SEMI-EMPIRICAL MODEL TO PREDICT THE SWELLING DUE TO THE DEVELOPMENT OF DELAYED ETTRINGITE FORMATION

Georges Nahas[1], Amal Rebhi[2], and Jacques Jabbour[3]

[1] Senior research engineer, IRSN, B.P. 17 - 92262 Fontenay-aux-Roses Cedex, France
(georges.nahas@irsn.fr)
[2] Trainee, IRSN, B.P. 17 - 92262 Fontenay-aux-Roses Cedex, France
[3] Research engineer, IRSN, B.P. 17 - 92262 Fontenay-aux-Roses Cedex, France,

ABSTRACT

Delayed Ettringite Formation (DEF) is a pathology that is likely to degrade concrete by causing swelling, cracking and major disorders in structures. It appears in concrete structures under specific conditions, mainly if the early age temperature exceeds 65°C, which leads to swelling and evolutionary cracking in the structure after several decades. In the nuclear field, this risk cannot be excluded, especially in the case of massive structures, such as the containment building of a Nuclear Power Plant (NPP). Current rheological Thermo-Hydro-Chimio-Mechanical laws include several parameters that are very difficult to identify. In this paper, we present a simplified, semi-empirical model to simulate the swelling due to DEF. This model is based on two important parameters identified in the literature. These parameters are the maximum temperature and the duration of heat treatment at the early age for a considered concrete mix. This semi-empirical model is developed based on test results realized on a full scale mock-up and laboratory samples. The validation of the approach is carried out by comparing the results of the model with the strains measured in a test case structure at different times.

INTRODUCTION

Among the phenomena involved in aging mechanisms, internal swellings reactions are pathologies likely to degrade concrete by causing swelling, cracking and major disorders in the affected structures. They include the Delayed Ettringite Formation (DEF) and the Alkali-Silicate Reaction (ASR). These pathologies are endogenous reactions, occurring as a result of the interaction between the initial components of the material. These interactions take place following the use of reactive aggregates in case of ASR or following a significant warm-up at the concrete's early age in case of DEF. They can appear in civil engineering structures several decades after their construction given certain thermodynamic conditions.

In nuclear facilities, the possibility of seeing these phenomena develop cannot be ruled out as they affect in priority massive reinforced concrete elements, such as containment building, for which a significant heating could have occurred at the early age. Therefore, the assessment of their behavior is of primary importance as they represent the third and last containment barrier against the possible release of radioactive products into the environment.

The assessment of the swelling due to DEF is a complex problem. According to the scientific literature, it depends on several parameters related to the concrete mix, the thermal conditions in the early age and the environment of the structure in the operating conditions. Several laws at the scale of the structure have been proposed in the literature. We note for instance: Salgues M. & al. (2014), Seignol J. F. & al. (2009) and Sellier A. & al. (2018). These laws require the knowledge of many parameters, often difficult to obtain without the use of elementary characterization tests specific to the concrete mix. However, in order to estimate the order of magnitude of the potential expansions at the scale of the structure affected by this

pathology, a simplified law seems necessary. It can be used to assess the risk associated with the pathology on the safety functions of the structure. The law must be easy to implement with a limited number of variables and easily identifiable. In this regard, a semi-empirical law for the DEF model has been developed based on the experimental data provided by Jabbour & al. (2021).

In this paper, we discuss the proposed semi-empirical law, the approach used to fit the model parameters and the results obtained. We evaluate as well the deviations from the strain measurements in a test case structure at different times.

THEORETICAL BASIS OF THE MODEL AND APPROACH USED

According to the scientific literature, the swelling due to the development of DEF depends on the temperature of the early age heat treatment and its duration of application. The research of Salgues M. & al (2014) shows that an increase of the maximum early age temperature from 3°C to 4°C produces 10 times more ettringite dissolution, while an increase of 10°C produces 1000 times more ettringite dissolution. This influences the magnitude of the swelling. In addition, the research of Kachakech B. & al. (2015) on the effect of the early age heat treatment and its duration confirm the importance of these parameters on the intensity of the DEF swelling. It proposes a new parameter named the effective thermal energy (Eu), defined as the integral of the temperature $T(t)$ over time t (in hours) of the concrete at early age when it exceeds a threshold value T_0. This threshold temperature was evaluated at 65°C.

