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Coupled constitutive equations for assessing mechanical effects of Internal Swelling Reactions

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Abstract

Diagnosis and prognosis of structures affected by ISR (Internal swelling reactions such as Alkali-silica reaction and Delayed Ettringite formation) are often based on numerical models. These models need to be precisely fitted to be relevant, which is often difficult to achieve since information about concrete or construction conditions can be scarce or missing in the case of ancient structures. The only trustable information are often the ones directly observed in situ: crack patterns or monitored displacements. Hence, this information shall be used to assess the relevance of the numerical model and its fitting, which requires first that the model is able to correctly simulate these phenomena.

This communication presents the foundations of a constitutive model developed within the framework of the finite-element method. In order to reach, in further step, a correct quantification of the visible crack patterns, we first develop a set of evolutive constitutive equations based on Larive's law and taking into account the main couplings that affect ISR in structures: chemical extent, available moisture, past and present temperature, and creep.

We first present the aims of this modelling framework by setting the set of constitutive equations and identifying material parameters on the base of observable data. Then we describe the evolution equation governing the chemical expansion. The third part focuses on coupling with various phenomena. Finally, we propose perspectives about material damage and cracking in concrete.

***Keywords**: constitutive equations; coupling; numerical model; parameter identification*

1. SCOPE AND MOTIVATION

Internal swelling reactions (*ISR*) in concrete can have significant impact on the long-term behaviour of massive concrete structures. Two kind of ISR pathologies are considered; the Alkali-Silica Reaction (*ASR*), and the Delayed Ettringite Formation (*DEF*). While for the former, the chemical reaction happens between alkalis in the cement paste and the reactive silica aggregates, the latter is caused by the formation of ettringite in concrete when subjected to high temperature during cement hydratation, and later exposed on to moisture. In both cases, the hardened concrete expands progressively which can potentially lead to cracking and structural disorders, to mention a few. It is then of major importance to build numerical tools that can simulate these expanding mechanisms and their consequences on the structural serviceability. For both phenomena, it is unanimously admitted that *ISR* develops when concrete is at high humidity above a certain threshold, or in contact with water.

Extensive research has been conducted so far to model the expansions caused by *ASR* [1–5]. Later on, models have been developed for *DEF* as well, see for example [6–8]. From the mathematical point of view, the models are mostly based on phenomenological approaches formulated in terms of internal variables that can be deployed to feed constitutive relations and evolution laws that must be integrated in a sound way within boundary-value problems that, in a last step, must be solved numerically for the response of concrete structures. This constitutes a good compromise between efficiency and representativity of the most of time complex concrete behaviour.

The *ISR* expansion is in general characterized by two important factors: amplitude, and kinetics. Both are in turn dependent on the humidity level, and on temperature. Hence, by nature, the complete problem at hand is a coupled one thermo-hydro-mechanics. Moreover, other phenomena must be accounted for, e.g. creep, damage, plasticity. In this contribution, details on the creep modelling are given through viscoelastic strain-like internal variables. The plasticity formulation is nowadays classical and is not described for the sake of clarity.

2. GENERAL FRAMEWORK FOR CONSTITUTIVE EQUATION

2.1 Kinematic behaviour

Within the continuum, the kinematical choice made in such developments is based on the additive split of the total strain tensor $\boldsymbol{\varepsilon}$ into an elastic part $\boldsymbol{\varepsilon}^{(E)}$ and complementary parts, each one corresponding to a specific phenomenon. we assume that the total strain is the sum:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{(E)} + \boldsymbol{\varepsilon}^{(T)} + \boldsymbol{\varepsilon}^{(H)} + \boldsymbol{\varepsilon}^{(\chi)} + \boldsymbol{\varepsilon}^{(C)} + \boldsymbol{\varepsilon}^{(P)} \tag{1}$$

where $\boldsymbol{\varepsilon}^{(T)}$ and $\boldsymbol{\varepsilon}^{(H)}$ are respectively the temperature-induced strain and the hygric-induced strain, $\boldsymbol{\varepsilon}^{(\chi)}$ is the free chemical strain, $\boldsymbol{\varepsilon}^{(C)}$ is the basic creep strain and $\boldsymbol{\varepsilon}^{(P)}$ is the plastic strain.

