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Numerical design of experiments applied to modelling structural element affected by DEF

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Abstract

In the case of structures affected by internal swelling reactions (ISR) such as AAR or Delayed Ettringite Formation (DEF), numerical modelling is a powerful tool to re-assess the serviceability and the safety of the structure, taking into account mechanical consequences of the pathology. Unfortunately, fitting these numerical models require a large set of information which might be difficult to obtain, especially in the case of ancient structures built several years ago. In the specific case of DEF, early-age temperature history is a critical parameter and is often difficult to evaluate due to lack of data regarding construction.

The technique known as "design of experiments" is applied to a multiphysics finite-element model of a reinforced concrete bridge-deck support affected by DEF. Using 2k-factorial design, we propose a meta-model to link critical outputs such as concrete swelling potential and stresses in steel rebars induced by concrete swelling to a large set of factors: cement hydration heat, environmental conditions during construction (external temperature, heat transfer through form...), concrete swelling potential and kinetics, mechanics properties, etc. This meta-model emphasizes the role of each factor and their interactions. Analysis of variance will then be used to focus on factors with highest importance, which deserve fine tuning, and to avoid using time and resources to estimate factors of lesser importance.

***Keywords**: delayed ettringite formation; design of experiments; numerical modelling; sensitivity analysis; structural assessment*

1. INTRODUCTION

When dealing with concrete structures affected by Delayed Ettringite Formation (DEF), numerical modelling is often required in order to re-assess the structural state and to set up a management policy or a repair program. Several models have been developed recently [1-3]. They all take into consideration the link between thermal history at early-age and formation of deleterious ettringite during the structure lifespan, as well as the concrete mechanical response to ettringite expansion in the hardened cement paste.

The correct fitting of these models often requires the identification of several parameters connected to the material properties, the conditions of construction (especially thermal conditions during concreting), etc. Achieving this task might be difficult or expensive: essential information are not always correctly recorded, or can be lost years or decades after construction, some difficult or costly laboratory investigations might be needed, as well as complex inverse analysis of degradations [4].

We propose to investigate which parameters really matter for numerical modelling, to be able to concentrate investigations on their identification. A common tool developed for industrial process will be used for this purpose: design of experiment.

We will first describe the main equations of the numerical models and their application to the reassessment of a bridge abutment cap beam affected by DEF. Then the principle of numerical design of experiment will be exposed. Finally, we will detail the sensitivity analysis of the first part of the re-assessment (early-age thermal problem) and sketch the principle of the second part (chemo-mechanical problem).

2. NUMERICAL MODEL FOR DEF-AFFECTED STRUCTURES

The numerical modelling of DEF-affected concrete structures is based on the following steps:

- assessment of thermal history in the days following concrete casting;
- computation of local swelling potential based on thermal history;

• application of long-term loads and computation of mechanical behaviour resulting from both external loads and internal swelling reaction.

2.1 Early-age thermal history

In the case of cast-in-place concrete elements, the temperature after pouring at each time *t* for each location *x* $T(x,t)$ is governed by the heat equation:

$$C_v \frac{\partial T}{\partial t} = -\nabla . q + l \frac{\partial \alpha_h}{\partial t} \quad (1a)$$

$$q = -K \nabla T \quad (1b)$$

Where C_v is the volumetric heat capacity, $\boldsymbol{q}$ is the heat flow, *l* is the latent heat per hydration degree, α_h is the cement hydratation (starting at 0 for dry cement, and equal to 1 when all the cement has been hydrated) and *K* is the concrete thermal conductivity.

The hydratation, responsible for the internal heat source, depends on temperature through Arrhenius' law:

$$\frac{\partial \alpha_h}{\partial t} = A(\alpha_h). exp\left(\frac{-E_h}{RT}\right) \quad (2)$$

for which *A* is the affinity function, E_h is the activation energy and *R* is the universal gas constant. Note that parameter *l* and function *A* depends on the nature of the concrete mix used, and can be obtained thanks to quasi-adiabatic test (QAB). Further details can be found in [5-7].

