From AAR to DEF: Numerical Modelling of Structures affected by expansive Reaction in Concrete

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FROM AAR TO DEF: NUMERICAL MODELING OF STRUCTURES AFFECTED BY EXPANSIVE REACTIONS IN CONCRETE

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Abstract

The recent detection in France of several scores of worrying Delayed-Ettringite Formation (DEF) affected cases in major concrete structures urged the need for developing numerical models adapted to the specificities of DEF. Recently discovered and identified as a possibly single and major origin of disorders, DEF is not so largely studied as Alkali-Aggregate Reaction (AAR). However, it presents strong similarities with AAR: concrete is subjected to expansive chemical reactions which induce cracks, abnormal deformations, stiffness decrease. As a unique feature, early-age thermal history plays a crucial role in forthcoming DEF development. This contribution explains how a numerical tool for DEF-affected concrete was built based on a macro-scale model developed for AAR. The focus is put on the AAR-features used as a starting point, and on the specific model developed to take into account early-age history.

Keywords: numerical model, delayed-ettringite-formation, chemo-mechanical coupling, structure re-assessment

1 INTRODUCTION

With a more-than-one-century-long history, concrete building has led to discover various pathologies. Amongst them, Alkali-Aggregate Reaction (AAR) has deserved a large attention for the last decades, impelling lots of research efforts with the view of understanding mechanisms and developing prevention, assessment and repair methods. Underlying the necessity to safely manage affected structures, several numerical models have been proposed to re-assess them. More recently discovered and identified as a possibly single and major origin of disorder, Delayed-Ettringite Formation (DEF) was not so largely studied up to now. The recent occurrence in France of some scores of worrying DEF-affected cases in major concrete structures urged the need for developing numerical models adapted to the specificities of DEF.

This pathology presents strong similarities with AAR: in both cases, concrete is subjected to expansive chemical reactions which induce cracks, abnormal deformations, stiffness decrease, and in case of DEF (or combined AAR and DEF) even more intense swellings may occur in a shorter delay with respect to the expectable structural service life.

If consequences are similar when observed at the structure scale, chemical mechanisms responsible for both pathlogies strongly differ. In particular, early-age thermal history plays a crucial role in forthcoming DEF development.

This contribution aims to explain how a numerical model for DEF-affected concrete structures was built based on a one developed for AAR-cases. After a brief survey of DEF characteristics and multi-physical and mechanical couplings as compared with those related to AAR, the numerical model and its implementation in a FEM-software are described. The focus is put on the AAR-features used as a starting point, as well as the specific model developed to take into account early-age thermal history. Lastly, as an illustrative example, the numerical reassessment of a real DEF-affected bridge pier is presented.

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2 DEF CHARACTERISTICS

2.1 What is DEF?

Most of the common cements contain small proportions of gypsum, which is composed of hydrated calcium sulfate ($CaSO_4, 2(H_2O)$). It plays an important role during cement hydration since its reaction with tri-calcic aluminate (C3A) and tetra-calcic ferro-aluminate (C4AF) prevents these two elements from reacting in flash setting and allow the development of C-S-H responsible for the hardened cement paste (HCP) mechanical properties. The reaction between gypsum and C3A or C4AF, called the set regulation, leads to the formation of an hydrated calcium tri-sulfoaluminate, also called ettringite [1], with expansive properties.

Ettringite is very sensitive to thermal conditions [2]. If submitted to temperatures higher than about 65 $^\circ$C, for example due to heat-emission during hydration of massive elements cast in-situ or thermal treatment of precast elements, it is destabilized and transformed into hydrated calcium mono-sulfoaluminate, releasing two SO_4^{2-} ions in the cement paste. When the thermal conditions turn back to normal, these ions can once again produce ettringite, but now this ettringite will develop in hardened cement paste, resulting into material expansion and crackings (this description is very simplistic; for more details, see for instance [3]).

