THERMO-CHEMO-MECHANICAL ANALYSIS OF CONCRETE STRUCTURES CONSIDERING AGING AND DAMAGE

Gustavo Luz Xavier da Costa[1], José Claudio de Faria Telles[1], Eduardo de Moraes Rego Fairbairn[1], Fernando Luiz Bastos Ribeiro[1]

[1]*Civil Engineering Graduate Program, Federal University of Rio de Janeiro*
Avenida Athos da Silveira Ramos, 21941-972, Rio de Janeiro, Brazil
gustavo.costa@coc.ufrj.br, telles@coc.ufrj.br, eduardo@coc.ufrj.br, fernando@coc.ufrj.br

Abstract. This paper will present Finite Element models to study the thermo-chemo-mechanical behaviour of concrete structures taking into account both aging and damage. The analysis is composed of two separated models, namely: thermo-chemical and thermo-mechanical with damage. First, the thermo-chemical model will be briefly presented. Then, the thermo-mechanical model with damage will be developed and the need for an incremental constitutive equation for modeling aging of concrete will be discussed. In order to avoid mesh-dependency due to strain localization, a nonlocal integral-type technique will be employed with few changes on the logical scheme of the Finite Element model. Finally, the thermo-chemo-mechanical analysis will be presented for a theoretical example: a concrete specimen. The results will show that residual stresses will take place due to both concrete aging and thermal strains. This, in turn, might lead to the premature collapse of the structure.

Keywords: Thermo-chemo-mechanical, Damage, Concrete.

1 Introduction

Concrete's properties are one of the main concerns of civil engineering community since its first usage as a structural material. One of its principal features is the ability to harden with time accompanied by the increase of its strength. However, this happens at the expense of considerable amount of heat generation. For massive concrete structures without reinforcement, for instance, this is responsible for cracking in the early age. In this context, the process of concrete hydration has been under intensive research by the scientific community because it will generally dictate the future behaviour of the structure.

2 Thermo-chemical model

In order to simulate temperature variations due to hydration of the cement paste, ULM and COUSSY [1] and ULM and COUSSY [2] proposed a theoretical framework based on the thermodynamics. It considers the cement paste as a chemically reactive porous media, as proposed by COUSSY [3]. This methodology was already employed by other researchers such as RITA *et al.* [4], EVSUKOFF *et al*. [5], FERREIRA [6], FERREIRA [7], SILVOSO [8], CERVERA *et al.* [9] and CERVERA *et al.* [10]. In this context, the present section will use the formulation proposed by ULM and COUSSY [1], ULM and COUSSY [2] and COUSSY [3] to develop a mathematical model that describes the kinetics of hydration reaction.

2.1 Finite Element formulation

Following the reasoning presented by ULM and COUSSY [1] and ULM and COUSSY [2], the governing equations for the thermo-chemical problem will be

$$\rho c_p \dot{T} = L\dot{\xi} + \nabla\left(k\nabla T\right) \quad \text{in} \quad \Omega_e \quad \text{(Temperature field)} \tag{1}$$

$$q = -k\nabla T \quad \text{in} \quad \Omega_e \quad \text{(Fourier's law)} \tag{2}$$

$$T = \bar{T} \quad \text{in} \quad \Gamma_D \quad \text{(Dirichlet boundary condition)} \tag{3}$$

$$-k\nabla T.n = \bar{q} \quad \text{in} \quad \Gamma_N \quad \text{(Neumann boundary condition)} \tag{4}$$

$$-k\nabla T.n = h\left(T - T_{ref}\right) \quad \text{in} \quad \Gamma_R \quad \text{(Robin boundary condition)} \tag{5}$$

with $L = \rho c_p[T(\infty)_{adiabatic} - T(0)_{adiabatic}]$ and $\xi = [T(t)_{adiabatic} - T(0)_{adiabatic}]/ [T(\infty)_{adiabatic} - T(0)_{adiabatic}]$. The Finite Element formulation is easily derived after employing the Galerkin's method and Euler-backward scheme for the time derivatives. In this case, the nonlinear system of equations will be given by

$$\left(M + \Delta t\left(K + H\right)\right)T^{t+1} = F_{ct} + F_{hf} + \Delta t\left(F_{chem} + F_{conv}\right) + MT^{t} \tag{6}$$