2.2 DEF-related swelling potential

For a given concrete, the swelling potential ε_∞ of DEF-affected material is governed by two parameters: the level of temperature reached by the material at early age, and the duration of its application. Based on experimental evidences, two models have been proposed and will be considered in this study. The first one is described in [8] and is expressed by:

$$\epsilon_{\infty,B} = \dot{\epsilon_m}. \int_{\tau_0}^{\tau_F} f\left(T(t)\right) dt \quad (3)$$

$$f(T) = \begin{matrix} 0 if T < T_s \\ exp\left(\frac{-E_a}{R}.\frac{1}{T-T_s}\right) else \end{matrix} \quad (4)$$

In equation (3), $\dot{\epsilon_m}$ is a material parameter representing the concrete composition, E_a is the activation energy of ettringite degradation and T_s is a threshold-temperature.

The second one (derived from the first one) is described by [9]:

$$\epsilon_{\infty,M} = \int_{\tau_0}^{\tau_F} \alpha\,(t). f\left(T(t)\right) dt \quad (5)$$

$$\alpha(t) = \lambda. \beta. t_{exp}(t)^{\beta-1} \quad (6a)$$

$$t_{exp}(t) = \int_{\tau_0}^{t} H\,(T(\tau) - T_s) d\tau \quad (6b)$$

where λ is a positive parameter, $\beta \in]0; 1[$ a second parameter (both depend on concrete composition) and *H* is the Heaviside step function.

In real conditions, this swelling potential might also be affected by moisture available in the material. For the present study, we will consider fully-saturated porous network in the whole structure.

2.3 Chemo-mechanical coupling

The mechanical influence of DEF is represented by a prescribed volumetric strain. Its amplitude varies with time t according to

$$\epsilon_\chi(x,t) = \epsilon_\infty(x) \frac{1 - exp(-t/\tau_c)}{1 + exp(\tau_l/\tau_c - t/\tau_c)} \quad (7)$$

where $\varepsilon_\infty(x)$ is the swelling potential given by expression (3) or (5) and τ_c and τ_l are two parameters for chemical kinetics, characteristic time and latency time respectively (alternative expressions of kinetics derived from the Larive's model, are not considered here for the sake of simplicity). This expansion is isotropic unless anisotropy is induced by stress state, see [10] for further details.

The second consequence of DEF, internal cracking, is represented by a damage variable *d* which modifies concrete stiffness:

$$E = E_0 \left(1 - d(\epsilon_\chi)\right) \tag{8}$$

and the evolution of *d* with chemical prescribed expansion is given by:

$$d(\epsilon_\chi) = d_{max}\left(1 - e^{\omega\langle\epsilon_\chi - \epsilon_0\rangle^{+1}}\right). \tag{9}$$

In this last expression, d_{max} is the maximal damage at the end of reaction, ω is a shape-parameter and ε_0 is the strain above which hardened cement paste starts to crack.

This chemo-mechanical model is then introduced in a more general mechanical model for concrete taking into account elastic and delayed deformation of material, see [1].

3. APPLICATION TO AN ABUTMENT CAP BEAM

In this study, the above-described model is applied to the re-assessment of a cast-in-place abutment cap beam. Although this case is fictious, it is inspired by real cases of DEF-affected elements in highway overpasses, such as described in [4]. An example of such a structure is shown on Fig. 3.1.

Figure 3.1: Example of abutment cap beam

3.1 Description of the structural element

The abutment cap beam is an 8-m long beam with rectangular 1 m × 1.5 cross-section. Bridge deck is supported by two 0.3 m × 0.4 m bridge supports and the abutment is founded on two piles (considered as rectangular cross-section to avoid excessive mesh complexity). Due to symmetries through longitudinal and transverse vertical planes, only one quarter of the structure is studied. The coordinate frame and the dimensions can be seen on Fig. 3.2.

3.2 Early-age thermal problem

The cap beam is cast in one step. Assessing its early-age thermal history consists in solving equations (1) and (2) with initial conditions:

$T(x, 0) = T_0, \forall x,$

$\alpha_h(x, 0) = 0, \forall x.$

Boundary conditions for heat equation are:

q = **0** for both symmetry plane,

q.***n*** = h_e ($T(x,t) - T_e(t)$) elsewhere (***n*** is the vector normal to faces).

