameters governing the damage evolution, the physical interpretations and calibration of which can be found in Nguyen (2005).

The damage loading function (42) becomes

$$y_d = \frac{1}{2}\int_{V_d} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} a_{ijkl}\varepsilon_{ij}\varepsilon_{kl}\,dV - F_1(\tilde{\alpha}_d) = 0 \tag{46}$$

So far we have not defined the volume V_d where dissipation takes place, and the weighting function $g(\|\mathbf{y}-\mathbf{x}\|)$ for the regularization operator L. These are required for the definition of the non-local damage criterion in (46). In the literature, V_d is a volume defined by a sphere of center $\mathbf{x}$ and radius R and $g(\|\mathbf{y}-\mathbf{x}\|)$ can be defined as the bell-shaped weight function:

$$g(r) = g(\|\mathbf{y}-\mathbf{x}\|) = \begin{cases} 0 & \text{if } r > R \\ \left(1-\frac{r^2}{R^2}\right)^2 & \text{if } r \leqslant R \end{cases} \tag{47}$$

or Gauss distribution function:

$$g(r) = \exp\left(-\frac{r^2}{2l^2}\right) \tag{48}$$

in which R is termed non-local interaction radius, and l is a length parameter of the Gauss distribution function (Jirásek, 1998). We adopt the definition (47) in this study.

As the damage criterion is specified here in strain space, this is the case in which the stress update can be carried out without spatial coupling between material states at several integration points. In other words, the damage increment can be directly determined from the rate form of the damage function, based on the strain rates at several integration points within a sphere (or circle) of radius R. The consistent non-local tangent stiffness matrix can be readily derived following Jirásek and Patzák (2002). This matrix is however non-symmetric due to the use of the non-local averaging in (26). In this study, local secant stiffness was used. As a consequence this significantly increased the computational costs. In addition, it should be noted here that the averaging scheme in (30) is unable to reproduce uniform field for bounded structure (Comi and Perego, 2001). This may lead to numerical difficulties in some models where the non-local damage variable is directly evaluated using that averaging scheme (Comi and Perego, 2001). This is however not the case here since the non-locality of damage is implicitly defined through its associated non-local thermodynamic force (see Eq. (46)). The implementation of the model is not of main concern here and therefore not presented. Numerical example demonstrating the mesh-independence of the model described above will be shown in Section 4.

3.2. A stress-based non-local damage model

We present here a non-local coupled damage-plasticity model formulated based on the non-local thermodynamic approach in Section 2.4. The Gibbs free energy function is assumed to be of the following form:

$$g = -\frac{D_{ijkl}\sigma_{ij}\sigma_{kl}}{2(1-\tilde{\alpha}_d)} \tag{49}$$

in which $\tilde{\alpha}_d$ is the non-local scalar damage variable, respectively; D_{ijkl} is the elasticity compliance tensor expressed in terms of elasticity modulus E and Poisson's ratio v as

$$D_{ijkl} = \frac{1+v}{2E}\left(-\frac{2v}{1+v}\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)$$

The dissipation here takes the form:

$$d = F_1^*(\tilde{\alpha}_d, \sigma_{ij})\dot{\tilde{\alpha}}_d \tag{50}$$

where $F_1^*(\tilde{\alpha}_d, \sigma_{ij})$ is a positive and monotonically increasing scalar-valued function associated with the damage process.

The derivation of the constitutive models here follows the same route illustrated in Section 3.1. The total strain and generalized stresses are derived from the energy function g as follows:

$$\varepsilon_{ij} = -\frac{\partial g}{\partial \sigma_{ij}} = \frac{D_{ijkl}\sigma_{kl}}{1-\tilde{\alpha}_{\mathrm{d}}} \tag{51}$$

$$\bar{\chi}_{\mathrm{d}} = -\frac{\partial g}{\partial \tilde{\alpha}_{\mathrm{d}}} = \frac{D_{ijkl}\sigma_{ij}\sigma_{kl}}{2(1-\tilde{\alpha}_{\mathrm{d}})^2} \tag{52}$$

In a similar way, the dissipative generalized stress χ_{d} is:

$$\chi_{\mathrm{d}} = \frac{\partial d}{\partial \dot{\tilde{\alpha}}_{\mathrm{d}}} = F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij}) \tag{53}$$