$$M = \int N^T \rho c_p N \, d\Omega_e \tag{7}$$

$$K = \int B^T k \, B \, d\Omega_e \tag{8}$$

$$H = \oint B^T h B \, d\Gamma_R \tag{9}$$

$$F_{ct} = -\left(M + \Delta t\left(K + H\right)\right)\bar{T}^{t+1} \quad \text{Contribution of Dirichlet BC on right-hand side vector.} \tag{10}$$

$$F_{hf} = \int B^T \bar{q} \, d\Gamma_N \tag{11}$$

$$F_{chem} = \int B^T L \, \dot{\xi}^{t+1} \, d\Omega_e \tag{12}$$

$$F_{conv} = \oint B^T h T_{ref} \, d\Gamma_R \tag{13}$$

with N as the matrix of interpolation functions, B the matrix of derivatives of interpolation functions, h the convection heat transfer coefficient and ξ the hydration degree.

3 Thermo-mechanical model with aging and damage

3.1 Constitutive equation for elastic materials with aging

For elastic materials with aging, the usual constitutive equation for solids $\sigma^{t+1} = \mathbb{C}^{t+1}\,\varepsilon^{t+1}_{elastic}$ is not valid anymore. According to MARQUES and CREUS [11], for materials that harden with time, one must employ the incremental constitutive equation $\dot{\sigma}^{t+1} = \mathbb{C}^{t+1}\,\dot{\varepsilon}^{t+1}_{elastic}$ because this will preclude that, for a constant stress state, strains decrease with time. This study will not focus on the derivation of the constitutive equation but rather on its usage. A good discussion regarding constitutive equations is presented in OTTOSEN and RISTINMAA [12], ODEN [13], BAŞAR and WEICHERT [14], TRUESDELL and DILL [15], TRUESDELL [16], LIU [17], HAUPT [18], CAPALDI [19], COMAN [20], REDDY [21], BYSKOV [22] and DIMITRIENKO [23].

3.2 Finite Element formulation

Using the concept of Effective Stress and the Principle of Strain-Equivalence along with the incremental constitutive equation $\dot{\sigma}^{t+1} = \mathbb{C}^{t+1}\,\dot{\varepsilon}^{t+1}_{elastic}$, it's possible to derive the constitutive equation (15) which encompasses both aging and damage. Thus, the governing equations will be

$$\nabla.\sigma^{t+1} + b^{t+1} = 0 \quad \text{for} \quad \Omega_e \quad \text{Equilibrium (momentum) equation} \tag{14}$$

$$\sigma^{t+1} = \left(1 - D^{t+1}\right)\mathbb{C}\,\Delta\varepsilon_{elastic} + \frac{\left(1 - D^{t+1}\right)}{\left(1 - D^{t}\right)}\sigma^{t} \quad \text{Constitutive equation} \tag{15}$$

$$\varepsilon^{t+1}_{total} = \Im u^{t+1} \quad \text{Strain} - \text{displacement equation} \tag{16}$$

$$u = \bar{u} \quad \text{(Dirichlet boundary condition)} \tag{17}$$

$$\sigma.n = \bar{t} \quad \text{(Neumann boundary condition).} \tag{18}$$

Using Galerkin's method, the Finite Element nonlinear formulation for equations (14) - (18) will be

$$K^{t+1}U^{t+1} = F^{t+1}_{cd} + F^{t}_{int} + F^{t+1}_{term} + F^{t+1}_{tf} + F^{t+1}_{dl} + F^{t+1}_{pd} \tag{19}$$

$$K^{t+1} = \left(1 - D^{t+1}\right)\int B^{T}\mathbb{C}^{t+1}B\,d\Omega_e \tag{20}$$

$$F^{t+1}_{cd} = \left(1 - D^{t+1}\right)\int B^{T}\mathbb{C}^{t+1}B\,d\Omega_e U^{t} = K^{t+1}U^{t} \tag{21}$$

$$F^{t}_{int} = -\frac{\left(1 - D^{t+1}\right)}{\left(1 - D^{t}\right)}\int B^{T}\sigma^{t}d\Omega_e \tag{22}$$

$$F^{t+1}_{term} = \left(1 - D^{t+1}\right)\int \alpha B^{T}\mathbb{C}^{t+1}\left(T^{t+1} - T^{t}\right)d\Omega_e \tag{23}$$