The second boundary condition represents Newton's convective heat transfer. For real cases, one should take into account difference between faces in contact with form and faces directly exposed to surrounding air (here, the upper face), as well as variations due to faces geometry and orientation (mainly, for free convection, the difference between horizontal and vertical faces). But since we are exploring the influence of various parameters, we will here assume a unique heat transfer coefficient h_e and check how its variations modify the model's output.

The problem is solved with finite-element software using 24 000 hexaedral elements and total duration of the simulation (τ_F = 7 days) is divided into 210 time steps: 56 15-min-long steps between t = 0 and t = 14 h, when temperature rises quickly in the structure, then 154 1-h-long steps between 14 h and 168 h, when temperature varies gently. These spatial and temporal discretizations have been chosen after several tests to make sure that discretization error will not have significant consequences on the sensitivity analysis exposed in the next section.

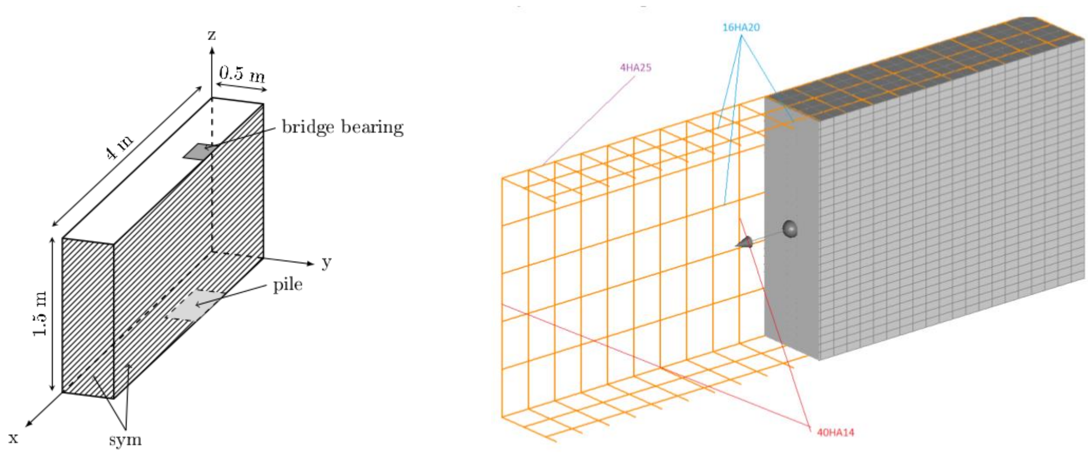

Figure 3.2: Quarter of the abutment cap beam and its reinforcement.

3.3 Mechanical problem

The mechanical problem represents the cap beam behaviour during 20 years after casting considering the evolution of DEF in the concrete. The concrete behaviour is elastic with linear creep and the structure is reinforced by rebars represented by elastic bar elements, as shown on Fig. 3.2. These elastic or visco-elastic behaviours are chosen because we are mainly interested in the consequences of DEF on serviceability of the structure; simulation is then supposed to be consistent with SLS evaluation.

The boundary conditions are: total embedding in the pile, normal displacements equal to zero on both symmetry planes. The initial stress-state $\sigma(x, 0)$ is computed by considering an elastic response to quasi-permanent combination of the dead weight (25 kN.m^{-3}) and to the permanent load applied through the bridge bearing (total load of 720 kN is transmitted by two .3 m × .4 m bridge bearings to the cap beam, hence a uniform pressure of 3 MPa).

As mentioned earlier, the whole cap beam is supposed to be saturated by moisture: first, this is a fair approximation of some real cases (cap beam is constantly submitted to water through direct contact with saturated soil and water ingress through dilatation joint at the deck extremity); second, this keeps the complexity of the study at a reasonable level. Of course, influence of variable and heterogeneous moisture field in the cap beam could be studied in further works.