The derivation of the damage criterion is a result of the degenerate Legendre transformation of the dissipation function (Houlsby and Puzrin, 2000, 2006):

$$y_{\mathrm{d}} = \chi_{\mathrm{d}} - F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij}) = 0 \tag{54}$$

We also have the following evolution rule for the scalar damage increment $\dot{\tilde{\alpha}}_{\mathrm{d}}$

$$\dot{\tilde{\alpha}}_{\mathrm{d}} = \lambda_{\mathrm{d}} \frac{\partial y_{\mathrm{d}}}{\partial \chi_{\mathrm{d}}} = \lambda_{\mathrm{d}} \tag{55}$$

The non-local form (30) of the orthogonality condition also holds:

$$\chi_{\mathrm{d}} = L^*(\bar{\chi}_{\mathrm{d}}) = \int_{V_{\mathrm{d}}} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \frac{D_{ijkl}\sigma_{ij}\sigma_{kl}}{2(1-\tilde{\alpha}_{\mathrm{d}})^2}\, \mathrm{d}V(\mathbf{y}) \tag{56}$$

turning the damage loading function (54) to

$$y_{\mathrm{d}} = \int_{V_{\mathrm{d}}} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \frac{D_{ijkl}\sigma_{ij}\sigma_{kl}}{2(1-\tilde{\alpha}_{\mathrm{d}})^2}\, \mathrm{d}V(\mathbf{y}) - F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij}) = 0 \tag{57}$$

In the above expression, choice of the scalar-valued function $F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij})$, which is of non-local form, is flexible, provided that it is non-negative to assure the thermodynamic admissibility of the dissipation process. The simplest choice of $F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij})$ could be $F_1(\tilde{\alpha}_{\mathrm{d}})$, as selected in the previous section. However, in general it can be in any other forms which can produce desired damage surfaces and damage evolution laws. Here the following form of $F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij})$ is adopted:

$$F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij}) = \begin{cases} 0 & \text{if } \sigma_{ij}(\mathbf{y}) = 0 \ (i,j = 1\ldots 3) \quad \forall\, \mathbf{y} \in V_{\mathrm{d}} \\ \left[\int_{V_{\mathrm{d}}} \dfrac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \dfrac{D_{ijkl}\sigma_{ij}\sigma_{kl}}{2(1-\tilde{\alpha}_{\mathrm{d}})^2}\, \mathrm{d}V(\mathbf{y})\right] \dfrac{F_1(\tilde{\alpha}_{\mathrm{d}})}{F_2(\omega(\mathbf{x}))} & \text{otherwise} \end{cases} \tag{58}$$

where $F_1(\tilde{\alpha}_{\mathrm{d}})$ and its parameters have been defined in (45); and the non-local function $F_2(\omega(\mathbf{x}))$ is defined here as a non-negative and scalar-valued function depending on the non-local energy-like ω at coordinate $\mathbf{x}$ of the material point under consideration. Substituting (58) into (57), we obtain:

$$y_{\mathrm{d}} = \left[\int_{V_{\mathrm{d}}} \frac{g(\|\mathbf{y}-\mathbf{x}\|)}{G(\mathbf{y})} \frac{D_{ijkl}\sigma_{ij}\sigma_{kl}}{2(1-\tilde{\alpha}_{\mathrm{d}})^2}\, \mathrm{d}V(\mathbf{y})\right]\left[1 - \frac{F_1(\tilde{\alpha}_{\mathrm{d}})}{F_2(\omega(\mathbf{x}))}\right] = 0 \tag{59}$$

As the first bracketed term in (59) is an energy-like term which is positive definite in non-zero stress states, its elimination in (59) is straightforward. Therefore, the damage function y_{d} can be rewritten in a simplified form as:

$$y_{\mathrm{d}} = F_2(\omega(\mathbf{x})) - F_1(\tilde{\alpha}_{\mathrm{d}}) = 0 \tag{60}$$

It is worthwhile to note here that the damage energy $\bar{\chi}_{\mathrm{d}}$ in Eq. (52) always involves in the dissipation process. This is because function $F_1^*(\tilde{\alpha}_{\mathrm{d}}, \sigma_{ij})$ turns out to be equal to $\bar{\chi}_{\mathrm{d}}$ when damage occurs under the criterion (60). In such cases $F_2(\omega(\mathbf{x})) = F_1(\tilde{\alpha}_{\mathrm{d}})$, and the dissipation rate due to damage becomes $\bar{\chi}_{\mathrm{d}}\dot{\alpha}_{\mathrm{d}}$. However, the activation and the evolution of damage are associated with the damage criterion (60). The technique presented above provides a useful way to integrate damage criterion with desired features into the thermodynamic framework used.