$$F^{t+1}_{tf} = \oint B^{T}\bar{t}^{t+1}d\Gamma_N \tag{24}$$

$$F^{t+1}_{dl} = \int B^{T}b^{t+1}d\Omega_e \tag{25}$$

$$F^{t+1}_{pd} = -\left(1 - D^{t+1}\right)K^{t+1}\bar{U}^{t+1} \quad \text{Contribution of Dirichlet BC on the right} - \text{hand side vector} \tag{26}$$

$$F^{t}_{int} = -\frac{\left(1 - D^{t+1}\right)}{\left(1 - D^{t}\right)}\int B^{T}\sigma^{t}d\Omega_e \tag{27}$$

with D as a scalar damage variable although the same reasoning also applies for tensorial damage models.

3.3 Lack of objectivity due to strain localization

Problems with softening suffer from lack of objectivity which means that, upon mesh refinement, it converges to results with less energy dissipation than expected. To circumvent this issue, it will be adopted the Nonlocal technique (cf. PIJAUDIER-CABOT and BAŽANT [24], JIRÁSEK [25] and JIRÁSEK [26]).

The next example explores this problem. It's consists in a bar loaded in tension by a prescribed displacement in the upper edge. Its properties are in Table 1 and its Finite element discretization is in Figure 1 (left). It's a pure mechanical problem and the Plane Stress theory was used to develop the FEM model. The hatched elements in the middle have tensile strength f_t = 1.47 MPa while the others have f_t = 1.50 MPa. Hence, as soon as stress reaches 1.47 MPa, the strains will localize in the hatched elements. The non-objective stress-strain curve are in Figure 1 (right).

Table 1. Properties of the bar.

Height	Width	Thickness	E
0.3 m	0.1 m	0.1 m	30 GPa

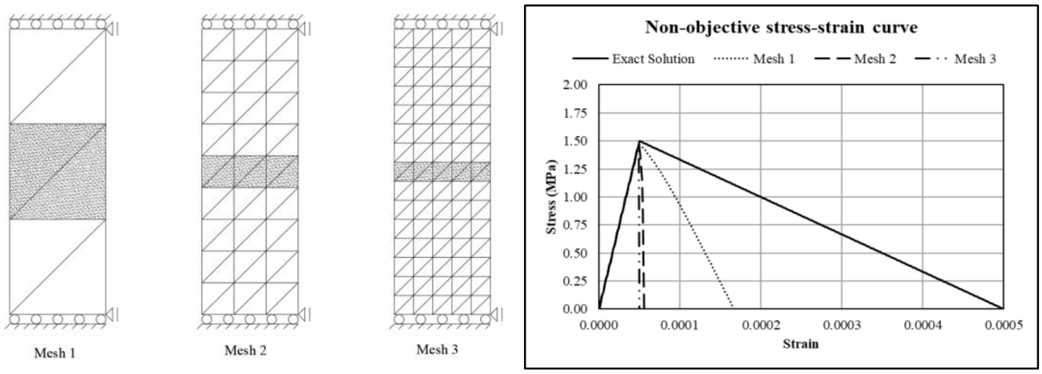

Figure 1. Meshes used (left) and their non-objective stress-strain curves (right).

Using the Nonlocal concept, the stress-strain curve becomes objective only changing the way equivalent strains are calculated. The Nonlocal concept is very useful since the main idea of the damage model remains almost the same. The only difference is that the equivalent strain of an element will be a weighted mean of the equivalent strain of near Gauss points. For linear elements, which is the case of the present study, the total number of Gauss points boils down to the total number of elements in the mesh. The Nonlocal equivalent strain $\bar{\varepsilon}_{eq}$ is evaluated as follows

$$\bar{\varepsilon}_{eq,k} = \sum_{l=1}^{\text{Number of Gauss Points}} w_l \left|J_l\right| \alpha_{kl}\, \varepsilon_{eq,l} \tag{28}$$

$$\alpha_{kl} = \frac{\alpha_0(x_k, x_l)}{\sum_{m=1}^{NGP} w_m \left|J_m\right| \alpha_0(x_k, x_m)} \tag{29}$$

$$\alpha_0(x_i, x_j) = e^{-\left(\frac{\left(\left\|x_i - x_j\right\|\right)^2}{2d^2}\right)}. \tag{30}$$

The Nonlocal technique was employed and the results are depicted in Figure 2.