$$Eu = \int (T(t) - T_0)\, dt \qquad\qquad (1)$$

This parameter can be correlated with different indexes used in the literature to quantify the final swelling of concrete, such as the ettringite formation index (I_{AFt}), the evolution of the available aluminates index (I_{Al}) and the absorbed sulfates index ($I_{sulfates}$). Therefore by using these two parameters (Eu) and (T_{max}) as surrogate variables for a given concrete mix and correlating them to a known swelling behavior for different early age heat treatments, we be able to quantify the swelling of the structure without using the other parameters (I_{AFt}, I_{Al}, $I_{sulfates}$...) more complicated to quantify. Thus, the proposed semi-empirical model is a function of these two variables: the maximum temperature (T_{max}) and the effective thermal energy (Eu). These surrogate variables have the advantage of being relatively simple to identify in the case of a structure affected by this pathology.

To define the parameters of the semi-empirical model, we used the experimental data provided by Jabbour J. (2018) in the framework of his PhD, in particular from the mock-up used to study the DEF pathology. The first step is to identify the spatial distribution of these two variables in the totality of the mock-up based on the measurements of the thermal sensors. The semi-empirical law is then developed based on these variables and the values of the expansions measured in the structure using the vibrating wires at five instants that characterize the evolution curve of the pathology. The verification of this law was then carried out by comparing the simulation results with the strain measurements obtained by optical fibers carried out at various times.

The simulation of the mechanical behavior of the mock-up and its evolution in time was performed using the OTTOSEN model with fictitious cracks based on the work of Dahlblom O & al. (1990). This model is available in the Cast3M software. The swellings calculated by the semi-empirical law are introduced as a loading with imposed deformations function of time. The mechanical characteristics of the concrete are assumed constant in the calculations. The validation of this approach was carried out by comparison with the measurements of the cracking indexes carried out on the face of the mock-up at various times.

EXPERIMENTAL DATA

As stated earlier, the main data used to define the parameters of the semi-empirical model are provided by the experimental program carried out by J. Jabbour (2018) on the accelerated development of DEF in massive concrete structures.

In this program, the DEF pathology was developed in a large-scale concrete mock-up without reinforcement whose dimensions are 2.40 m width, 1 m thickness and 1.40 m height. The concrete mix is presented in table 1. Shortly after the concrete is poured, the mock-up's core temperature reached 80°C due to the exothermic character of the cement hydration process. It was maintained at a plateau of 80°C for three days, hence generating a value of useful thermal energy of about 1800°C.h. This amplified the dissolution of ettringite at the early age which led to important expansions later on in the concrete structure.

The acceleration of the development of the DEF pathology was realized by immersion in water at ambient temperature in a tank of about 18 m³ for almost 1000 days. During this time, the cycled water was changed every 28 days to increase alkali leaching and accelerate DEF development.

The mock-up is instrumented with thermo-sensors to measure the internal temperature gradient at early age (see figure 1). Extensometers are disposed in three rosettes each containing three vibrating wires sensors to measure the strain in the concrete in the three directions (see figure2). An optical fiber was embedded within the mock-up in three different planes in the shape of a serpentine (see figure 3) in order to measure the strain evolution in 2D. Those measurements were performed at different times as well as cracking index measurements.

Table 1. Concrete mix used for DEF mock-up

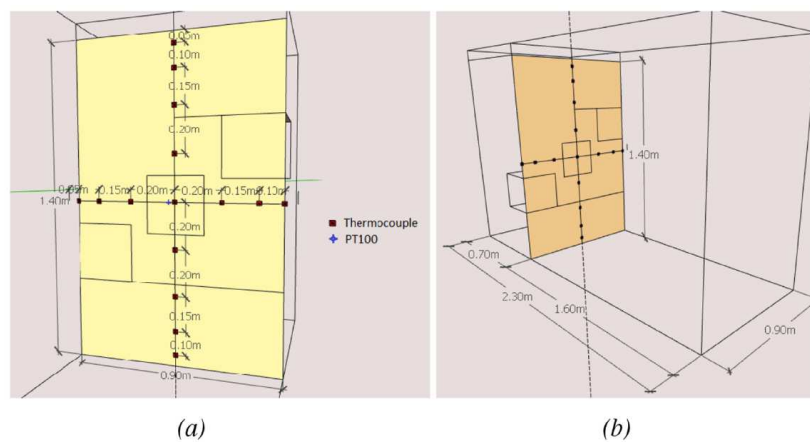|	Weight (Kg/m³)
Cement CEM II A-LL 42.5 R	400
Sand 0/5	772
Coarse aggregates 5/12.5	316
Coarse aggregates 12.5/20	784
Water	228
Plasticizer	1.4