4. NUMERICAL DESIGN OF EXPERIMENT - PRINCIPLES

4.1 Design of experiment

Considering a given phenomenon depending on various conditions, we call *experiment* the observation *y* of this phenomenon for a given set of parameters called *factors* $(p_i)_{i=1\dots k}$. Design of experiment (DOE) consists in choosing *n* experiments, represented by *n* vectors $\boldsymbol{p}^{(m)} = (p_1, \dots, p_k)^T$ (superscript ^{T} stands for transpose) with m = 1, ..., n, in order to learn information on the phenomenon by studying the relation between experiment results $(y^{(m)})_{m=1\dots n}$ and the values taken by the *k* parameters $(p_i)_{i=1\dots k}$.

Several techniques exist to find the optimal set of experiments $(\boldsymbol{p}^{(m)})_{m=1\dots n}$ to get as much information as possible on the phenomenon (see for instance [11-13]). These information are usually presented as a relation between the observation and the factors:

$$y = f(p_i) + e, \tag{10}$$

in this relation, function *f* of *k* variables is called *a priori* model, surrogate model or meta-model and it differs from the real phenomenon by an error *e* which represents both random error and lack-of-fit error.

4.2 Use of numerical design of experiment for sensitivity analysis

A numerical model can be considered as an experiment where the factors are the input of the model (initial conditions, boundary conditions, material properties...) and the observation is an output of the model with particular meaning (for instance stress in a critical location of the structure).

Note that in the case of numerical experiments, since no random exists in the relation between parameters p_i and model response *y*, the error *e* appearing in relation (10) is only lack-of-fit error. [14]

The use of DOE technique and the building of a meta-model allows to easily understand the role of each model inputs on the output, because usually the meta-model given by equation (10) is easier to study than the original numerical model.

In order to compare the role of each parameters, we will now consider only normalized factors $x_i \in [-1; 1]$.

They are defined as follow for numerical parameters p_i:

$$x_i = \frac{2p_i - (p_{i,max} + p_{i,min})}{p_{i,max} - p_{i,min}} \qquad (11)$$

where $p_{i,min}$ and $p_{i,max}$ are the lowest and highest value of p_i respectively. Qualitative parameters will be represented by $x_i = -1$ for conditions associated to a *low* level, and by $x_i = +1$ for a *high* level. Note that for all factors, the value $x_i = 0$ represents the median value of the parameter.

Once each parameter has been transformed into a normalized factor, we will build a meta-model with the following form:

$$y = a_0 + \sum_{i=1}^{k} a_i\, x_i + \sum_{i<j\leqslant k} a_{ij}\, x_i . x_j + \sum_{i<j<l\leqslant k} a_{ijl}\, x_i . x_j . x_l + \cdots + a_{12\ldots k} x_1 . x_2 \ldots x_k + e \qquad (12)$$

This kind of meta-model, also called response surface, is easy to interpret:

- a_0 is the mean value of output *y,*
- a_i is the *effect* of factor x_i,
- a_{ij} is the *interaction* between factors x_i and x_j, a_{ijl} the one between factors x_i, x_j and x_l, etc.,
- *e* is the lack-of-fit error.

Note that thanks to the transformation (11), all factors are dimensionless and with the same magnitude, hence their respective role in the output y can be easily compared by comparing their respective effects a_i.

4.3 Determination of the meta-model

1.1.1 Notations

As can be seen in equation (12), the building of the meta-model requires the determination of 2^k coefficients. Let denote by ***a*** the vector gathering all these coefficients:

$$a = (a_0, a_1, \ldots, a_k, a_{12}, \ldots, a_{ij}, \ldots, a_{12\ldots k})^T . \qquad (13)$$

Each experiment is represented by a vector $\boldsymbol{x}^{(m)}$:

$$x^{(m)} = \left(1, x_1^{(m)}, \ldots, x_k^{(m)}, x_1^{(m)} . x_2^{(m)}, \ldots, x_i^{(m)} . x_j^{(m)}, \ldots, x_1^{(m)} . x_2^{(m)} \ldots x_k^{(m)}\right)^{T.} \qquad (14)$$

and the whole set of experiments is then defined by matrix ***X***:

$$X = \begin{pmatrix} x^{(1)} \\ \vdots \\ x^{(n)} \end{pmatrix} . \qquad (15)$$

Finally, if we denote the observation of experiment *m* by $y^{(m)}$, the set of experiment observations is:

$$y = \left(y^{(1)}, \ldots, y^{(n)}\right)^T \qquad (16)$$

and the application of meta-model (12) leads to:

$$y = X.a + e \quad (17)$$

where ***e*** is a *n*-dimension vector the components of which are the lack-of-fit error for each experiment.