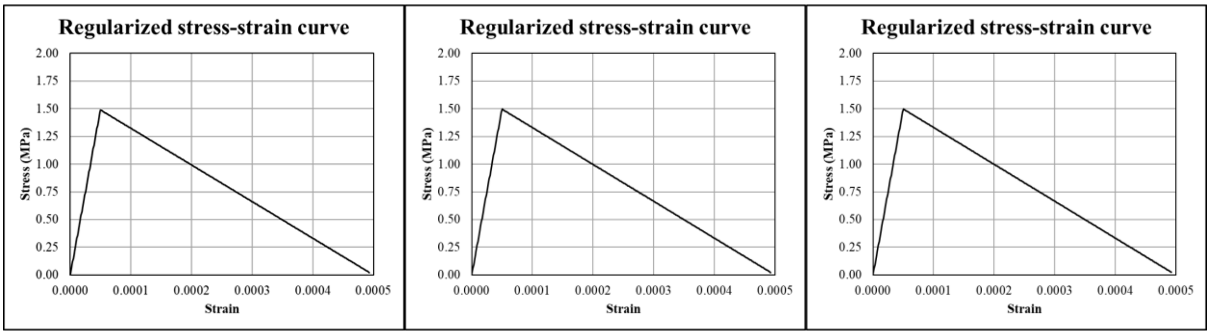

Figure 2. Objective stress-strain curves for Mesh 1 (left), Mesh 2 (center) and Mesh 3 (right).

4 Thermo-chemo-mechanical model with aging and damage

The general idea of the thermo-chemo-mechanical model is nothing but solving the thermo-chemical model first and followed by the thermo-mechanical model. The following example explores it and it's similar to the example considered in section 3.3. It consists in a bar with same geometry and boundary conditions of Figure 1 but, for the sake of simplicity, only Mesh 3 will be considered now. Its geometrical and physical properties are summarized in Table 2 below.

The bar is subjected to the hydration reaction. After 1500h, when hydration is already complete, the sample is loaded in tension by a prescribed displacement, similar to what was done in section 3.3. To avoid lack of objectivity, the Nonlocal technique was employed using the Gauss distribution and an interaction radius of 50 cm. In order to simulate the nonlinear behaviour, the Mazars damage model (MAZARS [27]) was adopted with parameters A_T and B_T also mentioned in Table 2. Parameters A_C and B_C are not important for this analysis since it is a pure tensile test. The Young's modulus was considered as a function of the hydration degree in order to take aging into account.

Table 2. Properties of the bar used in the thermo-chemo-mechanical analysis.

Properties	Values
Length (m)	0.30
Height (m)	0.10
Width (m)	0.10
Thermal conductivity ($W.m^{-1}.K^{-1}$)	2.00
Adiabatic temperature rise (°C)	25.60
Convective heat transfer coefficient ($W.m^{-2}.K^{-1}$)	0.85
Density ($kg.m^{-3}$)	2500.00
Specific heat capacity ($J.kg^{-1}.K^{-1}$)	800.00
Environment temperature (°C)	22.00
Specimen's initial temperature (°C)	22.00
Poisson's coefficient	0.30
Dilatation coefficient ($°C^{-1}$)	10^{-5}
Young's modulus (GPa)	30.00ξ

A_T	0.98
B_T	20000.00
Tensile strength for hatched elements (MPa)	1.47
Tensile strength for non-hatched elements (MPa)	1.50

The average evolution of the transverse strain is depicted in Figure 3. It was calculated as the mean strain of all elements. The evolution of stress measured on the support is in Figure 4 (left). The resulting stress-strain curve is in Figure 4 (right) and is compared with a curve without residual stresses.