There are very strong similarities of crack patterns observed in both DEF and AAR cases (see Figure 1), which is why recommendations aimed at detecting affected structures [4] insist on the need of SEM-analysis to clearly conclude on the problem nature. Indeed, chemical mechanisms responsible for each pathology are really different, as well as reaction localization at a microscopic scale (at the aggregate-cement paste interface or in aggregate cracks for AAR, rather diffuse in the cement paste for DEF at least for the first step), but, from the macro-scale which is relevant at the structure level, material expansive behaviour could be analyzed in a similar way.

2.2 Free expansion

As for ASR-affected concrete, it is possible to observe and quantify DEF-induced expansions on cylindrical concrete sample free of any loadings. The samples are stored in controlled conditions (see for example [5, 6]) and regular strain-monitoring leads to expansion-versus-time curves. These curves have an S-shape similar to what is observed for AAR-affected concrete. Explanations proposed by [7] for AAR seem relevant also for DEF: a first stage, called “latency”, corresponds to an active chemical process (DEF may start right after construction period) which is unable to induce consequences at macro-scale. Obviously, expansive reaction products are initially free to grow in the HCP porous network. Once these pre-existing spaces filled, the second stage starts, when the curve exhibits a growing strain-rate. Lastly, the phenomenom slows down, and eventually becomes stable, as for any chemical reaction in a closed system where reactants quantities are finite.

An important qualitative difference is although observed: the last stage of the curve, often considered as an horizontal asymptote in the case of AAR, tends to linearly grow, at a very low strain-rate, in the case of DEF [8]. But the main difference is quantitative: whereas AAR is often a very slow pathology (several decades are generally needed before the phenomenom stabilizes, although cases of quick AAR have also been observed), DEF is really quicker: expansion evidences can be observed on the structures from 5 to 15 years of age. Moreover, DEF also leads to larger swelling amplitude than AAR (expansion higher than 1% or 2% can be obtained with DEF, while AAR seldom causes swelling larger than 0.3 to 0.4%).

These differencies in kinetics and amplitude are of course of very important consequences when dealing with affected structures. But, from a modeling point of view, it is just a question of parameters setting and the similarities of the expansion-versus-time curves justify having used of an AAR-affected concrete model to develop a new one devoted to DEF cases.

2.3 Mechanical and physical couplings

AAR and DEF similarity is amplified by various physical and mechanical influences to be taken into account. Laboratory experiments and field-cases of AAR-affected structures show that observed chemical expansions can be linked to material free-swelling by taking into account:

- temperature influence, which can be modeled as thermo-activation according to Arrhenius law [9];
- moisture which affects both kinetics and swelling amplitude [10, 11, 12];
- stress-state which reduces expansion in the most-compressed directions but transfer it to directions less loaded [13].

The question of temperature is dealt with in section 3.2. Like AAR, DEF is strongly affected by moisture content in the concrete [1, 14]. A threshold value (about 90%) has been observed [15, 16].

Concerning stress-state, few experimental data are available with DEF-affected concrete, but several case-studies tend to indicate that observed strain and crack-opening are not the direct application of laboratory-measured expansions of stress-free samples. For instance, restraint due to reinforcement tends to lower or even stop expansion in the direction of the main rebars[17].

3 MODELING DEF-AFFECTED STRUCTURES

In the frame of studies aimed at giving support for structure owners dealing with expansive reactions, the main point is not to model the chemical phenomena in themselves but their mechanical consequences on the structure behaviour.

Due to AAR/DEF similitude, a new tool for DEF-affected structures was proposed based on the model developed at LCPC for AAR [18, 19, 20] and implemented in CESAR-LCPC finite-element software [21] as a module called ALKA.

3.1 Model for DEF-affected structures

Following the theoretical developments proposed by [20], a strain-additive constitutive equation is considered for AAR-affected concrete:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_s + \boldsymbol{\varepsilon}_\chi. \tag{1}$$

In this expression, concrete strain tensor $\boldsymbol{\varepsilon}$ is split into an elastic part $\boldsymbol{\varepsilon}_e$, connected to stress tensor $\boldsymbol{\sigma}$ by Hooke's law; a shrinkage part $\boldsymbol{\varepsilon}_s$, expressed as a linear function of the material saturation degree s [22]; a chemical part $\boldsymbol{\varepsilon}_\chi$ representing AAR-induced expansion. Note that the elastic part can be transformed into an elastoplastic one, considering Willam-Warnke model for the yield criterion. An isotropic thermal strain can also been added, linearly connected to the temperature variation. A similar model can be adopted for DEF-affected concrete.