(a)   *(b)*

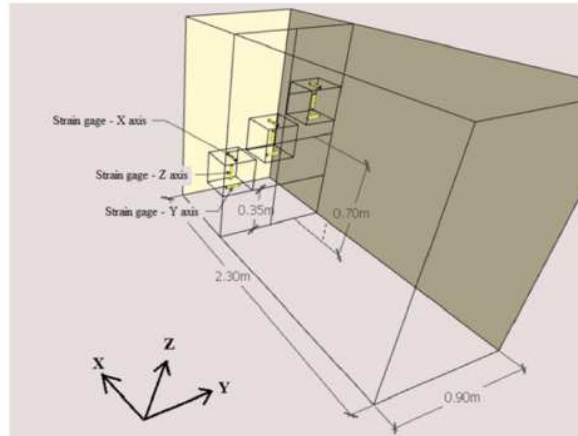Figure 1. (a) cross section and (b) Support showing the positioning of the thermo sensors

Figure 2. Vibrating wires placement in the structure (dimensions not including concrete cover
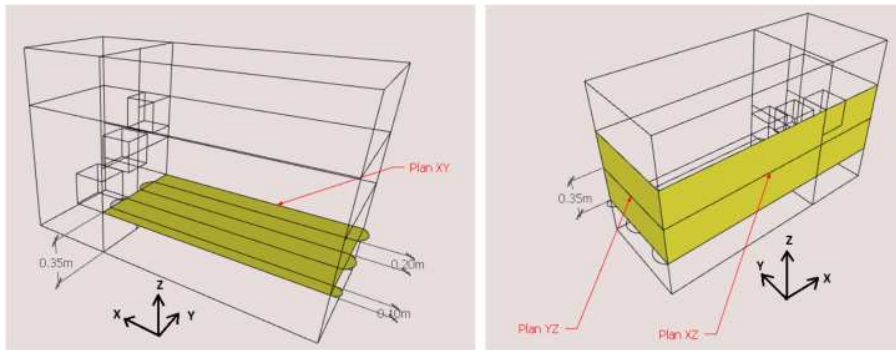