If θ_0 is defined as the reference temperature and θ as an arbitrary temperature, the thermal strains caused by a change in temperature of an unconstrained isotropic volume are given by:

$$\boldsymbol{\varepsilon}^{(T)} = k_T\,(\theta - \theta_0)\mathbf{1} \tag{2}$$

where k_T is the linear coefficient of thermal expansion. Following the same logic, the volumetric strain due to a change in the degree of saturation $\boldsymbol{\varepsilon}^{(H)}$ is given by:

$$\boldsymbol{\varepsilon}^{(H)} = k_S\,(S_R - S_{R,0})\mathbf{1} \tag{3}$$

with $S_{R,0}$ is the reference degree of saturation, S_R is an arbitrary value of the degree of saturation and k_S is the linear coefficient of hygric expansion. The concrete shrinkage/swelling can easily be expressed in terms of relative humidity too, rather than in terms of degree of saturation.

More complex relationships can be found in the literature for the drying of concrete and it is well known that k_S depends on the relative humidity since the physical mechanisms causing shrinkage change as the humidity decreases. Furthermore, a constant value of k_T neglects its dependence on both temperature and relative humidity. However, a linear relationship between relative humidity and drying shrinkage is a justified approximation in the case of humidity ranging from 50 to 100. Similarly, a constant value for k_T is a well-established approximation when analyzing concrete on a large scale.

The free volumetric ASR strain is given by:

$$\boldsymbol{\varepsilon}^{(\chi)} = \varepsilon^{\chi}\,\mathbf{1} \tag{4}$$

with $\varepsilon^{\chi} = \varepsilon^{\chi}(t,\theta)$ is the free chemical expansion.

2.2 Chemical kinetics

The macroscopic phenomena of *ASR* are modelled within the framework of the porous continua theory, extended to reactive partially saturated porous media [9]. Then, in order to take into account the diffusion conditions as the alkaline reaction develops, as well as accurately representing the sigmoidal chemical expansion-time curve, the model was calibrated on the basis of the extensive and rigorous experimental campaign published in [1].

It follows that the *ASR* strain-induced can be represented as:

$$\varepsilon^{\chi} = \varepsilon_{\infty}\,\frac{1 - exp(-\frac{t}{\tau_C})}{1 + exp(-\frac{t+\tau_L}{\tau_C})}\;; \tag{5}$$

From Equation (5) the chemical expansion can be represented through three parameters, namely, ε_{∞} which is the asymptotic volumetric expansion strain in the stress-free experiment, together with the characteristic time τ_C and the latency time τ_L of *ASR* swelling.

The previous formulation may also be extended to the case of structures affected by Delayed Ettringite Formation – *DEF*, see for instance [7, 8]. However, the difference lays in the asymptotic volumetric expansion strain; in case of *ASR* ε_{∞} is a constant parameter, deduced from experimental tests and depends on the type of concrete, in case of *DEF* $\varepsilon_{\infty} \equiv \varepsilon_{\infty}(\boldsymbol{x})$ is a field variable that depends on the thermal history.

In order to take into account this strong dependance the following model, based on experimental work by [10], has been proposed in [6, 7]:

$$\varepsilon_\infty = \alpha \int_0^{t_m} \begin{cases} 0 & if\ \theta \leq \theta_{DEF} \\ e^{\left[\frac{E_a^{DEF}}{R} \frac{1}{\theta - \theta_{DEF}}\right]} & if\ \theta > \theta_{DEF} \end{cases} dt \tag{6}$$

with α is a parameter which accounts for material properties influencing chemical expansion (cement, aggregates ...), θ_{DEF} is the temperature threshold above which *DEF* occurs, E_a^{DEF} is the activation energy, R is the universal gas constant and t_m is the maturation time. An alternative formulation can be found in [11, 12]. In any case, during the mechanical analysis, the field $\varepsilon_\infty(\boldsymbol{x})$ is known, which plays a key role in the design of the algorithm.

