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MODELING OF THCM BEHAVIOR OF CONCRETE: FROM MULTIPHASIC HYDRATION OF COMPOSED BINDERS TO EARLY AGE MECHANICAL BEHAVIOR IN REINFORCED STRUCTURES.

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1 INTRODUCTION

Sustainable development, economic considerations and technologic reasons lead to adopt more and more often blended cement for massive concrete structures. Most of the time slags are used combined or not with silica fume or fly ash. Hydration processes of these mixes are more complex than for single clinker cement. In fact activation energy is different for additions and clinker, so, the hydration kinetic of each component depends on the temperature during hydration. So, in large structures, hydration products, and consequently mechanical behavior, may be different in the core (which is subjected to higher temperature) than near the edge due to the difference of temperature of this zone during hydration.

This paper focus on particularity of models developed in LMDC Toulouse to take into account this aspect in order to predict early age poro-mechanics behavior of concrete. The dependence of hydrates nature on the temperature needs to consider the consequences in terms of mechanical properties and shrinkage. On purpose, a homogenization model coupled with the percolation theory is clarified. Once the poro-mechanics characteristics are supplied by the homogenization model, a water retention curve model allows computing capillary pressure from early age until long term. These results are applied to a mechanical model adapted to the prediction of chemically evolving concrete behavior (including effect of creep) in order to assess the risk of cracking at early age under restraining effects.

2 PREDICTION OF HYDRATED PHASES IN COMPOSED BINDERS

The prediction of the different hydrated phases of paste is performed using a multiphasic model of composed binder hydration [1] recently adapted for slag blended binders [2]. It is based on the coupled resolution of hydration kinetic, water mass balance and heat balance equations. This coupled solving allows taking into account the respective effects of temperature and watering content on reaction kinetic of each phase of the binder (additions and clinker) (see [1] for more details) This method, unlike the Avrami model [3], enables chemical interaction between hydrates to be considered.

In the system of constitutive equations, the variables managed at each time step and each point of the 3D finite element mesh are:

- The degree of hydration of each anhydrous phase (clinker and additions)
- The temperature

- The water content
- The porosity
- The volume of the different hydrated phases produced by each anhydrous
- The volume of portlandite (produced by clinker and consumed by additions).

The four last variables are the ones used in the homogenization model presented in this paper to assess the variation of paste mechanical properties through binder hydration. The model is applied here to CEM I based pastes but can easily be extended to composed binder as the hydrated phases of this kind of binder are predicted by the multiphasic model [1,3].

The fractions taken into account at this stage are the ones that compose the paste: anhydrous cement, water, void, portlandite, aluminates (grouping together AFm, ettringite and hexahydrate), and C-S-H gel. The calculation of the volume fractions of the different phases at each date requires the molar volumes (Table 1) of hydrates and the chemical equations.

Adding the Adenot stoichiometric hypothesis (ettringite formation only if there is enough $\bar{S}$), and the conservation of chemical species we can obtain the volume fraction of each compound for a degree of hydration of 1. These quantities are expressed according to oxide quantities in the system of equation (1).

$$\frac{\partial C_{1.7}SH_{2.5}}{\partial\alpha} = S$$

$$\frac{\partial CH}{\partial\alpha} = C - 1.7S - \bar{S} - 3A$$

$$\text{Hyp}\,1:\begin{cases}\dfrac{\partial C_3AH_6}{\partial\alpha} = A - \bar{S} \geq 0\\[2mm] \dfrac{\partial C_4A\bar{S}H_{12}}{\partial\alpha} = \bar{S}\end{cases} \tag{1}$$

$$\text{Hyp}\,2:\begin{cases}\dfrac{\partial C_6A\bar{S}_3H_{32}}{\partial\alpha} = 0.5\bar{S} - 0.5A \geq 0\\[2mm] \dfrac{\partial C_4A\bar{S}H_{12}}{\partial\alpha} = 1.5A - 0.5\bar{S}\end{cases}$$