1.1.2 Complete factorial experiment

We use complete two-level factorial experiments to assess the parameters of the meta-model. They consists in using the two extreme values of each factor x_i namely -1 and +1, and then testing all the possible combinations for *k* factors. Hence, the number of experiment *n* is also equal to 2^k.

Note that this choice has several advantages: it leads to a number of experiments equal to the number of parameters for the meta-model, it is easy to design and use, and it gives matrix ***X*** several interesting properties (for instance, ***X*** is a Hadamard matrix, see [11, 13] for more details).

1.1.3 Least-squares method

Once the n=2^k experiments have been realized and their results collected in the vector ***y***, the determination of *n* parameters of meta-model is obtained by finding $\hat{a}$ the estimation of a such that ***e*** in (17) is minimal. This minimization is equivalent to a linear regression based on the least-square criterion, and the solution is given by (see [15] for instance)

$$\hat{a} = (X^T.X)^{-1}X^T y. \quad (18)$$

In the particular case of two-level complete factorial experiment, equation (18) is simply:

$$\hat{a} = \frac{1}{2^k} X^T y. \quad (19)$$

5. SENSITIVITY ANALYSIS OF EARLY-AGE THERMAL PROBLEM

5.1 Factorial experiment

We apply the method described in the previous section to the determination of DEF-swelling potential in the abutment cap-beam due to early-age thermal history. Here, five factors will be considered, as described in table 5.1.

Table 5.1: Factors considered for the early age thermal problem.

x_i	Factor	Description	Unit	x_i = -1	x_i = +1
x_1	T_0	Initial temperature	° C	10.	30.
x_2	T_e	External temperature	° C	"cold"	"hot"
x_3	E_h/R	Arrhenius const.	K	4000.	7000.
x_4	QAB	Concrete mix exothermicity	° C	"low"	"high"
x_5	h_e	Heat transfert coef.	kJ/h/m^2/K	1.55	21.6

External temperature is considered as varying on a 24-hour basis. The *cold* case is a variation between 5 and 15° C, the *hot* one between 18 and 30° C. The *low* and *high* cases or concrete exothermicity are represented by temperature vs. time curves in adiabatic conditions as shown on Fig. 5.1

Note that volumetric heat capacity C_v and thermal conductivity are supposed to be easy-to-know parameters, hence they are not considered as variable factors. We chose classical values C_v = 2400 kJ/m^3/K and K = 6 kJ/h/m/K (they were considered as constant during the process of cement hydration, which is an approximation but with moderate consequences on the final result, see [16]).

The figure 5.2 represents isotherms in the cap beam 3 hours after casting for the simulation with $(x_1,x_2,x_3,x_4,x_5) = (+1,-1,+1,+1,+1)$. In this case, temperature reaches a maximum of 87° C in the centre of the structural element.

5.2 Analysis of meta-model

The 32 numerical experiments are realized, and, for each case, the thermal history $T_c(t)$ in the centre of the cap beam is considered. The observation *y* is the swelling potential obtained at this point:

$$y = \epsilon_{\chi}(T_c(t), 0 \leqslant t \leqslant \tau_F). \tag{20}$$

As presented above, we can choose between two models to bind DEF-swelling potential to thermal history: the one given by equations (3) and (4), or the one corresponding to (5) and (6). In this communication, we will only focus on the first one, but similar results were obtained with the second one [17]. The parameters used for assessing swelling potential are the same as found by [18] in his experimental study: $\dot{\varepsilon}_m = 6.510^{-4}$, $E_a = 438.5$ J/mol and $T_s = 43.3°$ C.

