MODELLING OF EARLY AGE CONCRETE CRACKING DUE TO THERMO-CHEMO-MECHANICAL COUPLINGS

F.-J. Ulm, A. Elouard, and P. Rossi,
Laboratoire Central des Ponts et Chaussées, Paris, France

Abstract
This paper aims at modelling early age concrete cracking due to thermo-chemo-mechanical couplings. The proposed modelling accounts explicitly for the hydration of cement in the constitutive modelling at the macro-level of material description (latent heat of hydration, hydration degree, thermal and autogeneous shrinkage), as well as for cracks as geometrical discontinuities (crack-width), and for the heterogeneity of the matter using a probabilistic approach. In the latter, the heterogeneity of concrete is taken into account by random distribution functions of the mechanical properties (Young's modulus, tensile strength). In the case of maturing concrete, these mechanical properties depend furthermore upon the hydration degree of concrete, and strains of thermal and chemical origin (autogeneous shrinkage) are taken into account. The proposed modelling accounts for the heterogeneity of maturing concrete (and thus for related size effects), and gives direct access to crack-patterns, crack-width and crack-spacing induced by thermo-chemo-mechanical couplings with a minimum of material parameters of clear physical significance and accessible by standard material tests.

1 Introduction

Hydration of cement is a highly exothermic and thermally activated reaction. The exothermic nature of the chemical reactions leads to heat generation, which, in the hours after pouring, may result in high temperature rises of up to 50° C in massive structures. The temperature evolution influences the kinetics of the hydration: the higher the temperature the faster occurs the reaction. As the rate of hydration slows down the temperature decreases resulting in a thermal shrinkage, which induces stresses of thermal origin. Moreover, the hydration of cement is at the base of the ageing phenomenon, which -at a macro-level of material description (i.e. scale of laboratory test specimen)- appears as a change of mechanical properties in time, and corresponds -at a micro-level of material description- to a change in the concentrations of the non-ageing constituents, i.e. the hardened cement gel. Furthermore, this change in concentration of the hardened cement gel is accompanied by a volume reduction, which results in a chemical shrinkage, coupled with a capillary shrinkage related to the formation of menisci due to water consumption through hydration. Finally, the shrinkage (if restrained) and the temperature gradients induce a severe state of stresses, which might be of a magnitude beyond the strength developed. The concrete then cracks, which effects the durability of the structure and requires often expensive treatments.

This paper aims at modelling early age concrete cracking due to thermo-chemo-mechanical couplings. We recall the thermodynamic framework of the modelling of thermo-chemo-mechanical couplings of concrete at early ages (Ulm and Coussy, 1995). It is combined with the probabilistic modelling of concrete cracking (Rossi et al., 1995) which models cracks as geometrical discontinuities and which takes into account the heterogeneity of concrete (and thus size effects), here extended to the case of maturing concrete.

2 Modelling of thermo-chemo-mechanical couplings

In this part we briefly recall the basic relations of the constitutive modelling of thermo-chemo-mechanical couplings to account at the macro-level of material description for a chemical reaction (Coussy, 1995). This framework allows to identify the hydration degree and the chemical affinity as internal state variable and conjugated forces, respectively, from mass conservation considerations and thermodynamics of open porous media, direct at the macro-level of material description

(Ulm and Coussy, 1995). In this part, the deformation of the skeleton is assumed continuous, leaving to section 3 the account for geometrical discontinuities, i.e. cracking.

2.1 Thermodynamic framework of chemical reactive porous media

Consider an *open* porous medium of initial volume $d\Omega$ composed of a matrix and a porous space which is saturated by two fluid phases, a reactant phase A and a product phase B. A chemical reaction may occur between them such that

$$A \rightarrow B \tag{1}$$

The observable strain is that of the skeleton and is denoted ε. The mass variation of the open system is due to the mass variations of fluid phases A and B per unit of macroscopic volume $d\Omega$, denoted m_A and m_B. The mass conservation for the two fluid phases reads

$$\frac{dm_A}{dt} = M^{\circ}_A - m^{\circ}_{A \rightarrow B} \qquad \frac{dm_B}{dt} = M^{\circ}_B + m^{\circ}_{A \rightarrow B} \tag{2}$$

where M°_i represents the external rate of fluid mass supply of each fluid phase. The quantity $m^{\circ}_{A \rightarrow B}$ is the rate of mass formation of product phase B due to chemical reaction (1) such that quantity $m^{\circ}_{A \rightarrow B} dt d\Omega$ is the mass of phase A which transforms into phase B during time interval dt. Note, that mass formation rate $m^{\circ}_{A \rightarrow B}$ is *a priori* not the time derivative of a function (*i.e.* $m^{\circ}_{A \rightarrow B} \neq dm_{A \rightarrow B} / dt$) since the mass increases of reactant and product phase may be due to external supply (*i.e.* the terms M°_A and M°_B).