The original part of the model summarized in equation 1 stands of course in the chemical part. This last one was built in order to be fitted on free expansion tests (*i.e.* without external load) performed on concrete samples (practically on sample cores drilled out of the studied structure). In ALKA, free expansion is given by

$$\boldsymbol{\varepsilon}_\chi(\mathbf{0}) = \varepsilon_\infty.\xi_a(t)\boldsymbol{A}_i. \tag{2}$$

In this expression, tensor $\boldsymbol{A}_i$ represents intrinsic anisotropy of the swelling (due to casting direction, for instance) and ε_∞ represents swelling potential, wich is supposed to be constant for a given concrete, taking into account various material parameters such as aggregate nature, alkali content, supplementary cementitious material effect, etc.

The function $\xi_a(t)$ is the reaction extent(the subscript $_a$ refers to AAR), responsible for modeling the pathology evolution versus time t. It is a scalar equal to 0 before deleterious phenomenon starts, and to 1 at the end, when all reactants have been transformed into AAR-gel. Its expression is based on works by Larive [7, 23]:

$$\xi_a(t) = \frac{1 - \exp(-t/\tau_c)}{1 + \exp\left(-\dfrac{t - \tau_l}{\tau_c}\right)}, \tag{3}$$

leading to the classical S-shaped curve (see Figure 2). Two parameters are used in the previous expression, latency time τ_l and characteristic time τ_c.

This model can easily be adapted for DEF-affected structures, assuming some minor changes. The first one deals with chemical extent versus time, as explained above. To take into account the quicker kinetics of DEF compared to AAR, numerical values for parameters τ_c and τ_l have to be lowered. Moreover, the continuous growing of expansion sometimes observed on DEF-affected concrete cannot be described by equation 3. Hence, a variation of this equation has been proposed [8, 24]:

$$\xi_s(t) = \frac{1 - \exp(-t/\tau_c)}{1 + \exp\left(-\dfrac{t - \tau_l}{\tau_c}\right)} \cdot \left(1 - \frac{\phi}{\delta + t}\right). \tag{4}$$

where ξ_s represents chemical extent in the case of DEF. The two previous parameters: characteristic time τ_c (which governs the rate of expansion during the fastest phase of the pathology) and latency time τ_l (corresonding to the duration of the first step of the phenomenom, during expansion is barely noticeable) have been kept but two corrective durations, ϕ and δ (with $0 < \phi < \delta$), have been added in order to correctly fit the end of the curve, as can be seen in figure 2.

3.2 The role of temperature

Early-age temperature:

For the reasons given *supra*, the triggering of DEF in concrete is strongly connected to the thermal history during the first hours or days after casting, *i.e.* the period during which cement hydration occurs. At this time, a raise in temperature (artificially caused by external heating for precast elements or due to insufficient evacuation of heat generated by hydration reaction in massive structure parts) can turn out to delayed ettringite formation.

At this point, it must also be taken into account that this early-age thermal history is seldom homogeneous, particularly in massive parts, where strong thermal gradients can be observed between quasi-adiabatic core and peripheric area where heat exange with environment can occur. See for instance Figure 3.

The swelling potential ε_∞ used in equation 2 cannot be anymore considered as uniform in the whole structure as for the case of AAR. It must be computed for any point of the structure (or, in practical cases, for any finite element of the mesh). A model was proposed by [25, 26] in order to locally link ε_∞ with thermal history at early-age $T_{ea}(\tilde{t})$, $\tilde{t} \in [0; t_m]$ where t_m represents the time where the whole structure is considered as mature (practically, it consists in chosing a time t_m large enough to ensure that the whole structure has reached a thermal equilibrium with its environment).