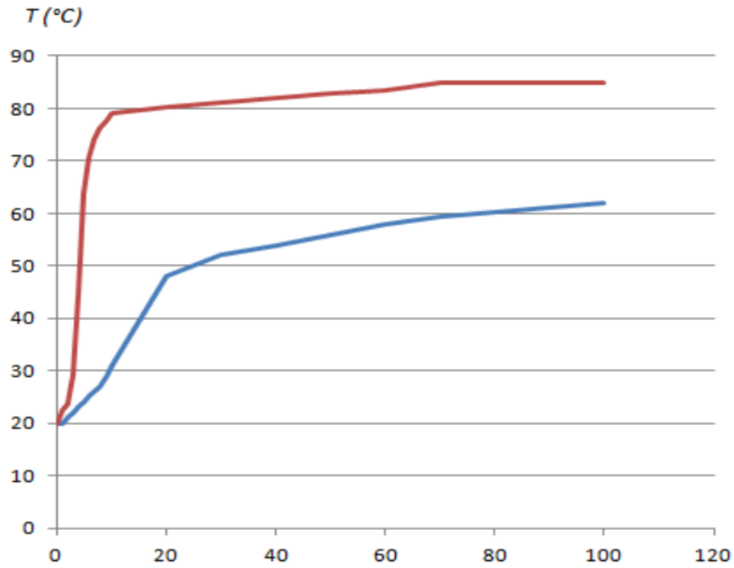

Figure 5.1: QAB-curves (temperature vs time in hours) for low and high cases

By using normal equation (19), the meta-model binding swelling potential to the five factors can be expressed. Here, we don't take into account effects or interaction lower than 1/100 of mean value $\alpha_0 = 4.75$ (swelling potentials are expressed in mm/m):

$$\begin{aligned} y = 4.75 + 3.11x_1 + 0.56x_2 + 3.37x_4 - 3.56x_5 + 0.19x_1.x_2 - 0.11x_1.x_3 \\ +0.17x_1.x_4 - 2.21x_1.x_5 + 0.33x_2.x_4 - 0.35x_2.x_5 - 0.05x_3.x_4 \\ -2.83x_4.x_5 - 0.13x_1.x_2.x_5 + 0.07x_1.x_3.x_5 - 1.02x_1.x_4.x_5 - 0.18x_2.x_4.x_5 \end{aligned} \tag{21}$$

(complete set of coefficients as well as detailed calculation can be found in [17].)

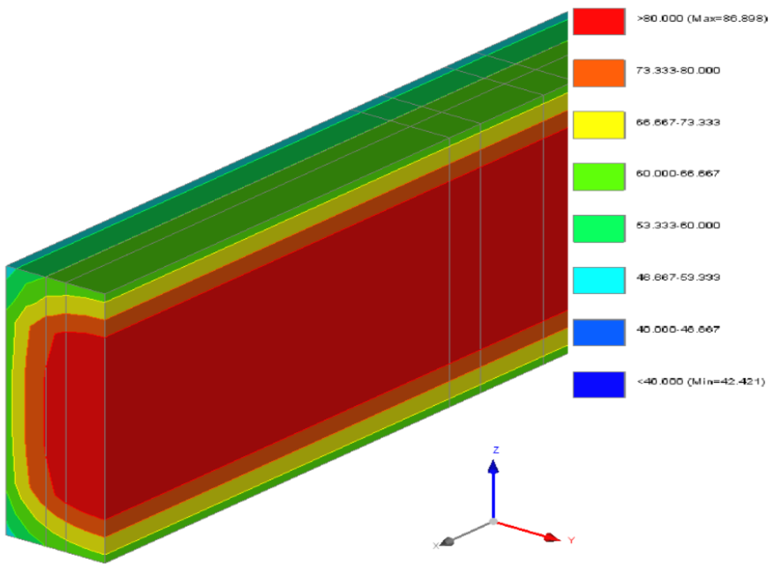

Figure 5.2: Example of isotherms in the cap beam 3 h after casting.

The meta-model (21) clearly shows the factors with high influence on the swelling potential (x_1, x_4 and x_5, namely initial temperature T_0, exothermicity of the mix and, with a negative effect, heat transfer through faces of the beam). The effect of outer temperature is six times smaller, and Arrhenius constant of the hydration reactions has no significant effect (this last point is not so clear because this factor is strongly linked to QAB-curve used for exothermicity, and shall deserve further investigations.)