Using thermodynamics of open porous continua, the generalized Clausius-Duhem inequality, which expresses locally the second law of thermodynamics, reads in the form

$$\Phi_1 + \Phi_{A \rightarrow B} \geq 0 \tag{3}$$

where Φ_1 is the intrinsic dissipation associated with the irreversible behaviour of the skeleton, which is zero in the case of a thermo-poro-elastic behaviour

$$\Phi_1 = \sigma : \frac{d\varepsilon}{dt} - S\frac{dT}{dt} + g^j_m \frac{dm_j}{dt} - \frac{d\Psi}{dt} = 0 \qquad j = A, B \tag{4}$$

and $\Phi_{A \to B}$ the dissipation associated with chemical reaction (1)

$$\Phi_{A \to B} = (g_m^A - g_m^B) m^\circ_{A \to B} \geq 0 \tag{5}$$

In intrinsic dissipation (4) σ, S and g_m^j are the stress tensor, the entropy and the chemical potentials or free enthalpies per mass unit of fluid phase j=A,B, associated to the rates of strain tensor ε, temperature T and fluid mass m_j (j=A,B), respectively. Furthermore, Ψ is the free energy of the open elementary system which defines the thermodynamic states of the system in terms of external variables, *i.e.* strain tensor ε, temperature T and fluid mass m_j (j=A,B)

$$\Psi = \Psi(T, \varepsilon, m_A, m_B) \tag{6}$$

Using Eq. (6) in (4) yields

$$\Phi_1 = \left(\sigma - \frac{\partial \Psi}{\partial \varepsilon}\right) : \frac{d\varepsilon}{dt} - \left(S + \frac{\partial \Psi}{\partial T}\right) \frac{dT}{dt} + \left(g_m^j - \frac{\partial \Psi}{\partial m_j}\right) \frac{dm_j}{dt} = 0 \tag{7}$$

and the constitutive equations are reduced to the sole state equations

$$\sigma = \frac{\partial \Psi}{\partial \varepsilon} \quad S = -\frac{\partial \Psi}{\partial T} \quad g_m^j = \frac{\partial \Psi}{\partial m_j} \quad \text{with} \quad j = A, B \tag{8}$$

Hence, in the case of an elastic skeleton behaviour, the dissipation is only due to the chemical reaction. It is given by inequality (5), where $g_m^A - g_m^B$ is the difference in chemical potentials between reactant phase and product phase. This gradient of free mass enthalpies expresses the thermodynamic imbalance between the chemical constituents involved in reaction (1). Chemical dissipation $\Phi_{A \to B}$ can be equally written in the form

$$\Phi_{A \to B} = A_m \xi^\circ \geq 0 \tag{9}$$

where $A_m = (g_m^A - g_m^B)$ is the affinity of the chemical reaction, and $\xi^\circ = m^\circ_{A \to B}$ its reaction rate. From Eq. (9), chemical affinity A_m is identified as the thermodynamic force associated in the (chemical) dissipation to reaction rate ξ°. It expresses the thermodynamic imbalance between the reactant and the product phase (= difference in chemical

potentials). This explicit identification holds irrespective of transport phenomena of the reactant and product phase through the structure and is essential when precising the kinetics of the chemical reaction considered at the macro-level of material description (*i.e.* scale of laboratory tests).

Consider now the elementary system as *closed* for the chemical constituents (*i.e.* $M^\circ_i = 0$, no external supply). Then, according to Eqs. (2), the rate of mass formation $m^\circ_{A \to B} = \xi^\circ$ is actually a time derivative:

$$M^\circ_i = 0 \quad \Leftrightarrow \quad m^\circ_{A \to B} = \dot{m}_{A \to B} = -\dot{m}_A = \dot{m}_B = \dot{\xi} \tag{10}$$

Closure condition (10) allows to reduce the number of state variables which characterise the thermodynamic states of the porous media. In fact, since intrinsic dissipation φ_1 of the closed elementary system reads

$$\varphi_1 = \sigma : \dot{\varepsilon} - S\dot{T} - \dot{\psi} \geq 0 \tag{11}$$

a comparison with Eqs. (3)-(5) allows to consider reaction extent ξ as an internal state variable since its evolution is spontaneous and cannot be controlled by external flow. In other words, in a closed system a chemical reaction is an internal process, and reaction extent ξ a measure of the progress of the reaction considered. Free energy ψ of the closed system then reads

$$\psi = \psi(T, \varepsilon, \xi) = \Psi(T, \varepsilon, m_a = -\xi, m_b = \xi) \tag{12}$$

and state equations (8) yield

$$S = -\frac{\partial \psi}{\partial T} \quad \sigma = \frac{\partial \psi}{\partial \varepsilon} \quad A_m = -\frac{\partial \psi}{\partial \xi} \tag{13}$$

where entropy S, stress tensor σ and chemical affinity A_m are the thermodynamic forces associated in intrinsic dissipation φ_1 with the rates of state variables T, ε and ξ. In contrast to the open elementary system, affinity A_m derives now explicitly from free energy ψ of the closed system.