Figure 3. Positioning of the optical fibers in the mock-up

Figure 4. Cracking index measurements in the DEF mock-up

Figure 5 presents the temperatures measured by the thermo-sensors during the heat treatment of the early age concrete and on the metallic formwork and figure 6 presents the deformations measured by the vibrating wires sensors due to the development of the DEF pathology.
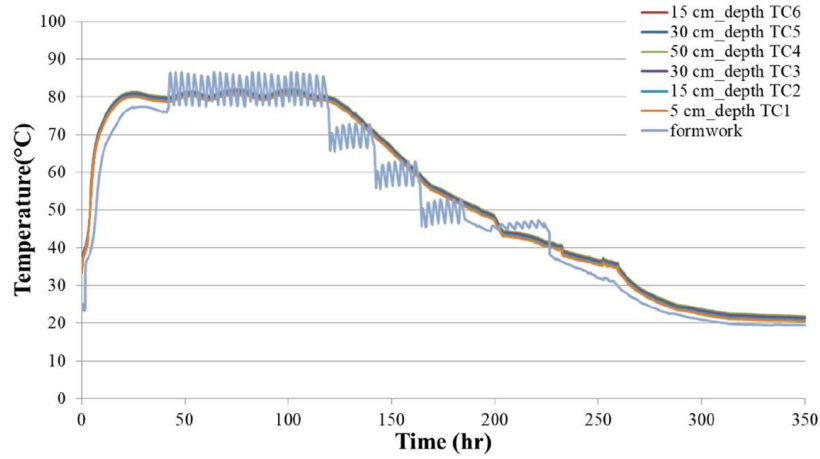
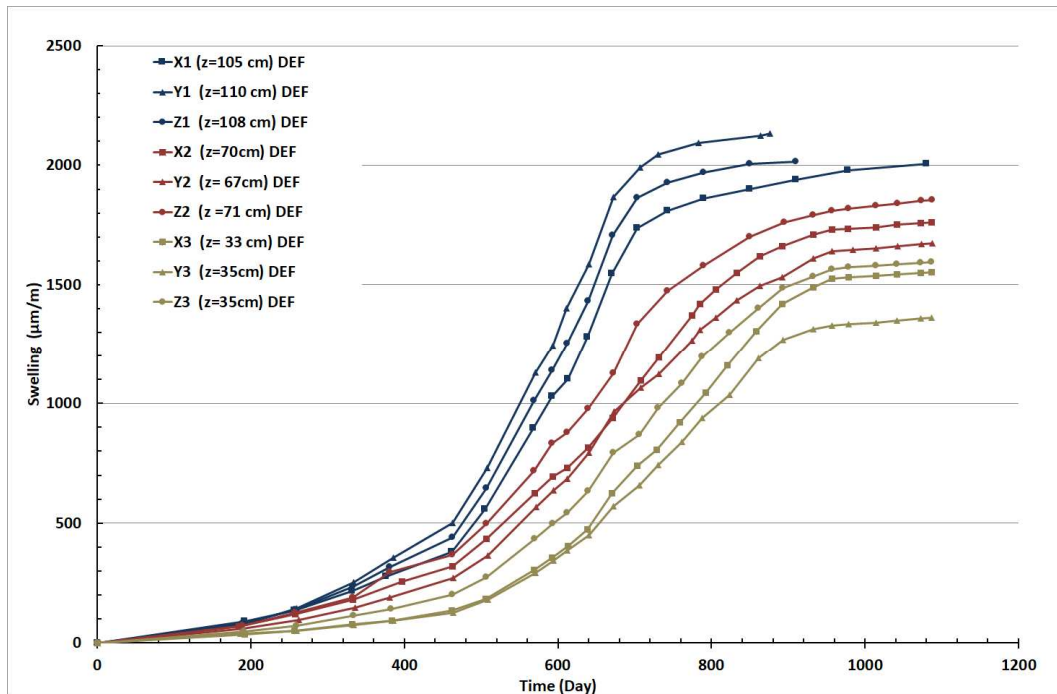Figure 5. The early-age heat profile of the mock-up

Figure 6. Strain measurements in the DEF mock-up

IDENTIFICATION OF THE MODEL COEFFICIENTS AND RESULTS

To determine the spatial distribution of the two variables in the mock-up structure, we used the temperature fields values measured by the thermo-sensors as a function of time. The spatial distribution of these temperatures in the mock-up was done by linear interpolation. Hence, we isolated the T_{max} (see figure 7-a) and calculated the Eu in the mock-up (see figure 7-b).

To define the parameters of the model, it is assumed that there exists β between 0.1 and 0.9 such that:

$$\varepsilon_{\infty DEF} = \beta \cdot \varepsilon_{\infty Tmax} + (1 - \beta) \cdot \varepsilon_{\infty Eu} \qquad (2)$$

Where :

$\varepsilon_{\infty DEF}$ is the final total expansion due to DEF,

$\varepsilon_{\infty Tmax}$ is the part of the final expansion due to T_{max}

$\varepsilon_{\infty Eu}$ is the part of the final expansion due to Eu

$$\varepsilon_{\infty Tmax} = 53.364T_{max}^3 - 12562T_{max}^2 + 984519T_{max} - 3E+07 \qquad (3)$$

$$\varepsilon_{\infty Eu} = 0{,}0206Eu^2 - 78{,}769Eu + 76683 \qquad (4)$$

β is determined by minimizing the difference between the calculated and measured strains in the vibrating wires. The value found is β = 0.5.

Table 2 presents the comparison between the final expansion found from the empirical model and the expansions measured experimentally.