In the case of constant or monotonically increasing temperature and humidity chemical strain can be expressed by Equation (5). In the case of variable temperature and humidity, characterised even by decreasing functions, the expansion should take into account its irreversibility during time. In the thermodynamic framework, developing the formulations presented in [1, 2], the chemical evolution equation can be expressed as follows:

$$\left[\tau_C\ \varepsilon_\infty \left(1 + e^{\frac{\tau_L}{\tau_C}}\right)\right] \dot{\varepsilon}^\chi + \left(e^{\frac{\tau_L}{\tau_C}}\right) \varepsilon^{\chi 2} + \left[\varepsilon_\infty \left(1 - e^{\frac{\tau_L}{\tau_C}}\right)\right] \varepsilon^\chi = \varepsilon_\infty{}^2. \tag{7}$$

2.2.1 Temperature dependance

In endothermic reactions, an increase in temperature normally increases the speed of reaction since the energy added to the system allows an easiest combination of reactive ions. This physical result is reinforced, for alkaline reactions, by the way in which accelerated testing is carried out, i.e., high storage temperatures are used in order to control the chemical expansion over a period of months, rather than years, time typically needed for AAR to develop within the concrete, [4, 13].

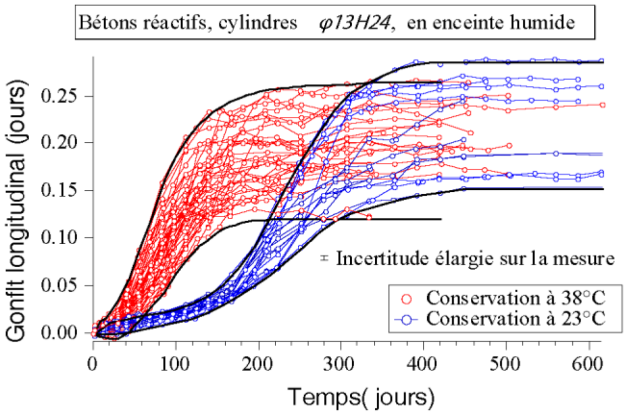

Figure 1: Free expansion from Larive's tests; [1]

The reaction kinetics are highly dependent on temperature, particularly it has been experimentally demonstrated that temperature dependance of time constants τ_C and τ_L matching the Arrhenius equation:

$$\tau_C(\theta) = \tau_C(\theta_0)\, exp[U_C(1/\theta - 1/\theta_0)] \tag{8}$$

$$\tau_L(\theta) = \tau_L(\theta_0)\, exp[U_L(1/\theta - 1/\theta_0)] \tag{9}$$

θ_0 is the reference temperature of expansion test, U_C and U_L are the activation energy constants which cause the thermo-activation of the characteristic and latent times respectively.

2.2.2 Variable moisture conditions

Water plays a dual role in the development of *ASR*: on the one hand, it acts as a carrier for the alkali and hydroxyl ions, allowing the reaction to progress; on the other hand, it is absorbed by the alkali-silica gel which swells, generating the pressure required to crack the concrete [14].

It is widely recognised that below a threshold value of relative humidity (RH = 80-85 %) *ASR* does not occur, [1, 15], and that above this value the expansion increases exponentially, Figure 2.

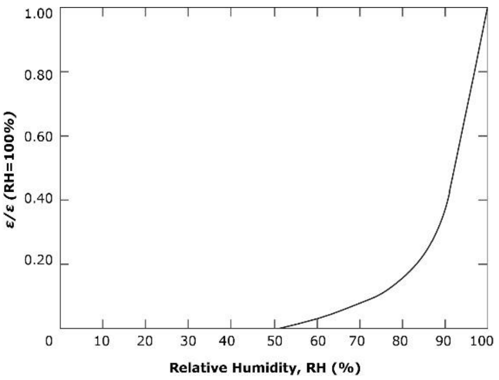

Figure 2: Influence of environmental conditions on chemical expansion: Effect of relative humidity, [16].

Experimental concrete affected by *ASR* also shows a significant dependence between free expansion and variable moisture conditions, [17–21].

In order to simulate the dependence of *ASR* on humidity, and more generally on environmental conditions, mathematical models have been proposed in literature, which take into account the humidity either by reduction functions, [22], or altering the kinetic laws, [20, 21, 23].

Within this framework, an alternative model able to take into account variable humidity conditions is proposed.