2.2 Application to the hydration reaction
Hydration of cement is a fairly complex set of competing chemical reactions of different kinetics and amplitudes, related to complex physico-chemical phenomena at the micro-level of material description.

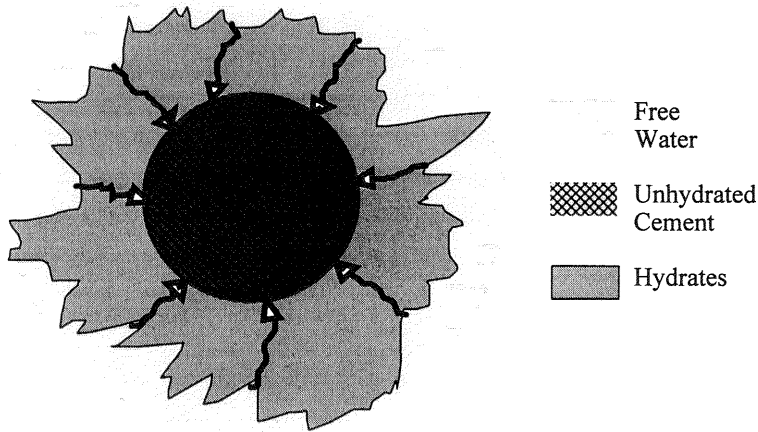Free Water

Unhydrated Cement

Hydrates

Figure 1: Diffusion of water through the layers of hydrates formed

At the level of the porous media, the hydration may be roughly viewed as follows (figure 1): at instant t, the solid part of the porous media is formed of unhydrated cement and hydrates. In order for the reaction to occur, water diffuses through the layers of hydrates already formed to the unhydrated cement. Once they meet, new hydrates are formed in an instantaneous manner relative to the time-scale of the diffusion process; then the water is chemically and/or physically combined. Hence, the diffusion of water through the layers of hydrates may be considered as the dominant mechanism of the hydration with respect to the kinetics. In terms of reaction (1), reactant phase A corresponds so to the free water, and product phase B to the water combined in the hydrates

$$\text{Free water} \quad \rightarrow \quad \text{Combined water} \tag{14}$$

Hence, mass formation rate $m^{\circ}_{A \rightarrow B}$ represents the mass rate of (non-evaporable) water combined in the solid phase. It is approximately proportional to the rate of mass formation of hardened cement gel. In this light, reaction rate ξ° can be considered as the hydration rate of the diffusion controlled reaction (14). It is controlled by the thermodynamic imbalance (affinity A_m) between free water and water combined in the solid phase, and amplified by thermal activation when the free water combines with unhydrated cement to form the hydrates. A kinetic law of the *Arrhenius type* may be adopted:

$$A_m = \eta \dot{\xi} \exp\left(\frac{E_a}{R\,T}\right) \tag{15}$$

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where E_a is the hydration activation energy and R the universal constant for ideal gas. From a pure empirical standpoint, evolution laws for maturing concrete based upon the Arrhenius concept are widely used since they have shown good agreement with experimental data. From a thermodynamic point of view, evolution law (15) refers to expression (9) of dissipation $\Phi_{A \to B}$, according to which the kinetics must be specified by a relation linking affinity A_m to hydration rate $\xi^\circ = \dot{\xi}$. From a physico-chemical point of view, the complementary evolution law (15) accounts for two distinct phenomena. First, that hydration rate $\dot{\xi}$ is controlled by the rate at which the free water diffuses through the layers of hydrates already formed. This diffusion rate depends upon the gradient between the free water and the water combined in the hydrates. At the macro-level of material description, this gradient is expressed by affinity A_m, whence the relation $A_m = \eta \dot{\xi}$. Second, that the combination of free water with unhydrated cement to form the hydrates is activation controlled, which the Arrhenius term $\exp(E_a / R T)$ takes into account. The first is at the basis of the chemical dissipation amplified by the latter thermal activation. Since viscosity η accounts for this micro-diffusion, it may not be constant, since the remaining free water has to bypass the layer of hydrates already formed (i.e. $\eta = \eta(\xi)$), in order to meet the unhydrated cement and to form new hydrates.