Table 2. Comparison between the final expansion model and the experimental values

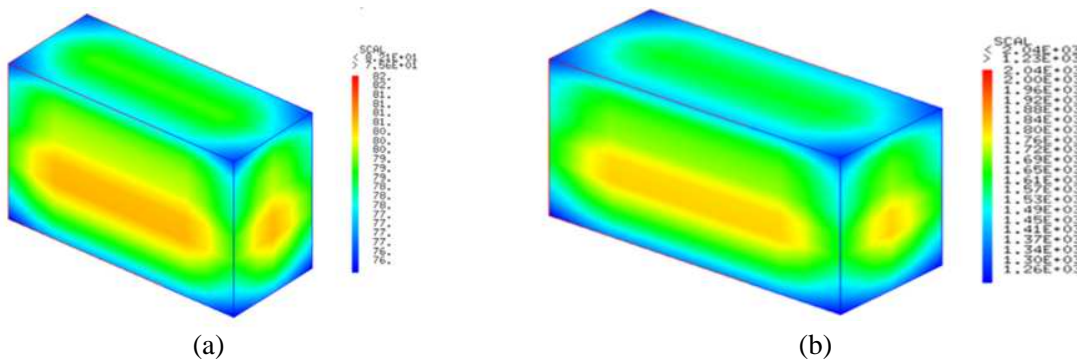| $\varepsilon_{\infty DEF-model}(\mu m/m)$	$\varepsilon_{\infty DEF-exp}(\mu m/m)$	Percentage error (%)
1871,56488	1987,4	6,19
2299,13177	2231	2,96
1977,01651	2031,3	2,75
1804,46823	1740	3,57
1657,90026	1650	0,48
1728,38537	1829,4	5,84
1663,50514	1537	7,60
1478,18913	1340,8	9,29
1472,41228	1578	7,17

Figure 7. (a) T_{max} field in the mock-up (b) Eu field the in the mock-up

A finite element model was implemented using the Cast3M software in order to evaluate the mechanical behavior of the mock-up and to assess the effect of the boundary conditions. The mesh represents the structure and its metallic support used as a lost formwork during the fabrication phase. The latter consists of a 6 mm thick metal plate welded to four I-profiles (IPE140) and two U-profiles (UPE140) steel beams connected by a 5 mm thick steel plate as depicted in figure 8.

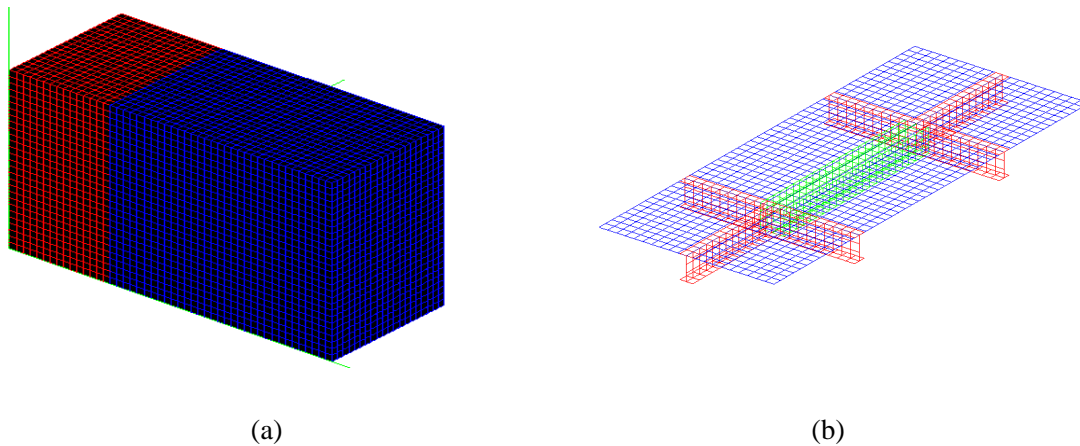(a)   (b)

Figure 8. (a) Mock-up mesh (b) Metallic support

The mechanical behavior of the concrete was simulated by using FEM (Finite Elements Method) and the Ottosen model with fictitious cracks based on the work of Dahlblom O & al. (1990). The swellings calculated by the semi-empirical law are introduced as a loading with imposed strain function of time. The dead weight of the mock-up and the pressure exerted by the water were considered in the modeling along with the expansion induced by the DEF.