Its main asumptions [25] are:

- as long as temperature remains below a threshold value T_0, there is no risk of delayed expansion;
- swelling potential grows with temperature reached at early-age according a relationship based on Arrhenius law [27];
- for a given temperature, swelling potential grows with the duration during which this temperature is maintained;

resulting in

$$\varepsilon_\infty = \dot{\varepsilon}_m . \int_{\tilde{t}=0}^{t_m} f\left(T_{ea}(\tilde{t})\right) \mathrm{d}\tilde{t}, \tag{5}$$

$$f(T_{ea}) = \begin{cases} 0 & \text{if } T_{ea} \leq T_0, \\ \exp\left(-\dfrac{E_a}{R}.\dfrac{1}{T_{ea} - T_0}\right) & \text{if } T_{ea} > T_0. \end{cases} \tag{6}$$

In equation 5, thermal history influence is given by the integral factor, while $\dot{\varepsilon}_m$ represents all the material properties influencing the pathology (cement nature, aggregates, formulation...). Equation 6 introduces activation energy E_a for ettringite decomposition (supposed constant for any concrete) and the threshold temperature T_0, R denoting the gas constant.

Temperature during structure life-span:

Contrary to AAR, different antagonist mechanisms are related to thermal effects on DEF, and their global effect remain difficult to assess. Essentially, raising concrete temperature should speed-up the pathology, thanks to Arrhenius effect; but at the same time it could destabilize delayed ettringite responsible for the expansion and hence inhibits the phenomenon.

Some tests performed by [24] with samples stored at 23 $^\circ$C and 38 $^\circ$C gave contradictory results and advocates for deeper researches.

3.3 Other couplings

Based on field experience, other parameters are taken into account in the model. However, due to the few experimental data available, the present version of the model couldn't be fitted on DEF-affected concrete. We instead used coupling relations developed in the frame of AAR.

Stress-state influence:

Expansion in stressed concrete is derived from free expansion through a model proposed by [13] for AAR, based on laboratory tests performed on samples submitted to axisymetric triaxial stress states. If $\boldsymbol{\sigma}$ denotes stress-state, its chemicaly-induced expansion is given by:

$$\boldsymbol{\varepsilon}_\chi(\boldsymbol{\sigma}) = \boldsymbol{A}_s(\boldsymbol{\sigma}).\boldsymbol{\varepsilon}_\chi(\mathbf{0}), \tag{7}$$

in which $\boldsymbol{A}_s.(\boldsymbol{\sigma})$ is a tensor varying with stress deviator, material tensile strength and Poisson's ratio.

Available moisture:

Several models had been proposed to represent moisture influence onto AAR development [12, 28]. All these models consider the two following features: expansion is stopped under a certain threshold value for moisture h; beyond this threshold value, expansion quickly grows with the available moisture.

Same observations tend to be drawn from experimental data [15, 16] on DEF-affected samples, with some differences. First, the threshold value might be higher (relative moisture of 90% for DEF, instead of 80% for AAR). Then the relation giving expansion versus moisture seems to be stiffer in the case of DEF. The parameters used in the various models should be fit accordingly.

Moreover, in the case of DEF, the coupling between moisture and chemical expansion is likely to be in both directions. In the case of AAR-affected concrete, no evidence of pathology on moisture transfer properties were found out [11]. With DEF-induced swelling, expansion and cracking are so important that it probably can increase material permeability [16]. This coupling will have to be taken into account in future model developments.

Damage:

Stiffness reduction due to crack opening is often observed in both AAR and DEF cases. To represent it in the model, we proposed [26] to introduce a dimensionless damage variable d such that, for a given level of expansion, concrete Young's modulus is equal to

$$E(d) = (1 - d).E_0, \tag{8}$$

where E_0 is the Young's modulus for sound concrete. Based on experimental results obtained by [8], [24] proposed the following expression for d:

$$d = d_{max}. \left(1 - e^{\omega.\langle\varepsilon_\chi - \varepsilon_0\rangle^+}\right). \tag{9}$$

In this equation, d_{max} represents the maximal damage, which can reach more than 60% in some case of DEF, ω governs the kinetics of degradation. The threshold value ε_0 represents the ability of the HCP to undergo a certain amount of expansion before cracking. It shall be noted that, for DEF-affected concrete, d damage evolution has to be based on chemical expansion ε_χ and not on the sole chemical extent ξ_s, since the proportionality between both variables varies from one point of the structure to another. Such problem did not arise for AAR-cases where ε_∞ is uniform.