2.3 State equations

In the framework of physical linearization, the expression of free energy ψ is limited to a second order expansion with respect to external state variables $\theta = T - T_o$ and $\boldsymbol{\varepsilon} = \mathbf{e} + \varepsilon \mathbf{1}$ (with $\varepsilon = \mathrm{tr}\boldsymbol{\varepsilon} / 3$). For an isotropic ageing material the following expression can be adopted

$$\psi = -A_{mo}\xi - 9K(\xi)\varepsilon(\alpha\theta + \beta\xi) + \frac{F(\xi)}{T_o}\theta - \frac{1}{2}\frac{C_\varepsilon}{T_o}\theta^2 + \frac{1}{2}\kappa\xi^2 \qquad (16)$$
$$+ \frac{9}{2}K(\xi)\varepsilon^2 + G(\xi)\mathbf{e}{:}\mathbf{e}$$

Using (16) in (13) and retaining in the derivation only terms of same order of magnitude the state equations read explicitly

$$\boldsymbol{\sigma} = 2G(\xi)\mathbf{e} + 3K(\xi)(\varepsilon - \alpha\theta - \beta\xi)\mathbf{1} \qquad (17)$$

$$T_o S = C_\varepsilon\theta + 9K(\xi)\alpha T_o\varepsilon - F(\xi) \qquad (18)$$

$$A_m = A_{mo} + 9K(\xi)\beta\varepsilon - f_\xi \frac{\theta}{T_o} - \kappa\xi \tag{19}$$

where $f_\xi = dF / d\xi$ with $F(\xi)$ the latent heat of hydration (see section 2.4). State equation (17) can be inverted reading

$$\varepsilon = \varepsilon^e + \varepsilon^t + \varepsilon^c = \left(\frac{s}{2G(\xi)} + \frac{\sigma}{3K(\xi)}\mathbf{1} \right) + \alpha\theta\mathbf{1} + \beta\xi\mathbf{1} \tag{20}$$

with subscripts e=elastic, t=thermal and c=chemical. The previous equation allows to identify coefficients α and β as the thermal and chemical dilatation coefficients which relate the dilatation of thermal and chemical origin to temperature variation θ and hydration degree ξ, respectively. More precisely, in (22), $\varepsilon^c = \beta\xi\mathbf{1}$ is the strain induced by shrinkage effects related to chemical volume changes (hydration shrinkage) and related capillary effects (capillary shrinkage) in the closed reactive porous medium (no exchange with the exterior, no drying). The hydration shrinkage is caused by the volume change due to the hydration of cement (Le Chatelier contraction). The consumption of water by the hydration reaction leads to the formation of menisci with an increasing pressure difference (capillary pressure) between the liquid phase and the gaseous phase saturating the porous space. Consequently, the skeleton suffers an increasing internal compression, inducing an overall (capillary) shrinkage which depends upon the quantity of water combined in the solid phase, and thus upon hydration degree ξ. With respect to this origin of autogeneous shrinkage, coefficient β accounts for involved capillary phenomena, by relating hydration degree ξ to strain ε^c induced by capillary effects.

Furthermore, the previous state equations account for ageing by considering the (instantaneous) elastic material properties at the macro-level of material description, bulk modulus K and shear modulus G, as a function of hydration degree ξ:

$$K(\xi) = \frac{E(\xi)}{3(1 - 2\nu)} \qquad G(\xi) = \frac{E(\xi)}{2(1 + \nu)} \tag{21}$$

where E=Young's modulus and ν =Poisson's ratio. Ageing formulation (21) derives its essential characteristics from the thermodynamic framework of reactive porous media, as briefly presented above, since it relates explicitly the actual change of macro-mechanical properties

through Eq. (10) to the change in the concentration of the non-ageing constituents, i.e. the hardened cement gel.