In order to capture the moisture effect on the chemical evolution, we use the concept of effective time t_{eff}, introduced in [24, 25], such as:

$$\dot{t}_{eff} = \dot{t}_{eff}(S_R, t) \quad \in [0,1] \tag{10}$$

Now, if $S_{R,\mathrm{thrs}}$ denotes the degree of saturation for which the reaction occurs, we have that:

$$\begin{cases} \varepsilon^{\chi} = 0 & if\ S_R < S_{R,thrs} \\ \dot{\varepsilon}^{\chi} > 0 & if\ S_R \geq S_{R,thrs} \end{cases} \tag{11}$$

Where $\dot{\varepsilon}^{\chi}$ is the chemical strain due to *ASR*, and in the case of constant or monotonically increasing temperature and humidity can be expressed by Equation (5).

The following is a possible option for embedding humidity dependence in chemical evolution equation:

$$t_{eff} = \int_0^t \left(\frac{\langle S_R - S_{R,thrs} \rangle_+}{1 - S_{R,thrs}} \right)^m dt \tag{12}$$

where m is a parameter that depends on the degree of saturation and $\langle \quad \rangle_+$ denotes the positive part. Furthermore, and besides on the above features, if the final expansion amplitude depends on the level of saturation too, a possible choice to link could be:

$$\varepsilon_\infty(S_R) = \varepsilon_\infty\left(S_{R,1.0}\right) \cdot \left(\frac{\langle S_R - S_{R,thrs} \rangle_+}{1 - S_{R,thrs}} \right)^{m_\infty} \tag{13}$$

where m_∞ is a material parameter that can be identified from free expansion tests carried out at different degree of saturation.

2.3 Viscoelastic behaviour

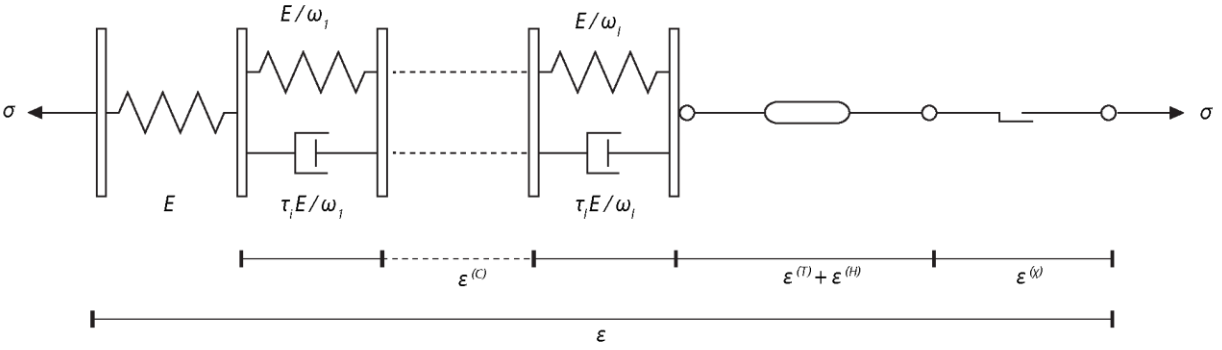

Figure 3: One-dimensional viscoelastic rheological model.

In this framework, creep strain $\varepsilon_{ij}^{(C)}$ is treated as an internal variable, and can be composed of as many contributions as necessary as follows:

$$\boldsymbol{\varepsilon}^{(C)} = \sum_{i=1}^{l} \boldsymbol{\varepsilon}_i^{(C)} \tag{14}$$

Where the $i = 1, \dots l$ hidden variables $\boldsymbol{\varepsilon}_i^{(C)}$ characterize viscoelastic processes with corresponding relaxation times $\tau_i \in [0, +\infty[,\ i = 1, \dots l$. The way all these internal variables evolve is motivated by the generalized Kelvin-Voigt rheological model, Figure 3. In this case, the complementary evolution equations that govern the creep strain components are given by, (for further information see [26]),

$$\dot{\varepsilon}_i^{(C)} + \frac{1+\omega_i}{\tau_i}\,\mathbb{N} :\, \varepsilon_i^{(C)} + \frac{\omega_i}{\tau_i} \sum_{j=1,\ j\neq i}^{l} \mathbb{N} \colon \varepsilon_j^{(C)} = \frac{\omega_i}{\tau_i}\,\mathbb{N} : (\varepsilon - \varepsilon^{(T)} - \varepsilon^{(H)} - \varepsilon^{(\chi)}), \qquad i = 1, \dots l \tag{15}$$

where $\omega_i, i = 1, \dots l$ are material parameters. Here $\mathbb{N}$ is the fourth-order tensor which depends solely on the Poisson's ratio ν. In Voigt engineering notation, it is given by:

$$\mathbb{N} = \frac{1}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & & & \\ \nu & 1-\nu & \nu & & & \\ \nu & \nu & 1-\nu & & & \\ & & & 1-2\nu & & \\ & & & & 1-2\nu & \\ & & & & & 1-2\nu \end{bmatrix} \tag{16}$$