The C-S-H gel is sub-divided in two kinds of hydrates: high density areas (HD) and low density areas (LD). The amount of LD C-S-H is calculated using the ratio rLD of the mass of LD C-S-H to the total mass of C-S-H predicted by the hydration model. As précised in the equation (2), this ratio is expressed according to the water to cement ratio and to hydration degree α .

$$r_{LD} = (3.017 \times \frac{W}{C} \times \alpha) - (1.347 \times \alpha) + 0.538 \tag{2}$$

Finally, 7 fractions are used in the homogenization procedure to predict paste elastic properties (anhydrous cement, water, voids, portlandite, aluminates, LD C-S-H and HD C-S-H).

3 PERCOLATION FUNCTION FOR THE PREDICTION OF CONCRETE HYDROMECHANICAL PROPERTIES

Predicting the elastic properties of concrete requires three different levels of homogenization:

- Paste: The first stage is the prediction of the paste elastic modulus. Using the chemical composition of cement, the proportion of each type of hydrate (aluminates, C-S-H, portlandite) is evaluated. The principal originality of the proposed approach is the use of a percolation function applied to all solid phases (as detailed in §2.2).
- Mortar: Knowing the elastic properties of the paste, the Mori-Tanaka scheme is applied with the paste as matrix and the sand as elastic inclusions.
- Concrete: Finally the Mori-Tanaka scheme is applied using the mortar as matrix and the aggregates as elastic inclusions

3.1 An original percolation function for the homogenization at paste level

The homogenization at the paste level is performed using the self-consistent scheme, which proves to be the most suitable for this stage [4]. This scheme requires two implicit equations (3) and (4) to be solved using a numerical Newton-Raphson method.

$$k_{\text{hom}}^{est} = \frac{\sum_{r=1}^{n} f_r k_r (1+\alpha_0^{est}(\frac{k_r}{k_0}-1))^{-1}}{\sum_{r=1}^{n} f_r (1+\alpha_0^{est}(\frac{k_r}{k_0}-1))^{-1}}$$

$$\mu_{\text{hom}}^{est} = \frac{\sum_{r=1}^{n} f_r \mu_r (1+\beta_0^{est}(\frac{\mu_r}{\mu_0}-1))^{-1}}{\sum_{r=1}^{n} f_r (1+\beta_0^{est}(\frac{\mu_r}{\mu_0}-1))^{-1}} \quad (3)$$

Where:

$$\alpha_0^{est} = \frac{3k_{\text{hom}}^{est}}{3k_{\text{hom}}^{est} + 4\mu_{\text{hom}}^{est}}$$

$$\beta_0^{est} = \frac{6(k_{\text{hom}}^{est} + 2\mu_{\text{hom}}^{est})}{5(3k_{\text{hom}}^{est} + 4\mu_{\text{hom}}^{est})} \quad (4)$$

The mechanical properties of each phase that compose a CEM I based paste are summarized in [4] or [5] and recalled in Table 2.

Table 1: Mechanical properties of constituents

	K (GPa)	μ (GPa)
Water	2.2 (*undrained conditions*)	0
Void	0	0
Portlandite	34.2	15.32
Aluminates	33.33	15.38
C-S-H LD	12.82	8.06
C-S-H HD	19.23	12.1
Anhydrous cement	112.5	51.92

Dynamic ([6] and [7]) and static ([8]) measurements give a modulus equal to zero before setting. The overvaluation of the modulus is a consequence of the hypothesis that all the solid phases are cohesive. The solid percolation thus leads to increased mechanical performance. To reproduce the behavior of the material at early age, it is necessary to consider a gradual change of the cohesion and to use the notion of "mechanical percolation". Here, we propose to define a percolating function which takes a percolated fraction into consideration among the total fraction of hydrates. The entire solid fraction could transmit compressive forces but unpercolated hydrates cannot transmit shear stress. For this reason, we suggest setting the shear modulus of the unpercolated phase of hydrate to zero and maintaining the bulk modulus at its normal value (the same value for the percolated and unpercolated phases).