Finally, using Eq. (19) in kinetic law (17), leads to:

$$A_{mo} + 9K(\xi)\beta\varepsilon - f_\xi \frac{\theta}{T_0} - \kappa\xi = \eta\dot{\xi} \exp\left(\frac{E_a}{R\,T}\right) \tag{22}$$

which shows that the thermodynamic imbalance between the free water and the water combined in the hydrates depends *a priori* on strain and temperature variations. In other words, strain and temperature variations can induce a thermodynamic imbalance, and thus influence the amplitude of hydration. Here we assume them negligible, which leads to the kinetic law in the form

$$A_{mo} - \kappa\xi = \eta\dot{\xi} \exp\left(\frac{E_a}{R\,T}\right) \tag{23}$$

with an asymptotic hydration degree which depends only on the initial affinity A_{mo}, i.e. upon characteristics relative to the concrete mix design as for instance the water/cement ratio w/c, placing temperature T_0, etc.:

$$A_m(\infty) = 0 \quad \Leftrightarrow \quad \xi(\infty) = \frac{A_{mo}(w/c, T_0, ...)}{\kappa} \tag{24}$$

2.4 Latent heat of hydration

The field equation which expresses the locally the entropy balance is the thermal equation

$$T_0\dot{S} = Q^\circ + \varphi_1 \tag{25}$$

where $Q^\circ = R - \text{div}\mathbf{q}$ represents the external rate of heat supply to the elementary system provided by conduction (term $-\text{div}\mathbf{q}$ with $\mathbf{q} = -k\mathbf{1}.\text{grad}T$ the heat flux vector, when adopting a linear isotropic heat conduction law) and by eventual external volume heat sources (term R). Using (18) in (25), and retaining in the derivation of entropy S with respect to time only first order terms, leads to

$$C_\varepsilon\dot{T} + 9K(\xi)\alpha T_0\dot{\varepsilon} - f_\xi\dot{\xi} = Q^\circ + A_m\dot{\xi} \tag{26}$$

Equations (26) and (18) allow to identify $F(\xi)$ as the latent heat of hydration, and $f_\xi = dF(\xi)/d\xi$ as the latent heat per unit of hydration extent dx, which is in general assumed constant. Note, that the rate of heat given out by the hydration reaction, is due to latent heat effects (term $\dot{F}(\xi) = f_\xi \dot{\xi}$), as well as to the chemical dissipation $\varphi_1 = \Phi_{A \to B} = A_m \dot{\xi}$ as given by Eq. (9) or (11), even though the latter may be considered as negligible with respect to the former in the exothermic reaction considered (i.e. $\Phi_{A \to B} \ll \dot{F}(\xi)$). Hence, assuming the heat due to intrinsic dissipation, as well as the latent heat due to deformation (term $9K(\xi)\alpha T_0 \varepsilon$) negligible with respect to the exothermic latent hydration heat, Eq. (26) becomes

$$C_\varepsilon \dot{T} = Q^\circ + f_\xi \dot{\xi} \qquad (27)$$

which is the field equation generally used. The latter lends itself readily for the experimental determination of the latent heat of hydration from calorimetry tests, for instance under adiabatic or isothermal conditions (i.e. $Q^\circ = 0$ or $\dot{T} = 0$ in Eq. (27)), and leads on account of hydration kinetic (23) to the experimental determination of viscosity η as a function of hydration degree ξ. Then the thermo-chemical coupling is completely defined.

Finally, for the numerical application, the coupled thermo-chemical problem consists in solving simultaneously field equation (27) and (local) kinetic law (23), -independent of the mechanical problem- and leads to the numerical determination of the temperature-field and hydration degree. Here, standard numerical procedures can be applied: a discretization in space by the finite element method with standard boundary conditions concerning the temperature and a Cranck-Nicholson integration scheme in time for both temperature and hydration degree evolution.

3 Modelling of cracking

So far, the modelling of thermo-chemo-mechanical couplings left cracking beside, by assuming an elastic behaviour (non-linear due to ageing) of the skeleton within the hypothesis of continuity. However, the shrinkage (if restrained) and the temperature gradients induce a severe state of stresses, which might be of a magnitude beyond the strength developed. Two phenomena are in competition: stress-development due

to thermal and chemical/capillary shrinkage *versus* strength growth, both related to the kinetics of hydration. Note however clearly the different time-scales of chemical and crack-evolution: the evolution of hydration degree ξ (and thus the evolution of autogeneous shrinkage, ageing of both elastic and strength material properties) is related to the time scale of the reaction kinetics, while cracking occurs simultaneously with any variation in loading reaching a crack threshold.