The numerical simulations (figure 9) show that the metallic support on which the structure has been cast generates stress while the concrete expands. Hence, the upper part of the mock-up can expands freely whereas the lower part is hindered by the friction with the support. This boundary condition explains the different strain measurements obtained at different heights in the DEF mock-up (figure 6).
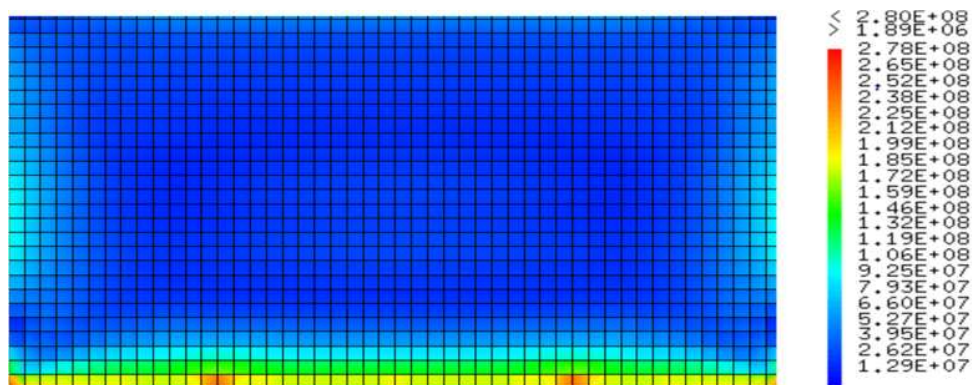

Figure 9. Stress fields in the XY plane

Figures 10 and 11 compare between the strains measured by optical fiber (Figure 10 a) or by vibrating wire extensometer with those obtained numerically using the FEM.

The results show that the developed semi-empirical model allows to estimate correctly the strains measured in the structure. A small disparity is found which is most probably due to the hypothesis formulated at the boundary conditions and the lack of data for the mock-up's edge expansion.
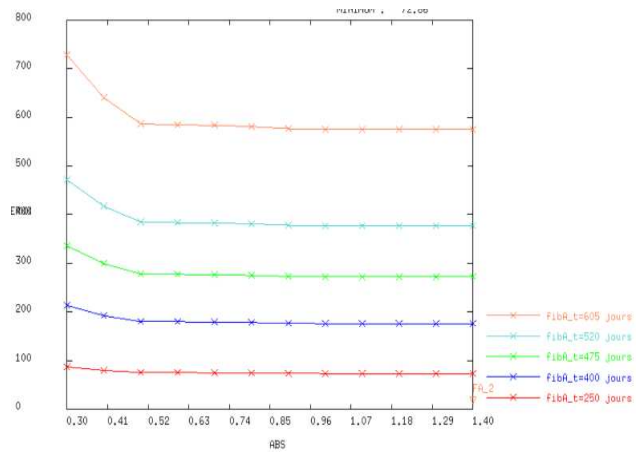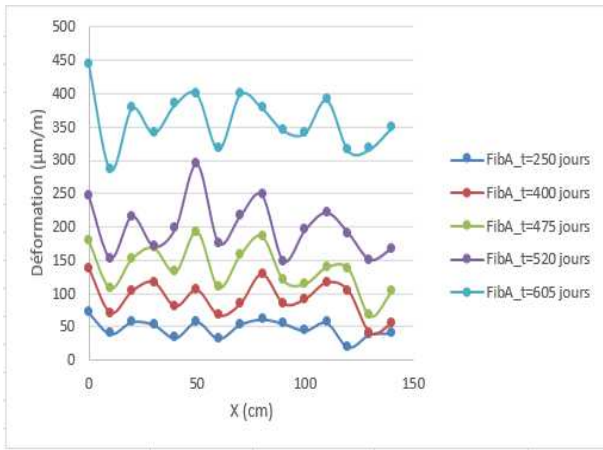
(a)   (b)