As the proposed approach is based on probabilistic considerations (percolation if a cohesive solid phase is in contact with a solid phase), a Weibull-type law is used:

$$P_P = \left(\frac{\alpha}{\alpha_{cr}} \times \frac{1}{1-\phi_g}\right)^{1/m} \leq 1 \quad (5)$$

Where: αcr is a parameter named the critical degree of hydration

m is a fitting parameter

ϕ_g is the volume fraction of aggregate in the material (paste, mortar or concrete)

When the degree of hydration (α) reaches the critical value (αcr), the function is equal to 1 regardless of the aggregate fraction (ϕ_g) and all the solid phases can transmit shear stress (they are all on the percolation path). m is the parameter that influences the slope of the percolation function curve between 0 and αcr.

If α is smaller than αcr, the percolation probability depends on the aggregate fraction ϕ_g because of "percolation bridges" generated by aggregates. These values enable us to fit all the values of elastic modulus measured at the early age and for cement pastes of various W/C ratios, mortar and concrete.

The percolation probability tends towards 1 faster for concrete than for cement paste and mortar even if the W/C ratio is the same.

Because of this method, the solid phases are split into two parts (percolated and non-percolated) and five more phases are defined with the same bulk modulus but a zero shear modulus (non-percolated phases). **Figure 1** presents the results of the homogenization method including the percolation function concerning the evolution of modulus on cement pastes cast with different W/C ratios (experimental results of dynamic modulus from Boumiz [6]). This figure shows that, through the use of the percolation function, the model is able to reproduce the evolution of the elastic modulus even at early age and for W/C ratios different from 0.5.

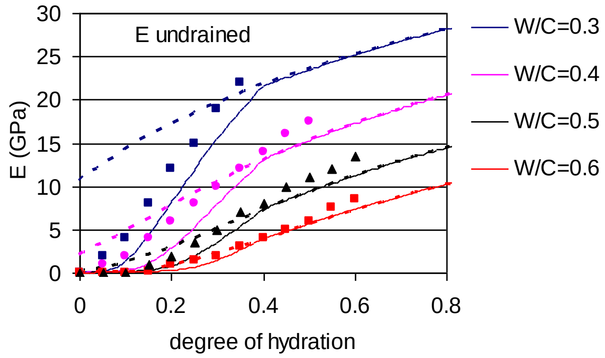

Figure 1: Evolution of undrained Young's modulus (αcr =0.4 m=5) compared with experimental values from [6] (dotted line is the self-consistent scheme without Percolation function).

3.2 Mortar and concrete homogenization levels

The Mori-Tanaka scheme requires the fractions and mechanical properties of inclusions, and the mechanical properties of the matrix. The matrix properties are provided by the previous homogenization level. First for the mortar, the matrix is the cement paste with the properties previously calculated by the self-consistent scheme and the function of percolation.

For concrete, the matrix to consider is the mortar and the inclusions are the aggregates for which the properties are evaluated according to their mineral nature [4].

Figure 2 illustrated the results obtained on paste, mortar and concrete with the same W/C ratio in order to test the capability of the model to reproduce the evolution of mechanical properties at each homogenization level.

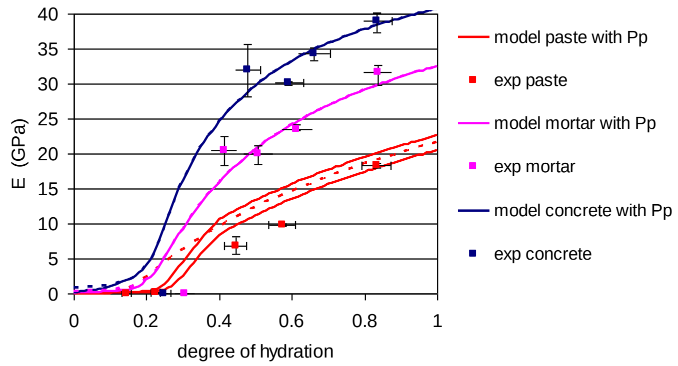

Figure 2: Young modulus evolution for paste, mortar and concrete.