3.1 Strength growth as chemical hardening

To account for strength growth within the theoretical framework of closed reactive porous continua presented above, the following modified expression for the free energy is adopted

$$\psi = \psi(T,\varepsilon,\xi) + U(\chi,\xi) \tag{28}$$

where $\psi(T,\varepsilon,\xi)$ is the free energy of the elastic ageing material given for the isotropic case by (16), and $U(\chi,\xi)$ the energy related to the chemical hardening phenomenon, i.e. the (elastic) energy *frozen* in the skeleton at the micro-level of material description induced by the formation of hardened cement gel. At the macro-level of material description, these irreversible micro-level phenomena are modelled by hardening variable χ. Using (28) in (11) together with state equations (13), the intrinsic dissipation on account of chemical hardening phenomena reads

$$\varphi_1 = A_m\dot{\xi} + \zeta\dot{\chi} \geq 0 \quad \text{with} \quad A_m = -\frac{\partial\psi}{\partial\xi} \quad \zeta = -\frac{\partial\psi}{\partial\chi} \tag{29}$$

which allows to identify ζ as the hardening force associated in the dissipation to the rate of hardening variable χ. A detailed discussion of this phenomenon of *chemical hardening* within the theory of chemo-poro-plasticity can be found in Coussy and Ulm (1995). Here for the particular application to concrete cracking a linear coupling of hydration degree ξ and hardening phenomenon is assumed

$$U(\chi,\xi) = -\xi\chi\zeta_o \quad \text{and} \quad \zeta = \xi\zeta_o \tag{30}$$

where ζ_o = the hardening force at complete hydration ($\xi(\infty) = 1$), i.e. for the hardened concrete. The particular expression (30) of frozen energy $U(\chi,\xi)$ corresponds to the case of a pure chemical hardening, i.e. hardening force ζ depends only on hydration degree ξ. In return, on

account of the chemical hardening phenomenon, the evolution of hydration degree ξ may now depend on hardening variable χ, i.e.

$$A_{mo} + \chi\zeta_0 + 9K(\xi)\beta\varepsilon - f_\xi \frac{\theta}{T_o} - \kappa\xi = \eta\dot{\xi}\,\exp\!\left(\frac{E_a}{R\,T}\right) \tag{31}$$

where $\chi\zeta_0$ is identified as the thermodynamic imbalance induced by irreversible skeleton evolutions (for instance micro-crack and void creation). Yet, little has been reported on this subject. In a first approach we assume this coupling negligible, referring thus to kinetic law (23) instead of (31).

Together with stress tensor σ hardening force $\zeta = \zeta(\xi)$ describes the admissible stress states with respect to the crack-criterion $f(\sigma,\zeta)$, and defines the elasticity domain D_E of maturing concrete, i.e.

$$\sigma \in D_E \quad \Leftrightarrow \quad f(\sigma,\zeta(\xi)) \le 0 \tag{32}$$

and in the particular case of a mode-I crack opening:

$$f(\sigma,\zeta) = \sigma_N - \zeta(\xi) \le 0 \tag{33}$$

where mode-I hardening force $\zeta(\xi)$ is the local tensile strength $f_t(\xi)$ in the maturing concrete, and σ_N the stress normal to the fracture plane, which is obtained from state equation (17)

$$\sigma_N = \mathbf{n}.\sigma.\mathbf{n} = 2G(\xi)(\lambda - \varepsilon) + 3K(\xi)\big(\varepsilon - \alpha\theta - \beta\xi\big) \tag{34}$$

with $\lambda = \mathbf{n}.\varepsilon.\mathbf{n}$ the principal extension normal to the fracture plane oriented by unit normal $\mathbf{n}$.

3.2 Probabilistic modelling of early age concrete cracking

It is generally admitted, that the cracking of hardened concrete is strongly influenced by the heterogeneity of the matter: the tensile strength of concrete is mainly related to that of the hardened cement paste, which -in turn- is governed by the presence of voids, microcracks etc. created during the concrete hardening by non-uniform shrinkage of thermal and capillary origin at the scale of the heterogeneous material, i.e. at the scale of the concrete aggregates. This heterogeneity of the matter constituting concrete can be considered to be at the basis of apparent size effects, governing the overall cracking behaviour at the macroscopic scale of

material description. This has led to the development of the probabilistic modelling of concrete cracking over the last decade (Rossi and Wu, 1992), which accounts for the heterogeneity of hardened concrete by random distribution functions of the mechanical properties of the material (Young's modulus, tensile strength) with experimentally determined standard deviation and mean values which depend upon the volume ratio of coarsest grain to test specimen size (V_g/V_t) for a given apparent compressive strength $f_c(\infty)$, (Rossi et al., 1992):

$$E(\infty) = E\left(\frac{V_g}{V_t}, f_c(\infty)\right) \qquad f_t(\infty) = f_t\left(\frac{V_g}{V_t}, f_c(\infty)\right) \tag{35}$$