2.4 Constitutive equations and mechanical equilibrium

In the case of a linear elastic relationship for reversible material behaviour, the constitutive relationship can be expressed as follows:

$$\boldsymbol{\sigma} = \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{(T)} - \boldsymbol{\varepsilon}^{(H)} - \boldsymbol{\varepsilon}^{(\chi)} - \boldsymbol{\varepsilon}^{(C)} - \boldsymbol{\varepsilon}^{(P)}) \tag{17}$$

where $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{C}$ is the fourth-order elasticity tensor within which a damage mechanism can be introduced as:

$$\mathbf{C} = (1 - d_\chi)\mathbf{C}_0 \tag{18}$$

where $\mathbf{C}_0$ is the elastic modulus for the undamaged concrete and d_χ is a damage variable in the sense of continuum damage mechanics. Indeed, the latter can be related to the chemical expansion explicitly as a function of the quantity $\varepsilon^{(\chi)}$ as follows [7]:

$$d_\chi = 1 - exp\left[-\beta\ \langle \varepsilon^{(\chi)} - \varepsilon_{thrs} \rangle_+\right] \tag{19}$$

where $\varepsilon_{thrs}$is the strain-like chemical damage threshold, and $\beta \geq 0$ is a parameter that determines chemical damage occurrence, i.e. for $\beta = 0$ no chemical damage occurs.

2.5 Outlines of the F.E. approximation

2.5.1 Variational formulation

If we consider the weak form of mechanical equilibrium, without taking into account the effects of creep or plasticity, then we will have at the actual time t_{n+1}:

$$\int_{\boldsymbol{B}} \nabla^s\, \delta\boldsymbol{u} : \boldsymbol{C}_{n+1} : \nabla^s \boldsymbol{u}_{n+1} dV = G_{n+1}^{ext}(\delta\boldsymbol{u}) + \int_{\boldsymbol{B}} \nabla^s\, \delta\boldsymbol{u} : \boldsymbol{C}_{n+1} : (\boldsymbol{\varepsilon}_{n+1}^{T} + \boldsymbol{\varepsilon}_{n+1}^{H} + \boldsymbol{\varepsilon}_{n+1}^{\chi}) dV \tag{20}$$

Which must hold for any variation of displacements $\delta\boldsymbol{u}$, and where ∇^s is the symmetric gradient operator. Here G_{n+1}^{ext} is a shorthand notation for the virtual work of the external loads embedding both of the volumetric forces in the body $\boldsymbol{B}$ and traction forces on part of its boundary $\delta_t\boldsymbol{B} \subset \delta\boldsymbol{B}$ applied at time t_{n+1}. Equation (20) is to be solved for the actual displacement field $\boldsymbol{u}_{n+1}$.

The evaluation of the chemical strain $\boldsymbol{\varepsilon}_{n+1}^{\chi}$ in Equation (20) is carried out through the concept of effective time t_{n+1}^{eff}, which is updated locally at each time step as:

$$t_{n+1}^{eff} = t_n^{eff} + \left(\frac{\langle S_{R,n+1} - S_{R,thrs}\rangle_+}{1 - S_{R,thrs}}\right)^{m_{n+1}} \Delta t \tag{21}$$

Where $\Delta t = t_{n+1} - t_n$ is the real time increment, and m_{n+1} is evaluated at the saturation degree value $S_{R,n+1}$. Consequently, the effective time is treated as an internal field variable ; $t^{eff} = t^{eff}(\boldsymbol{x}, t)$.