3.3 Prediction of hydro mechanical properties

The realism of the bulk modulus assessment obtained by the previous homogenization stages is of first importance to assess realistically a Biot coefficient. To obtain the Biot coefficient (defined by eq 6), homogenization is first done once with the real fraction of solid and the void but without the free water, in order to obtain the drained bulk modulus Kd; and secondly without the void to assess the skeleton bulk modulus Ks. The Biot coefficient b is deduced classically from these two homogenization calculi.

$$b = 1 - k_d / k_s \tag{6}$$

Where kd and ks are the drained bulk modulus and the bulk modulus of the solid phase.

5 INDUCED EVOLUTION LAWS OF MECHANICAL PROPERTIES AT EARLY AGE

In the case of a 3D finite element modeling of massive structures, the variation of the elastic characteristics according to hydration development is usually modeled by equation (7). These laws were inspired by the Young's modulus variation law proposed by De Schutter [9].

$$E(\alpha) = E_\infty \left\langle \frac{\alpha - \alpha_s}{1 - \alpha_s} \right\rangle^{P_E} \tag{7}$$

Where: - E_∞ is the theoretical elastic modulus of the completely hydrated concrete.

- α_s is the hydration degree that characterizes the percolation threshold

- $\langle X \rangle$ is the positive part of X (X if X>0, 0 elsewhere).

The variation of the creep parameters is similar to that of the instantaneous elastic parameter. The parameters related to the creep model are thus proportional to the instantaneous elastic modulus. This assumption has been previously proposed in De Shutter's works [9], and implies that the characteristic time of creep is independent of the hydration degree.

But the fitting of these evolution laws requires numerous mechanical (and hydro mechanical) tests especially at very early age which are not so easy to do. We propose thus, to use the model of prediction of mechanical properties presented here to replace experimental measurements in the fitting.

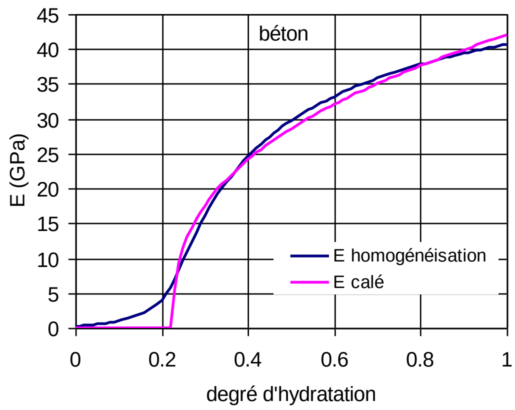

Figure 3: Fitting of Young's modulus law on homogenization results

The results of the percolation based homogenization model shows that, under drained conditions (which is the case in static mechanical tests), the Poisson's ratio does not significantly evaluate (see illustration in next figure). So the evolution of this characteristic is neglected.

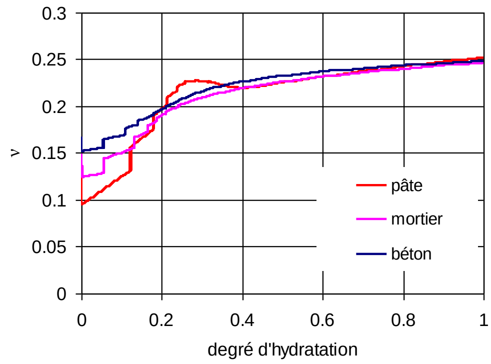

Figure 4: Homogenization results of Poisson's ratio according to hydration degree

The Biot coefficient used to predict the autogenous shrinkage of concrete is also modeled using a law as De Schutter's laws and the parameter are fitted on homogenization results as presented below.