Since the heterogeneity of the hardened concrete, as modelled by relations (35), results from void and micro-crack creation induced by non-uniform shrinkage of thermal and capillary origin during hardening, i.e. by chemo-mechanical couplings, the probabilistic modelling can be extended to the case of maturing concrete by:

$$E(\xi) = E(\infty)\, g_E(\xi) \qquad f_t(\xi) = f_t(\infty)\, g_\zeta(\xi) \tag{36}$$

where $E(\infty)$ and   are the Young's modulus and the tensile strength of the hardened material, which account for the heterogeneity of the matter, i.e. relations (35), and $g_E(\xi)$ and $g_\zeta(\xi)$ the ageing and the chemical hardening function according to (21) and (30). The previous expression assumes a homothety of maturing material properties with respect to the hardened one, and is widely used in the experimental determination of apparent material characteristics of maturing concrete. Note however, that in the framework of the probabilistic modelling, this homothety implies the homothety of the heterogeneity of the hydrating matter constituting concrete, i.e. the cement paste. This needs still to be confirmed, and the proposed modelling is just a first attempt to model size effects in maturing concrete.

Finally, the probabilistic modelling of early age concrete cracking can be readily used in finite element application within an explicit crack approach with special contact elements that interface the solid elements. The Young's modulus and the tensile resistance are distributed randomly on all mesh elements, by replacing in the experimentally determined random distribution function (35) the volume of the test specimen V_t by the volume of each singular solid finite element. This is consistent with physical evidence: the smaller the scale of observation (respectively the modelling scale) with respect to that of the structure, the larger the

fluctuation of the local mechanical characteristics, and thus the (modelled) heterogeneity of the matter. This renders the numerical results mesh-independent. In the case of maturing concrete, the (randomly distributed) Young's modulus and the tensile strength in the mesh are updated in each time step on account of the hydration degree ξ locally developed. A crack opens according to crack criterion (33). With crack opening the local tensile strength $f_t(\xi)$ is set to zero (local irreversible fragile tensile behaviour): the strength is not recovered when the crack re-closes.

4 Example: Cracking in a casting cycle

Economic and environmental constraints have led over the last decade to an increasing use of fast cements for short casting times. The cracking risk at early ages may thus increase when little precautions are taken concerning thermal conditions once the hydration rate slows down. One illustrative example is shown hereafter.

Two blocks of concrete of 1x1x1 m^3 are casted in a casting cycle of 12 hours. The couring conditions are shown in figure 2a, and the finite element mesh in figure 2b. The concrete is a high strength concrete with a compressive strength greater than 80 MPa. The high cement rate ($530\,kg/m^3$), together with a low water cement ratio (w/c $\approx 0,3$), leads to high temperature rises in the massif blocks ($\Delta T = 60\,K$ within 168h in an adiabatic experiment), furthermore to an important autogeneous shrinkage due to the water consumption in the hydration reaction ($\varepsilon^c(\infty) = \beta\xi(\infty) \approx -10^{-5}$ for $\xi(\infty) \approx 0,8$, determined from (28)).
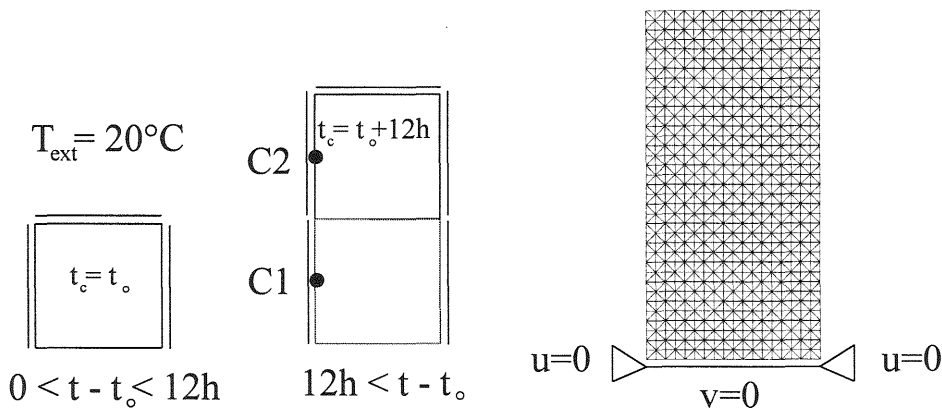