2.5.2 Iterative resolution procedure

In order to extend the use of Equation (20) to non-linear phenomena, such as creep, plastic behaviour, damage mechanics, among others, its resolution is based on an iterative resolution. Hence, assuming a known state $\boldsymbol{u}_{n+1}$ at time t_n, one then solves iteratively the following linearized form for the increment $\Delta\boldsymbol{u}$ of the displacement field:

$$\int_{\boldsymbol{B}} \nabla^s\, \delta\boldsymbol{u} : \widetilde{\boldsymbol{C}}_{n+1} : \nabla^s(\Delta\boldsymbol{u}) dV = G_{n+1}^{ext}(\delta\boldsymbol{u}) - \int_{\boldsymbol{B}} \nabla^s\, \delta\boldsymbol{u} : \boldsymbol{\sigma}_{n+1}^{(i)}\, dV \tag{22}$$

Where, initially for $i = 0$, $\boldsymbol{\sigma}_{n+1}^{(0)} = \boldsymbol{\sigma}_n$. The right-hand side in Equation (22) constitutes the residual of the mechanical balance that is used to test the convergence of the iterative process, and $\widetilde{\boldsymbol{C}}_{n+1}$ is the tangent modulus, whether algorithmic or continuous, computed as:

$$\widetilde{\boldsymbol{C}}_{n+1} = \frac{\boldsymbol{\sigma}_{n+1}^{(i)}}{\partial\boldsymbol{\varepsilon}} \tag{23}$$

Equation (22) is solved together with the appended local evolution equations to update the set of internal variables, i.e. plasticity and/or creep and/or damage. At the end of each global iteration, the displacement field is updated as:

$$\boldsymbol{u}_{n+1}^{(i+1)} = \boldsymbol{u}_{n+1}^{(i)} + \Delta\boldsymbol{u} \tag{24}$$

3. NUMERICAL EXAMPLES

In this section, two numerical examples are given within the framework of the finite element method. The first one shows the coupling between creep and expansion of a concrete sample, while the second one shows the structural effects of internal reinforcement.

3.1 Basic creep coupled to ISR

It is well known that creep plays a dominant role in the long terms response of concrete structures subjected to constant loads. It is suspected that under chemical expansion, the coupling with creep can be more evident. In this first example, we consider cylindrical samples submitted to two levels of axial compression, with uniform relative humidity; one under the swelling threshold where only basic creep takes place, and one at complete saturation where *ISR* is full evolving. More precisely, the following four computations are considered:

(i) Compression tests at $10\ MPa$, with and without *ISR*;
(ii) Compression tests at $20\ MPa$, with and without *ISR*.

For the concrete, we use $E = 20.5\,GPa$ for the Young's modulus, and $\nu = 0.2$ for the Poisson's ratio. For the chemical expansion we choose the parameters:

$$\varepsilon_\infty = 0.4\%,\ \tau_C = 70\ days, \text{ and } \tau_L = 0,$$

And for the basic creep, we use only one mechanism with parameters: $\omega_1 = 1.5$ and $\tau_1 = 150\ days$.

Figure 4 shows the four curves. One can see that, from these computations, the expansion due to *ISR* shows a decrease due to the compressive stress.

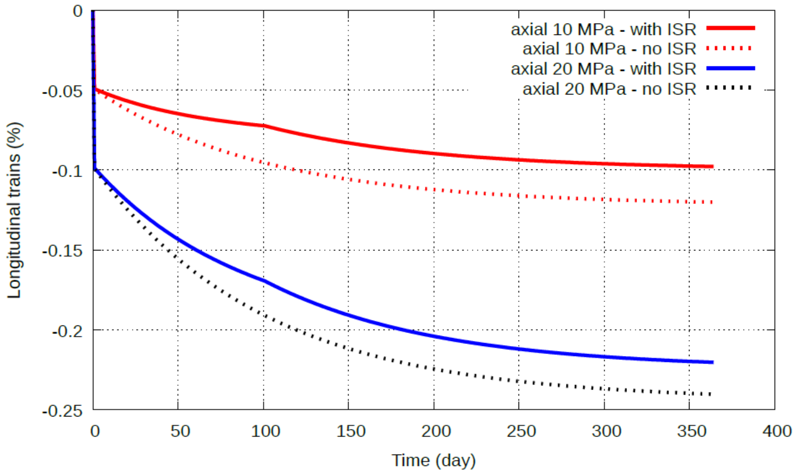

Figure 4: Creep simulations: longitudinal strain evolution for the different compression levels.