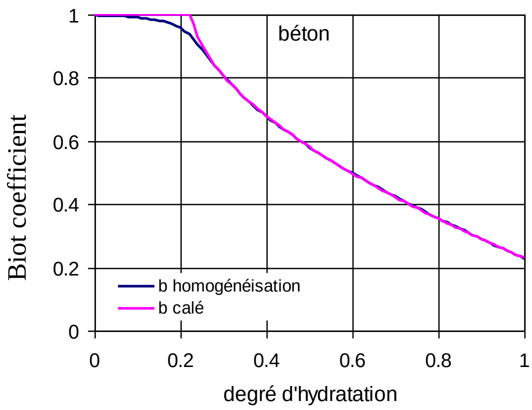

Figure 5: Fitting of Biot coefficient law on homogenization results

6 APPLICATION TO A MASSIVE REINFORCED STRUCTURE

The proposed test is named RG8 and is part of the French national project CEOS.fr. This project deals with the study of the cracking in special reinforced concrete structures under various conditions.

This test more particularly deals with the cracking occurring at early age under THM loading and its influence on the mechanical behavior of the structure.

It is a massive structure with a special form chosen to use two metallic struts in order to restrain the contraction of the central part of the structure and consequently provoke cracking at early age.

Figure 6: Restrained shrinkage specimen

The concrete used in the RG structure is a C50/60 concrete casted with a CEM I 52.5N cement. The formulation is given in the following table.

Table 2: Formulation of CEOS concrete

	Quantities (kg/m3)
CEM I 52,5N CE CP2 NF	400
Sand 0/4 GSM LGP	785
Gravel 4/20 GSM LGP	980
Superplastifiant Axim 4019	5,4
Total water	185

The structure is subjected to a THM loading (temperature elevation in the isolated structure). It is placed in its environment and the strains of the structure are globally restrained by two struts.

During the first 2 days after casting, the structure is isolated. Then the isolation and the formwork are removed and the structure is conserved during 2 months in the environment.

The test process was the following:

- 07 April 2010, 10:30: beginning of the casting (Tini concrete = 17°C)

- 07 April 2010, 12:00: end of the casting

- 09 April 2010, 9:00: prestressing of the “heads” of the structure

- 09 April 2010, 10:00: removing of the isolation and the formwork on all the faces

All specimens were fully instrumented, externally and internally (9 points for internal temperature measurement, 24 vibrating cord sensors for local internal or external deformation measurement, 3 internal optical fiber sensors and 12 electrical strain gauges placed on reinforcement bars).

The external temperature, the solar radiation and the exposition of the specimen were also measured during the test.

The structure has been modeled using a non-linear mechanical model coupling creep and damage [10]. This model is adapted to the prediction of early age behavior using an adapted numerical formulation [11] and the evolution laws fitted on homogenization results. All the reinforcement was modeled as illustrated in **Figure 7** and the steel-concrete bond was modeled and is expressed according to hydration development.

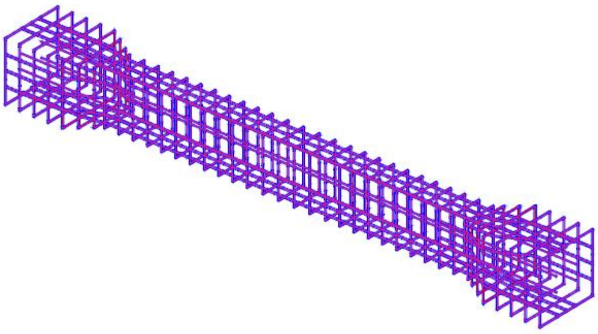

Figure 7: Mesh of the reinforcement

The results obtained with the numerical modeling of this THM test is successfully compared with experimental results in terms of concrete and steel strains (**Figure 8** and **Figure 9**) and in terms of forces induced in the struts (**Figure 10**).