The choice of function $F_2(\omega(\mathbf{x}))$ is flexible here to obtain the desired shape of the damage surface. In the proposed model here, we define it as a non-local stress-based function, evaluated at position $\mathbf{x}$ of the material point:

$$F_2(\omega(\mathbf{x})) = L(\omega) = L\left(\frac{(1+p_t)\sigma_{ij}^+\sigma_{ij}^+ - p_t\langle\sigma_{kk}\rangle\langle\sigma_{ll}\rangle}{2E(1-\tilde{\alpha}_d)^2}\right)$$
$$= \frac{1}{G(\mathbf{x})}\int_{V_d} g(\|\mathbf{y}-\mathbf{x}\|)\frac{(1+p_t)\sigma_{ij}^+\sigma_{ij}^+ - p_t\langle\sigma_{kk}\rangle\langle\sigma_{ll}\rangle}{2E(1-\tilde{\alpha}_d)^2}\,dV(\mathbf{y}) \tag{61}$$

in which L is the regularization operator defined in (15); $\langle\ \rangle$ denotes the Macaulay bracket; p_t is a parameter controlling the shape of the damage surface in stress space (Nguyen, 2005); and σ_{ij}^+ is defined as the positive part of the total stress tensor σ_{ij}, which in turn is decomposed into positive and negative parts using the eigenvalue decomposition (Ladeveze, 1983; Ortiz, 1985):

$$\sigma_{ij}^+ = \sum_{m=1}^{3}\langle\sigma^m\rangle p_i^m p_j^m \tag{62}$$

where $\mathbf{p}^m$ is the unit vector of the mth principal direction and σ^m is the mth principal stress. Further details and some properties of the decomposition can be found in Ladeveze (1983) and Ortiz (1985). Use of other more complicated forms for $F_2(\mathbf{x})$ is possible, but not pursued in this study to preserve the simplicity yet the practicality of the proposed constitutive model.

It is noted here that in principle, the adjoint regularization operator L^* or any other form of non-local averaging can be used in (61). In all cases, the thermodynamic admissibility of the model is always strictly satisfied, through the enforcement of the non-local form (30) of the orthogonality condition. This is an interesting feature of the approach presented here, allowing the flexibility in the formulation of non-local constitutive models.

The non-local damage model described in this section however suffers some computational drawbacks due to the non-symmetry of the non-local tangent stiffness matrix and the coupling between integration points. It is difficult, or even impossible, to derive the non-local consistent stiffness matrix and the stress update process is very complicated and time consuming. This is due to the use of an implicit law for damage evolution and the coupling between integration points. In particular, the stress update algorithm leads to a system of non-linear equations to be solved at every iterative step. The size of this system of equations depends on the size of the damage zone, with damage spreading due to non-locality. On the other hand, local stiffness matrix was used for the numerical simulation, due to difficulty in deriving the non-local consistent stiffness matrix. Therefore the computational cost increases considerably during the simulated failure process. Details on this can be found in Nguyen (2005). The finite element implementation of a constitutive model with the non-local damage criterion (60) has been described in Nguyen (2005) and Nguyen and Houlsby (2007b) and therefore is not presented here.

4. Numerical examples

Some numerical examples are used here to demonstrate the mesh objectiveness of the numerical solutions of structural problems, captured by the non-local damage models presented in Section 3. More demonstrations on the mesh independency of those models can be found in Nguyen (2005) and Nguyen and Houlsby (2007b). In addition, the constitutive behaviour of those models along with the calibration of model parameters has been described in other papers (Nguyen, 2005; Nguyen and Houlsby, 2007a,c). The analytical proof for the regularization effects of non-local models derived within the proposed non-local thermodynamic approach is a subject of another study and not incorporated here.