Figure 2a:
Couring and casting conditions

Figure 2b:
FE-mesh and boundary conditions

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The latter together with the thermal shrinkage during cooling lead to a severe state of tensile stresses at the boundaries (pts. C1,C2-Fig.2a), as shown in figure 3, when assuming an elastic behaviour of the bulk material. These stresses are beyond the strength developed and lead to cracking as shown in figure 4a and 4b, obtained with the probabilistic model of early age concrete cracking.
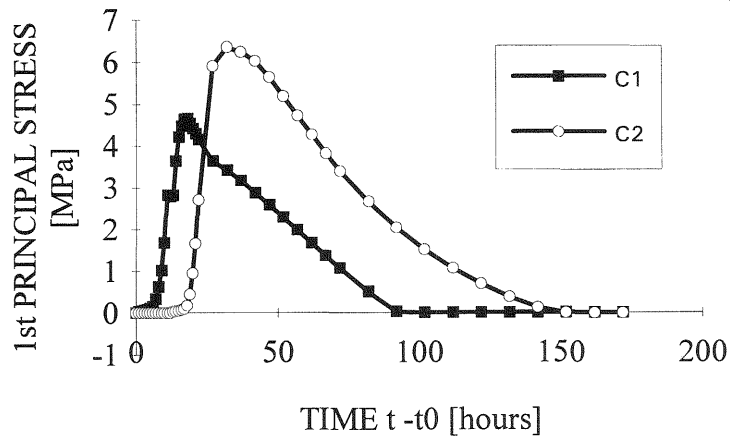
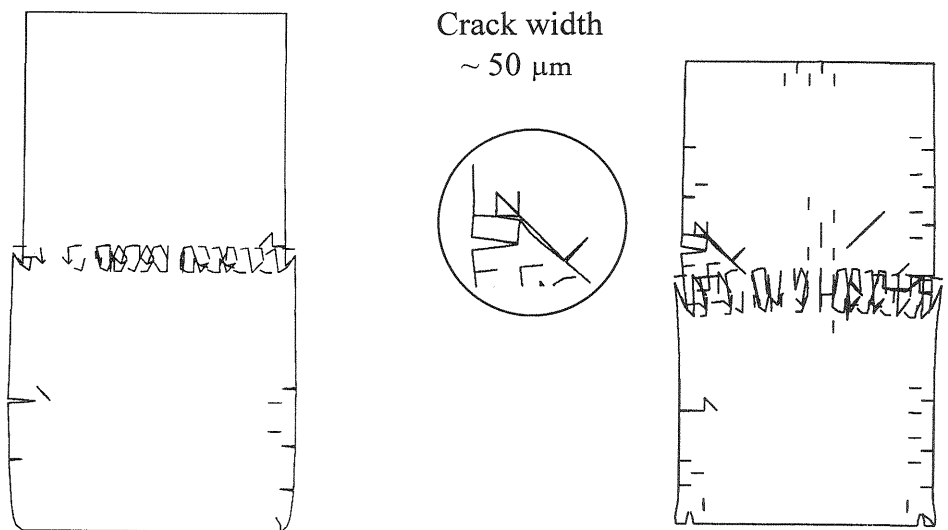Figure 3: Principal (tensile) stress-evolution *versus* time

Fig. 4a: Cracks at $t = t_o + 13h$ Fig. 4b: Cracks at $t = t_o + 172h$

5 Conclusion

This modelling of early age concrete cracking gives direct access to crack-patterns, crack-width and crack-spacing induced by thermo-chemo-mechanical couplings with a minimum of material parameters of clear physical significance and accessible by standard material tests. For the thermo-chemical problem a calorimetric test result is needed, in order to determine the kinetics of hydration, while for the mechanical problem using the probabilistic modelling of concrete cracking, the compressive strength of the hardened concrete and the size of the aggregate is required.

Finally, by assuming that the hydration affinity does not depend on the strain, creep effects were eliminated in the modelling. Note, however, that this hypothesis concerns only the thermodynamic imbalance related with the hydration reaction (i.e. between the free water and the water combined in the solid phase). Other physico-chemical phenomena may be at the origin of a stress induced thermodynamic imbalance, which gives rise to creep effects. Here the frontier between material mechanics and physical chemistry needs still to be explored.

6 References
An updated literature review on the topic of modelling of early age concrete can be found in Ulm and Coussy (1995).

Coussy, O. (1995) **Mechanics of porous continua.** John Wiley & Sons, Chichester, England.

Coussy, O. and Ulm, F.J. (1995) Creep and plasticity due to chemo-mechanical couplings, in **Computational Plasticity** (eds D.R.J. Owen, E. Onate and E. Hinton), Pineridge Press, Swansea, 925-944.

Rossi, P. and Wu, X. (1992). Probabilistic model for material behaviour analysis and appraisement of concrete structures. **Magazine of Concrete Research**, 44, No. 161, 271-280.

Rossi, P., Wu, X., Le Maou, F. and Belloc, A. (1994) Scale effect on concrete in tension. **Materials and Structures**, 27, 437-444.

Ulm, F.J. and Coussy, O. (1995) Modeling of thermochemomechanical couplings of concrete at early ages. **ASCE J. Eng. Mech.**, Vol. 121, No. 7 (July) (*with an updated literature review on the topic*).