3.4 Numerical implementation

This model for DEF-affected concrete structures was developped in the finite-element software CESAR-LCPC as a module called RGIB (abbreviation of the French name meaning "Internal swelling reactions in concrete"). It allows to connect the chemo-mechanical computation with other modules used for the structure assessment. Four steps are needed, all realized on the same FE-mesh.

- The first computation tends to assess the early-age temperature evolution in the structure by resolving heat equation coupled to hydration reaction extent. It returns for each discrete time $(\tilde{t_i})_{i=1..m}$ in $[0; t_m]$ the early-age temperature fields $T_{ea}(\tilde{t_i})$.
- In each point of the structure, this thermal history $T_{ea}(\tilde{t_i})_{i=1..m}$ is transformed into swelling potential in accordence with equations 5 and 6.
- A second modeling based on Fick's equation (with non-linearity due to moisture-dependant permeability) allows to evaluate saturation degree fields $s(t_j)$ at each discrete instants chosen during the structure life-span $(t_j)_{j=1..n}$.
- Finally, swelling potential and saturation degree are used to compute chemical strain increment for each discrete time $(t_j)_{j=1..n}$; this increment is used as prescribed strain in a mechanical model to assess displacements and stresses in the whole structure.

4 APPLICATION TO A REAL STRUCTURE

The modeling of a bridge pier cap affected by DEF is briefly presented. More detailed example can be found in [26].

4.1 Pier cap affected by DEF

We apply the above-described model to the assessment of a pier, part of a road girder bridge. The massive pier cap was cast during summer in South of France, hence submitted to temperature high enough to trigger DEF. Structure owner was alarmed by large cracks, especially at the end of the bent exposed to rain and permanent humidity. Laboratory investigations confirmed DEF when the structure was about 20-year-old [17].

4.2 Preliminary models

A finite-element mesh with about 6,000 nodes is used to assess early-age temperature during the 300 hours following casting. With an outside temperature of maximum 23 ˚C, the core of the element reached 74 ˚C, whereas the ends of the piece never reached more than 58 ˚C. Results can be seen on Figure 4, where one shall remark the strong heterogeneity between the core and the peripheral part of the pier cap. The modeling was also performed onto the pier shaft (not represented here). Due to lesser transverse dimensions, the temperature in the pier shaft never reached high values. This difference was confirmed by laboratory tests on samples from both cap and shaft, since no DEF-evidences were found out in the pier shaft.

The same mesh was used for moisture field computation, which allows to take into account various exposure to the rain, according to prevailing winds and cover provided by the bridge deck (this particular aspect was aimed at reproducing the asymetric crack-pattern observed on the bent).

4.3 Chemo-mechanical coupling

The evolution during 22 years of prescribed chemical strain is introduced into a mechanical model of the pier cap, taking into account the connection with the shaft, the dead-weight and the load applied by the bridge-deck and the rebars. It allows to assess stress fields in the concrete, resulting from mechanical actions, rebars over-stresses due to interaction with swelling concrete and strong heterogeneity of the expansions due to initial thermal-history (difference between core and skin) and moisture conditions (difference between East and West parts). Figure 5 shows an example of longitudinal stress in the middle plane.

5 CONCLUSION

This contribution has presented a numerical model aimed at reassessing concrete structures affected by DEF. It was based on a previous one devoted to AAR case, due to strong similarities in both pathology when considered from a structure point of view. The step-by-step building of the model was presented and the stress was put on:

- the features which can be directly transposed from AAR to DEF;
- the coupling relations which have to be adapted to the specificity of DEF, such as the reaction kinetics or the influence of available moisture on expansions;
- the development specific to DEF, especially the model aimed at taking into account the early-age thermal history to assess the heterogeneous swelling potential in the structure.

An application to a real case was also provided.