4.1. Double-edge notched specimen under tension using non-local isotropic damage model

In this numerical example, the numerical simulations of a double edge notched specimen under tension (Shi et al., 2000; Fig. 1) are presented. In the numerical models, the specimen is fixed in both directions at the bottom edge, and in horizontal direction at the top edge. The numerical analyses were carried out using two meshes of 6-node triangular finite elements, with prescribed vertical displacements on the top edge of the specimen.

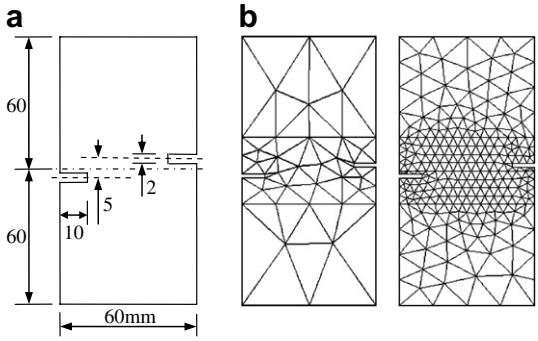

Fig. 1. Double edge notched specimen (10 mm thick) – geometry (a) and FE meshes (b).

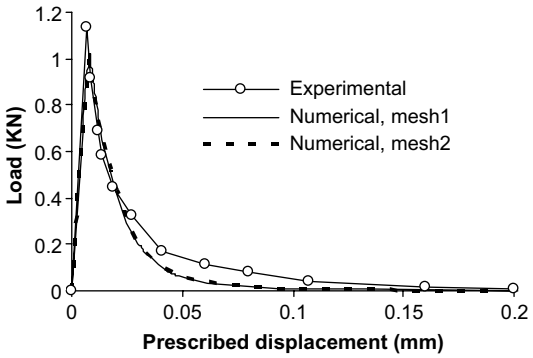

Fig. 2. Load–displacement curves.

The material properties and model parameters used are: Young's modulus $E = 24$ GPa, Poisson's ratio $v = 0.2$, tensile strength $f_t = 2.4$ MPa, fracture energy $G_f = 0.059$ N/mm, non-local interaction radius $R = 8$ mm, $E_{pt} = 3779$ MPa and $n_t = 0.29$ (see Nguyen and Houlsby (2007a,c) for details on the choice of model parameters). The isotropic strain-based damage model in Section 3.1 was used for the numerical simulation.

The numerical results are depicted in Fig. 2, showing the agreement in the load–displacement curves obtained from different finite element meshes, thus proving the lack of mesh dependence of the proposed model. In addition, the overall shape of the numerical load–displacement curves is consistent with the experimental one.

4.2. Three-point bending test using stress-based non-local damage model

The numerical simulations in this example are carried out on a notched beam in a three point bending test, aiming at investigating mode I fracture and crack propagation (Fig. 3). The geometrical data and material

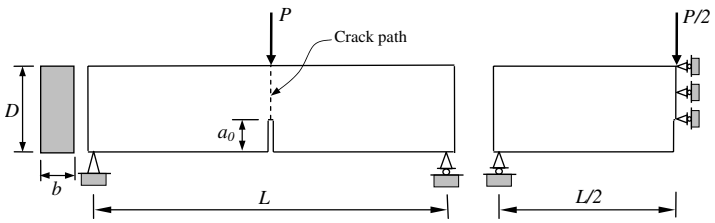

Fig. 3. Geometrical data and half beam model used in the numerical analysis.

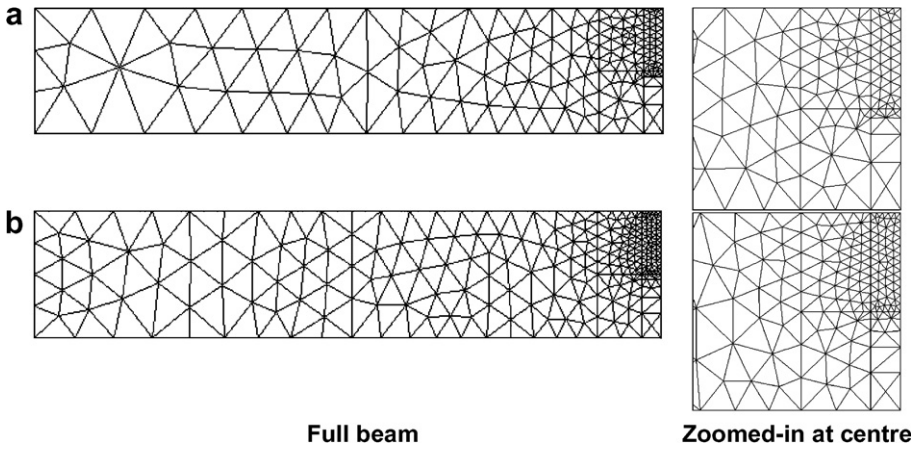

Fig. 4. Finite element meshes: coarser (a) and denser (b).