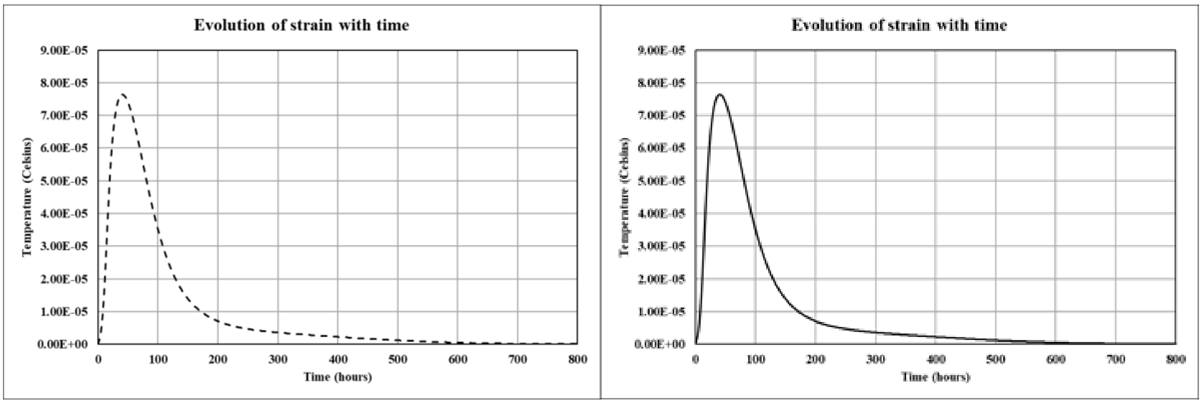

Figure 3. Average evolution of strains for non-incremental (left) and incremental (right).

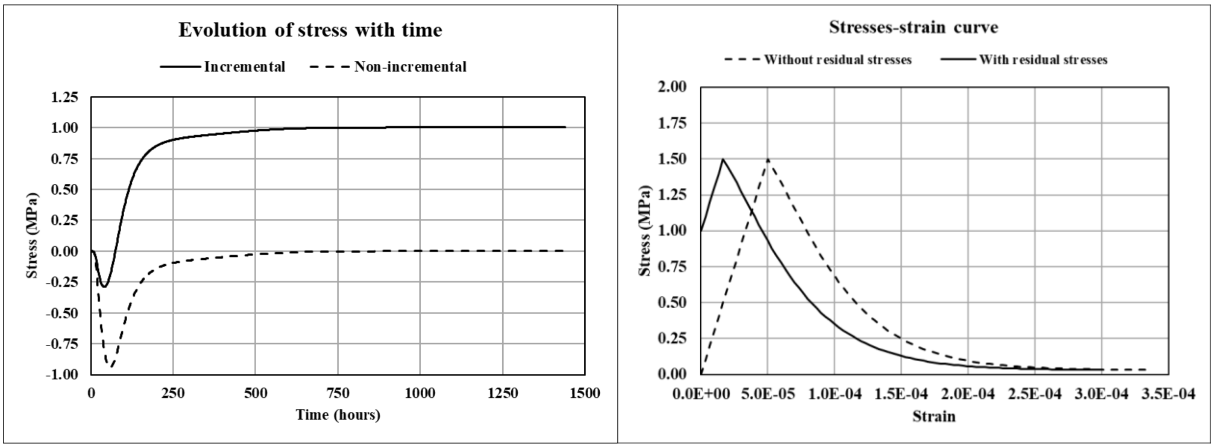

Figure 4. Stress evolution measured on the support (left) and influence of residual stresses on the stress-strain curve (right).

Figures 3 and 4 demonstrate the necessity of an incremental constitutive relation for aging materials like concrete. From Figure 3, one can conclude that the strain development in the specimen are the same for both incremental and non-incremental equations. However, Figure 4 (left) shows that, when using the incremental constitutive equation, remaining stresses take place (correct) while for non-incremental relation it does not happens (incorrect).

Figure 4 (right) exhibits what was expected: the specimen collapses before the one without residual stresses. This situation is dramatic because such premature collapse is caused by strains lower than theoretically predicted. Therefore, this pathological behaviour should be avoided or at least took into account already in the design stage given the difficulty to measure stresses accurately in daily concrete structures.

5 Conclusions

The present paper showed the influence of concrete's hydration on the response of the structure. To this end, it was developed Finite Element models that take into account aging and damage in the thermo-chemo-mechanical behaviour. It demonstrated that undesirable aspects might take place such as the presence of residual stresses. This pathological behaviour must be avoided since they will likely lead to the premature collapse of the structure.

Acknowledgements. This study was financed in part by the Brazilian Agency Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) —Finance Code 001. The support of Brazilian funding agencies Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ) are also gratefully acknowledged.

Authorship statement. The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

References

[1] F. J. Ulm and O. Coussy, "Modeling of thermochemomechanical couplings of concrete at early ages," *J. Eng. Mech.*, 1995, doi: 10.1061/(ASCE)0733-9399(1995)121:7(785).

[2] F. J. Ulm and O. Coussy, "Strength growth as chemo-plastic hardening in early age concrete," *J. Eng. Mech.*, 1996, doi: 10.1061/(ASCE)0733-9399(1996)122:12(1123).