The model presented here can already be applied to various structures affected by DEF, but this paper also emphasise the work still to do: experimental data have to be collected to check and improve various part of the model, especially the role of moisture and stress-state on the development of expansions. The influence of present temperature on DEF kinetics and amplitude deserves deeper inquiry. Last, a new model should be developed to adress the cases where both AAR and DEF simultaneously affect a structure.

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Figure 1: Typical crack pattern for DEF, very similar to AAR ones

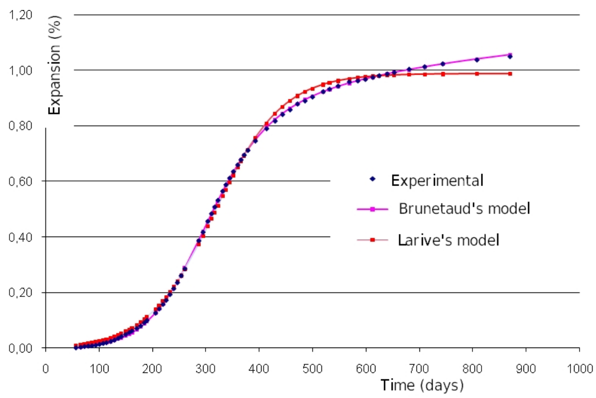

Figure 2: Experimental results from expansion test fitted with Larive's model for AAR and Brunetaud's for DEF

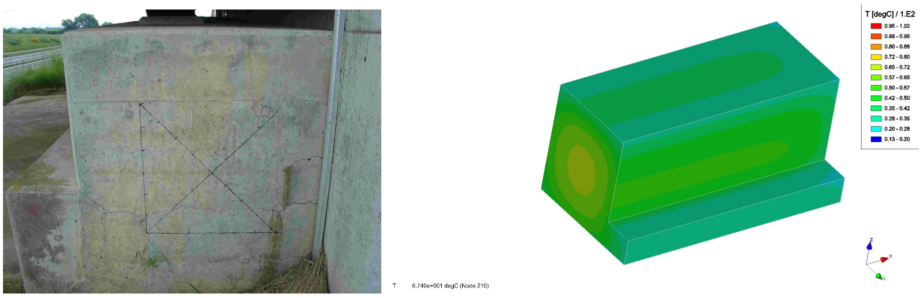

Figure 3: Bridgedeck support affected by DEF and numerical modeling of its temperature after casting

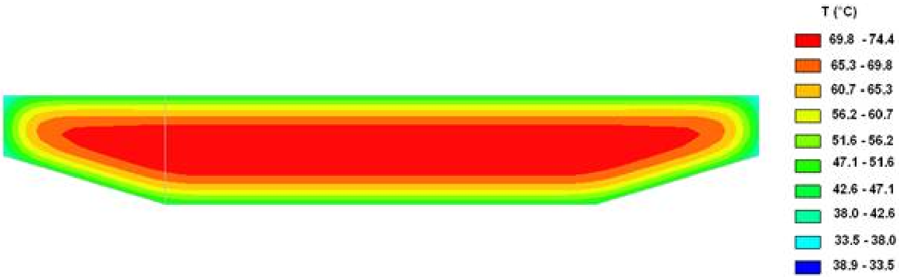

Figure 4: Plot contour for temperatures at early-age in the bent

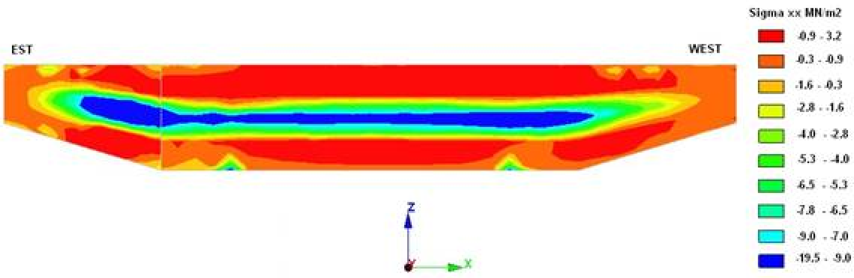

Figure 5: Plot contour for the horizontal stress σ_{xx} in the middle plane of the bent