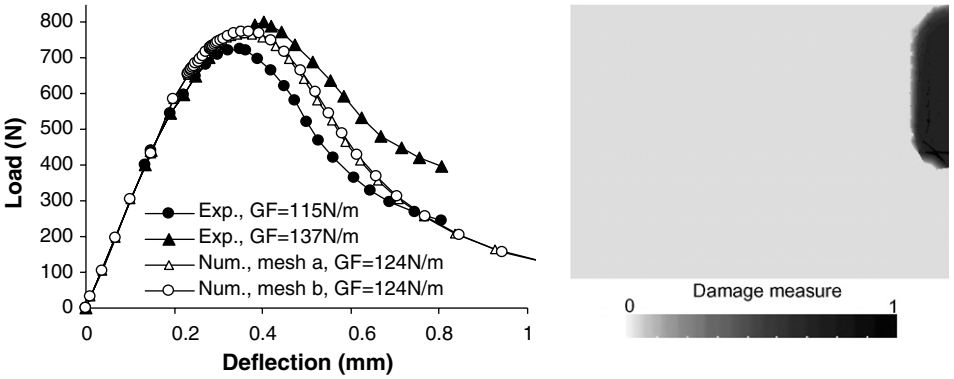

Fig. 5. Load-deflection curve and damage pattern at very late stage of the numerical analysis (mesh b, zoomed-in at center part of the half-beam).

properties are taken from the experimental test of Petersson (1981): $L = 2000$ mm, $D = 200$ mm, $b = 50$ mm, $a_0 = 100$ mm, $E = 30{,}000$ MPa, $v = 0.2$, $f'_t = 3.33$ MPa, $G_F = 0.124$ N/mm, with the fracture energy being measured eliminating the effect of the beam's self weight (see Petersson, 1981).

The nonlocal interaction radius was taken as 2.0 times the maximum aggregate size ($d_{max} = 8$ mm, Petersson (1981)), resulting in $R = 16$ mm and the following model parameters (see also Nguyen and Houlsby, 2007a,c): $E_{pt} = 6899$ MPa and $n_t = 0.32$. The numerical analyses were carried out using two different finite element meshes of six-node triangular elements, with different mesh densities. Because of symmetry, only half of the beam was modelled (Fig. 4). Numerical results, in the form of load–deflection curve and damaged pattern, are shown in Fig. 5. The damage process zone can be clearly seen in the figure and the numerical crack path agrees well with the experimental one in Fig. 3. The numerical load–deflection curves obtained from different meshes are almost identical, again demonstrating the lack of mesh-dependency of the proposed model. In addition, they also match quite well the experimental curves.

5. Concluding remarks

The key point of the approach proposed in this study is the incorporation of the concept of non-locality residual into a well defined thermo-mechanical framework. Energy exchanges between material points in the dissipation zone are therefore taken into account. This results in a non-local form of the orthogonality condition (Ziegler, 1983; Houlsby and Puzrin, 2000) and allows in principle the definition and formulation

of any non-local constitutive model. In particular, explicit link between dissipation potential and yield/damage function and way to introduce non-local damage function with desired features into the proposed non-local approach were presented (Sections 2.5 and 3.2). The derivation of any non-local damage model then requires the specification of only two energy potentials and follows procedures consistently established beforehand. This helps to simplify the formulation of complicated thermodynamically-consistent non-local models. The application to non-local constitutive modelling of concrete illustrates the capability of the proposed non-local thermodynamic approach. However the computational aspects of non-local models presented in this study have only been briefly discussed and therefore should be a subject for more research. In addition, further research is also required on the incorporation of different coupled dissipation mechanisms within the presented non-local thermodynamic framework, as well as the localization analysis for various non-local models derived within this framework.

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