[3] O. Coussy, *Mechanics of Porous Continua*. 1995.

[4] M. Rita, E. Fairbairn, F. Ribeiro, H. Andrade, and H. Barbosa, "Optimization of mass concrete construction using a twofold parallel genetic algorithm," *Appl. Sci.*, 2018, doi: 10.3390/app8030399.

[5] A. G. Evsukoff, E. M. R. Fairbairn, É. F. Faria, M. M. Silvoso, and R. D. Toledo Filho, "Modeling adiabatic temperature rise during concrete hydration: A data mining approach," *Comput. Struct.*, vol. 84, no. 31–32, pp. 2351–2362, 2006, doi: 10.1016/j.compstruc.2006.08.049.

[6] I. A. Ferreira, "Modelagem numérica do acoplamento térmico-químico-mecânico no concreto jovem," Universidade Federal do Rio de Janeiro, 1998.

[7] I. A. Ferreira, "Solução em paralelo de um modelo termo-químico-mecanico para concreto jovem," Universidade Federal do Rio de Janeiro, 2008.

[8] M. M. Silvoso, "Otimização da Fase Construtiva de Estruturas de Concreto em Face dos Efeitos da Hidratação via Algoritmos Genéticos," Universidade Federal do Rio de Janeiro, 2003.

[9] M. Cervera, J. Oliver, and T. Prato, "Thermo-chemo-mechanical model for concrete. II: Damage and creep," *J. Eng. Mech.*, 1999, doi: 10.1061/(asce)0733-9399(1999)125:9(1028).

[10] M. Cervera, R. Faria, J. Oliver, and T. Prato, "Numerical modelling of concrete curing, regarding hydration and temperature phenomena," *Comput. Struct.*, 2002, doi: 10.1016/S0045-7949(02)00104-9.

[11] S. P. C. Marques and G. J. Creus, *Computational viscoelasticity*. Springer International Publishing, 2012.

[12] N. Ottosen and M. Ristinmaa, *The Mechanics of Constitutive Modeling*. Elsevier Inc., 2005.

[13] J. T. Oden, *An Introduction to Mathematical Modeling: A Course in Mechanics*. John Wiley & Sons, Inc, 2011.

[14] Y. Başar and D. Weichert, *Nonlinear Continuum Mechanics of Solids*, 1st ed. Springer, 2000.

[15] C. Truesdell and E. H. Dill, *The Elements of Continuum Mechanics*. 1968.

[16] C. A. Truesdell, *A first course in Rational Continuum Mechanics*, 2nd ed. Academic Press, Inc, 1991.

[17] I. S. Liu, *Continuum Mechanics*, 1st ed. Springer, 2002.

[18] P. Haupt, *Continuum mechanics and theory of materials*, 2nd ed. Springer, 2002.

[19] F. M. Capaldi, *Continuum mechanics: Constitutive modeling of Structural and Biological materials*, 1st ed. Cambridge University Press, 2012.

[20] C. D. Coman, *Continuum Mechanics and Linear Elasticity: An Applied Mathematics introduction*, 1st ed. Springer, 2019.

[21] J. N. Reddy, *An introduction to Continuum Mechanics with applications*, 1st ed. Cambridge University Press, 2008.

[22] E. Byskov, *Elementary Continuum Mechanics for everyone: with applications to Structural Mechanics*, 1st ed. Springer, 2013.

[23] Y. I. Dimitrienko, *Nonlinear Continuum Mechanics and large inelastic deformations*, 1st ed. Springer, 2011.

[24] G. Pijaudier-Cabot and Z. P. Bažant, "Nonlocal damage theory," *J. Eng. Mech.*, vol. 113, no. 10, pp. 1512–1533, 1987, doi: 10.1061/(ASCE)0733-9399(1987)113:10(1512).

[25] M. Jirásek, "Damage and smeared crack models," in *CISM International Centre for Mechanical Sciences, Courses and Lectures*, 2011.

[26] M. Jirásek, "Nonlocal damage mechanics," *Rev. Eur. génie Civ.*, vol. 11, no. 7–8, pp. 993–1021, 2007.

[27] J. Mazars, "Application de la mecanique de l'endommagement au comportement non lineaire et a la rupture du beton de structure," Universite Pierre et Marie Curie, 1984.