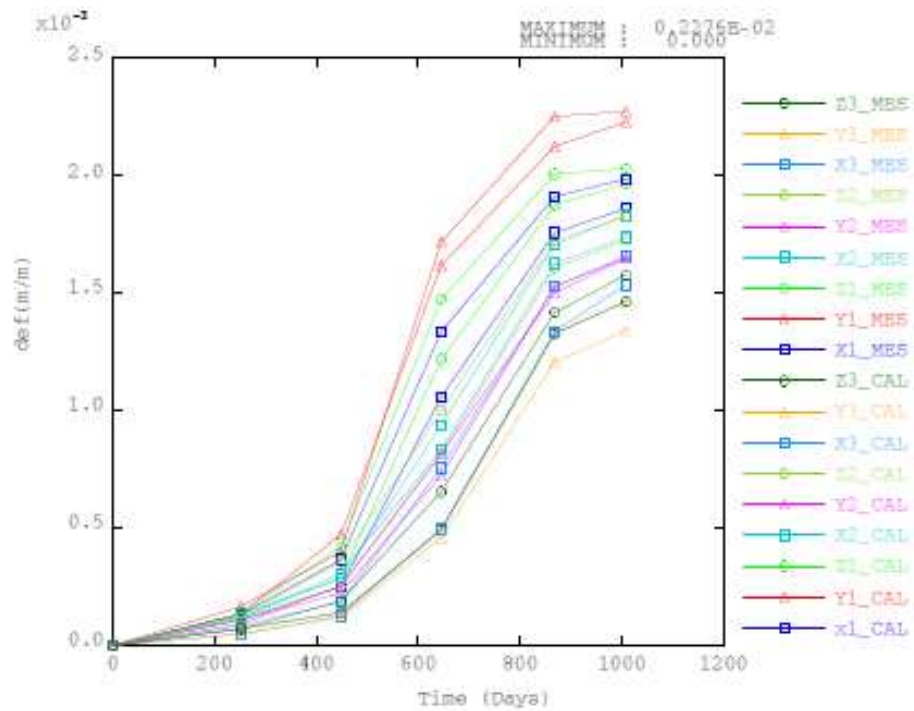Figure 10. (a) Strains measured by optical fiber (b) Strain calculated by FEM

Figure 11. Comparison between measured and calculated strains at vibrating wire

GENERALIZATION OF THE MODEL

Despite the good results obtained in the framework of this numerical application, the generalization of the model is necessary to be able to study the behavior of the structures affected by this pathology. In this test case, the fluctuation of the maximum temperature measured in the DEF mock-up used is relatively low: it varies from 79.10°C to 82.10°C leading to a variation of the associated effective thermal energy from 1624°C.hr to 2042°C.hr. Hence, the developed model is therefore restricted to this data range.

The analysis of different data sets available in the scientific literature, especially those obtained by Kchakech B. & al. (2015), offers the possibility to generalize the model. The before mentioned experimental program considers two different concrete mixes and is conducted on prismatic samples (11x11x22 cm^3). Two temperature plateau are used in this study: one at 70°C and another at 80°C. The heat treatment durations vary from one day to 28 days hence providing swelling results over a large range of effective thermal energies. Based on the results of this program, the authors proposed a master curve that gives the final swelling as a function of the effective thermal energy for a considered concrete mix (figure 12-a). By reverse analyzing these results and by correlating those to the maximum temperature T_{max} variable (figure 12-b) the master curve is transformed into a master surface linking the measured concrete swelling to the two variables of the developed semi-empirical model: the maximum temperature (T_{max}) and the effective thermal energy (Eu) (figure 13).
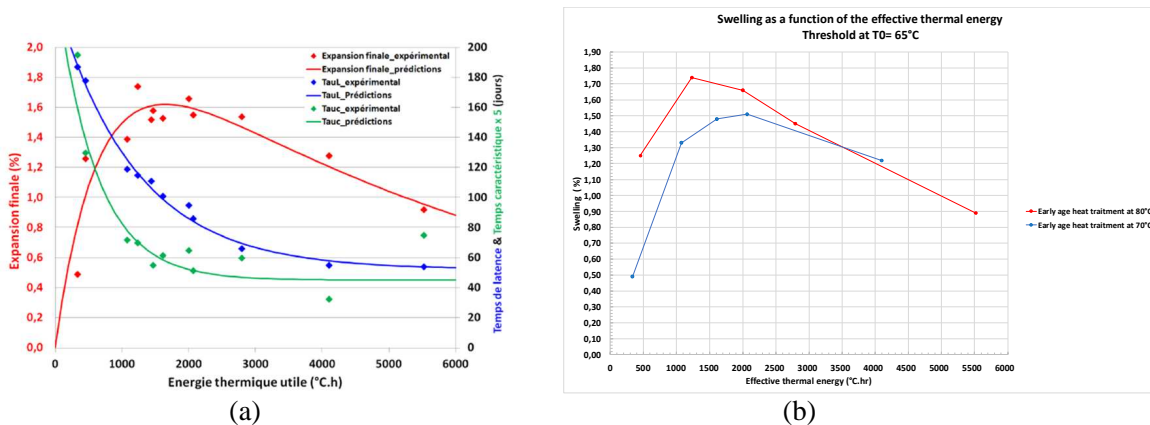