Some interactions have also significant consequences on the swelling potential: the largest one involve, once again, x_1, x_4 and x_5.

A first conclusion on this meta-model is then proposed: the swelling potential due to DEF in the middle of the cap beam is mainly governed by the initial temperature of the fresh concrete, the QAB-curve of the mix and the convection through faces; these 3 factors have same order of influence. The outer temperature also plays a role, but smaller.

6. TOWARDS SENSITIVITY ANALYSIS OF MECHANICAL PROBLEM

The next step of this work (still in progress) consists in applying the same technique of numerical design of experiment to the chemo-mechanical problem. The question is to determine which factors play a large role in re-assessing the bearing capacity of the DEF-damaged cap beam.

6.1 Factorial experiment

This study will only focus on the loss of bearing capacity induced by DEF at the end of the pathology, and not on how fast this situation could occur. This is why the study is restricted to factors influencing the magnitude of the swelling, and not to the ones responsible for its kinetics.

The previous design of experiment allows to conclude that, concerning early-age thermal history, the main factors are concrete mix exothermicity, initial temperature and heat transfer coefficient.

We will then consider the 3 parameters involved in equations (3) and (4): $\dot{\varepsilon}_m$, T_0 and E_a which bind thermal history to swelling potential.

Finally, in what concerns to the mechanical problem, we can consider that properties such as resistance f_c and f_t as well as stiffness E_c is known with good confidence, but other parameters are more difficult to estimate, so their influence on final result must be determined. We will consider ω and d_{max} involved in equation (9) for chemical damage and creep coefficient k_{fp} from the model described in [19] for AAR which is applied here to DEF.

Note that factors modifying the swelling anisotropy are considered here since it depends on creep coefficient (which "softens" the concrete in the most compressed directions). Anisotropy also depends on tensile strength and Poisson's ratio, but both can be considered as trusty estimated.

The 9 factors studied in this numerical experiment as well as their range are presented in table 6.1

Table 6.1: Factors considered for the chemo-mechanical problem.

x_i	Factor	Description	Unit	x_i = -1	x_i = +1
x_1	T_0	Initial temperature	° C	10.	30.
x_2	QAB	Concrete mix exothermicity	° C	"low"	"high"
x_3	h_e	Heat transfert coef.	kJ/h/m^2/K	1.55	21.6
x_4	T_s	Threshold temperature	° C	40.	55.
x_5	E_a	Activation energy	J/mol	400.	500.
x_6	$\dot{\varepsilon}_m$	Material param.	h^{-1}	5.10^{-7}	4.10^{-6}
x_7	d_{max}	Maximal chemical damage	-	.5	.9
x_8	ω	Shape param. for damage	-	2.	4.
x_9	k_{fp}	Creep coefficient	Pa$^{1/2}$	2.10^{-3}	8.10^{-3}

Other parameters needed for the numerical simulations take the following fixed value: Young modulus for concrete E_c = 30 GPa, Poisson's ratio ν = 0.2, compressive strength f_c = 30 MPa, Young modulus for rebars E_s = 190 GPa, characteristic time for DEF-kinetics τ_c = 500 days, latency time τ_l = 2500 days.

6.2 Output

The numerical simulations are performed over a 20-year-long period and, at the end, the deformation of the cap beam is similar to the one presented on figure 6.1.