3.2 Effect of internal reinforcement

This second example is inspired by a JCI-benchmark example carried out on alkali-aggregate expansion experiments, see for example [27]. Here cylindrical specimens have been considered instead of prismatic ones. They have been constrained uniaxially as shown in Figure 5. Rigid plates on the samples' ends are linked by a steel rebar. Three cases are considered in this set of examples:

(i) a rebar of diameter 6 mm that corresponds to a steel ratio of 0.22%;
(ii) a rebar of diameter 13 mm that corresponds to a steel ratio of 0.88%;
(iii) a rebar of diameter 19 mm that corresponds to a steel ratio of 1.99%.

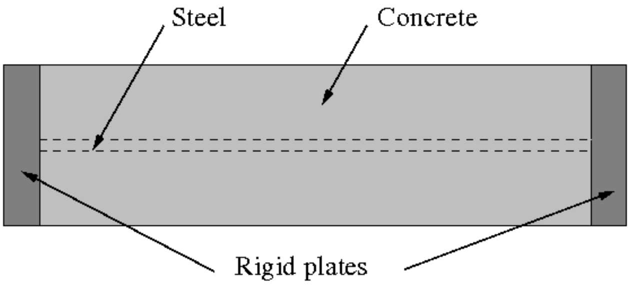

Figure 5: Expansion specimen with a steel rebar

For the sound concrete, we use $E = 25\,GPa$ for the Young's modulus, and $\nu = 0.2$ for the Poisson's ratio. For the chemical expansion we choose the parameters:

$$\varepsilon_\infty = 0.7\%,\ \tau_C = 40\ days, \text{ and } \tau_L = 0.$$

Under fully saturated hydric conditions, the concrete "free" expansion is shown in Figure 5, red curve. Notice that as constant thermo-hydric conditions are considered in all that follows, there is no need to specify the values of the parameters k_T and k_S for the thermo-hydric strains.

For the steel rebars, we consider an elastic/perfectly plastic constitutive relation with the von Mises yield criterion. The parameters we choose are:

$$E_S = 210\,GPa,\ \nu_s = 0.2, \text{ and yield stress } \sigma_y = 550\,MPa.$$

The problem has been discretized by using an axisymmetric analysis. Figure 6 shows the evolutions of the mean longitudinal strain of the concrete for different rebar ratios.

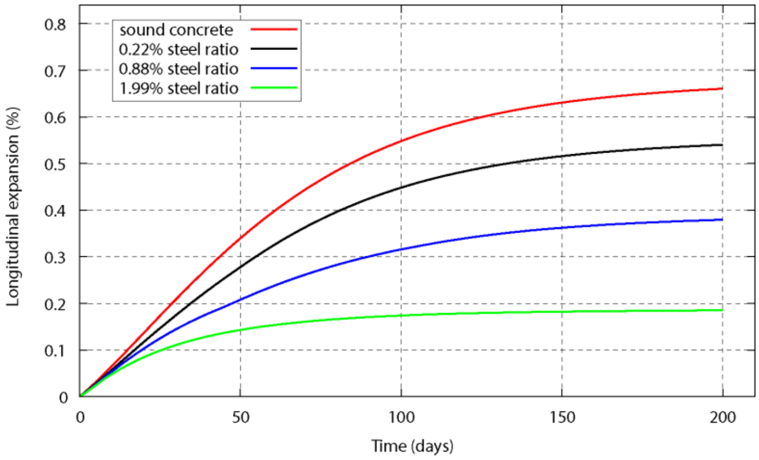

Figure 6: Longitudinal expansions evolutions for the different steel ratios.

4. CONCLUSION AND PERSPECTIVES

In this study, we have presented and numerically tested an efficient tool for the modelling of the influence of relative humidity on the development of *ISR* expansions. Within a sound mechanical basis, couplings with phenomena as basic creep and plasticity have been drawn for efficient structural computations. Numerical examples have been given to show the effectiveness of the present framework.

Future work will be to test the link between internal swelling and visible opening cracks on the structure edges. This would open the door on a field where engineering could give precise diagnostics on existent structures such like bridges, dams, nuclear plants to mention a few.

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