Figure 12. (a) Master curve provided by Kachakech B. & al. 2015 (b) With temperature effect
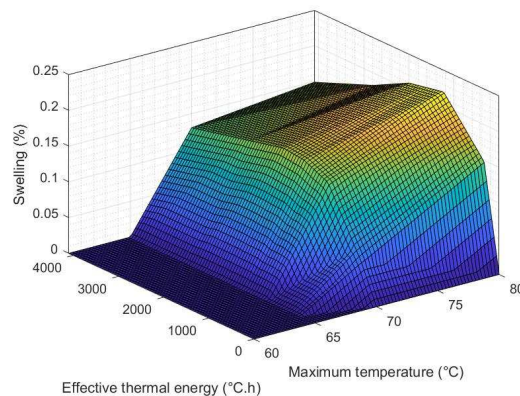

Figure 13. Master surface with two variables ($Tmax$ and Eu)

This master surface is the key to generalizing the model to various structural configurations present in the nuclear civil engineering framework.

CONCLUSION AND PERSPECTIVE

This research study presents the first step for the modeling of Delayed Ettringite Formation on a macroscopic scale and the possibility to evaluate its consequences on the mechanical behavior of the structure. It sheds light on the necessary data, the numerical models and the difficulties to carry out these simulations. For that purpose, a representative massive structure subject to DEF is selected as a test case and simulated using a detailed finite-element model (FEM).

The experimental and numerical investigations allowed the development of a master surface linking the two variables of the developed semi-empirical model (the maximum temperature (T_{max}) and the effective thermal energy(Eu)) with the final concrete swelling.

The semi-empirical model developed is relatively simple to use and allows the assessment of the stress-strain state of the considered structure by correlating it to a defined swelling function of the early age temperature profile and the concrete composition. The generalization of this approach to other cases is underway in the ODOBA project, Marquié & al. (2019).

REFERENCES

Dahlblom O., Ottosen N. S. (1990). *Smeared crack analysis using generalized fictitious crack model*, Journal of Engineering Mechanics, Volume 16.

Jabbour J. (2018). *Méthodes d'essais de vieillissement accéléré des bétons à l'échelle des ouvrages*, PhD, ENS Paris-Saclay, France.

Jabbour J., Darquennes A., Divet L., Bennacer R., Torrenti J. M., Nahas G. (2021). *New experimental approach to accelerate the development of internal swelling reactions (ISR) in massive concrete structures,* Construction and Building Materials. Volume 313.

Kchakech B., Martin R. P., Metalssi O., Toulemonde F. (2015). *Experimental Study of the Influence of the Temperature and Duration of Heat Treatments at an Early Age on the Risk of Concrete Expansion Associated with Delayed Ettringite Formation,* CONCREEP 10 Vienna, Austria. Page 455-465.

Marquié C., Dauzeres A., Richard B., Nahas G. (2019). *Concrete aging in containment building and deep geological disposal facilities: the ODOBA Project,* SMiRT-25 Charlotte, NC, USA, Division IX

Salgues M., Sellier A., Multon S., Bourdarot E., Grimal E. (2014). *DEF modelling based on thermodynamic equilibria and ionic transfers for structural analysis*. European Journal of Environmental and Civil Engineering. 18 (4). pp. 377–402.

Seignol J. F., Baghdadi N., Toulemonde F. (2009). *A macroscopic chemo-mechanical model aimed at re-assessment of delayed-ettringite-formation affected concrete structures.* 1st International conference on computational technologies in concrete structures CTCS'09, Jeju, Korea

Sellier A., Multon S. (2018). *Chemical modelling of Delayed Ettringite Formation for assessment of affected concrete structures* - Cement and Concrete Research, Volume 108, Pages 72-86