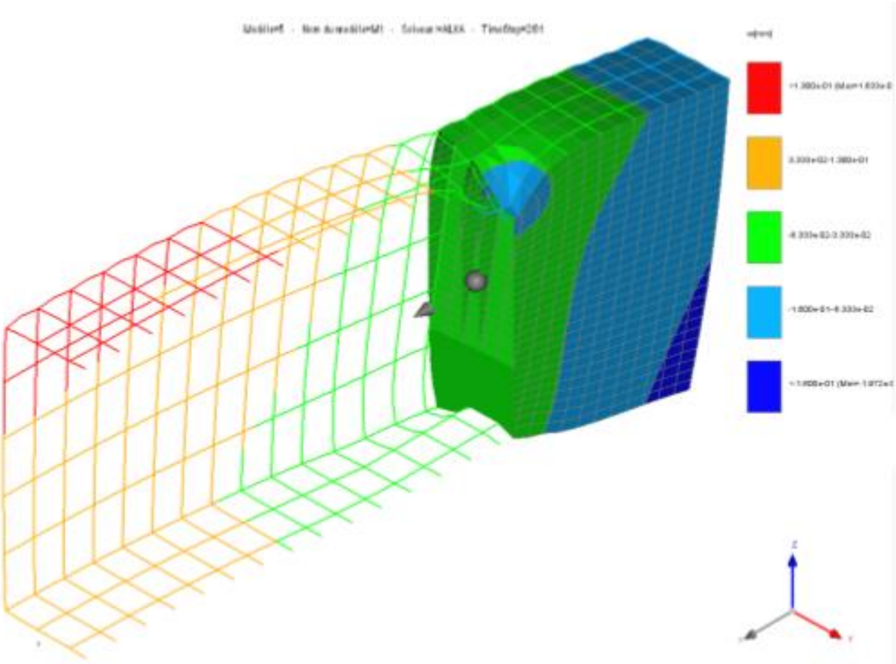

Figure 6.1: Deformation of the cap beam.

These simulations can be used to re-assess the bearing capacity of the cap beam when damaged by DEF. In that context, the most important outputs are the tensions induced by concrete expansion in the reinforcement. For this study, we will focus on two rebars: one is a longitudinal 20-mm rebar located just under the bridge bearing (because it is in charge of transmitted deck load to the cap beam), the other one is a 14-mm stirrup located in the middle of the cap beam (in the symmetry plane where concrete is the more likely to swell).

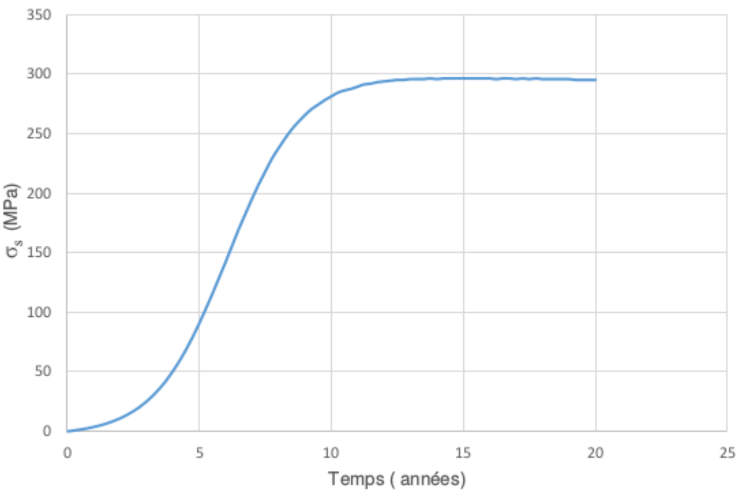

Figure 6.2: Stress (in MPa) vs. time (in years) in the stirrup in the middle of the cap beam

As can be seen on figure 6.2, the stress in the stirrup can rise to significant value (around 300 MPa) due to concrete swelling after 20 years of DEF.

We will then try to build metal-model connecting $y = \sigma_s(20\ \text{y})$ to the 9 factors from table 2.

7. CONCLUSION

When managing structures damaged by DEF, often years or decades after their building, it is difficult to obtain fair and accurate information to correctly fit the numerical models used for their re-assessment. Hence it is crucial to know which parameters really matter, to be able to concentrate investigations on their identification. In this communication, we present a work-in-progress consisting in quantifying the influence of various parameters on the numerical modelling of a bridge abutment cap beam affected by DEF.

The technique of numerical design of experiments proves to be efficient to achieve this goal: use of simple numerical methods provide quantified information on the effects of each studied factors as well as their interaction.

The future steps of this work will consist: first in completing the building of the meta-model for chemo-mechanical problem and analysing the obtained meta-model, second in testing various design of experiments techniques, especially kriging approach which is supposed to be particularly well adapted to numerical experiments [14], and last in using the obtained meta-model for global sensitivity analysis and uncertainty propagation, as presented, for instance, in [20].

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