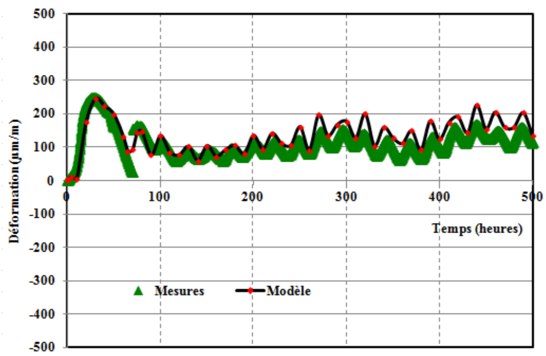

Figure 8: Comparison of concrete strain measurements with numerical results (at core)

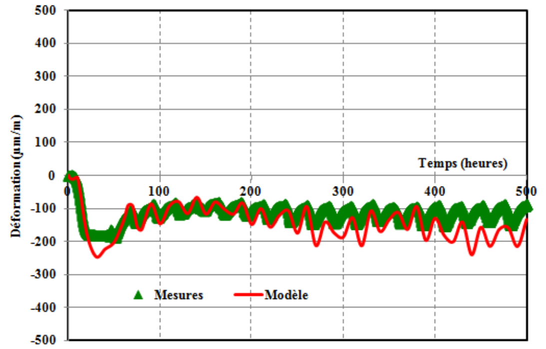

Figure 9: Comparison of steel strain measurements with numerical results (central section)

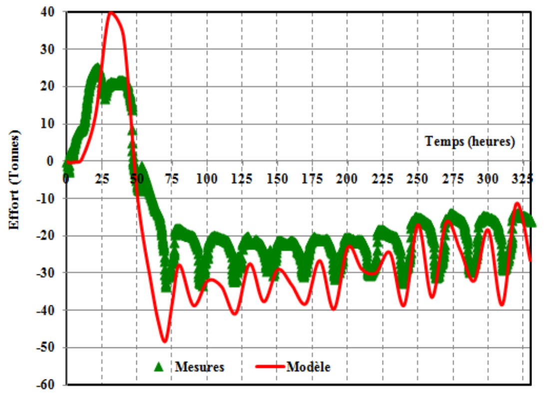

Figure 10: Comparison of strut force measurements with numerical results

The crack pattern at the end of the THM test is also globally well reproduced (**Figure 11**) and the first cracking is numerically obtained 70 hours after casting which correspond to the in situ observations.

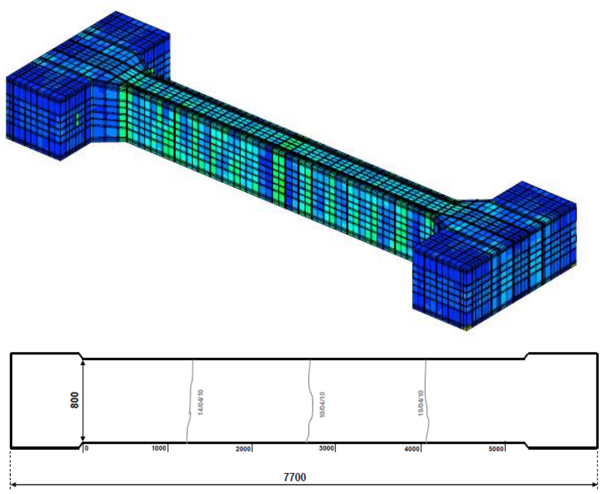

Figure 11: Comparison of crack pattern with numerical results

Concerning the crack width, the order of magnitude is respected but it is underestimated (about 50 microns for numerical results and about 100 observed in situ for the central crack).

12 CONCLUSIONS

This paper presents an original approach to predicting the evolution of elastic properties of paste, mortar and/or concrete during hydration. The proposed approach is based on three homogenization levels, as is usually done for cementitious materials, but with the use of a new percolation function for the paste.

At the first stage of homogenization, the elastic properties of the paste are determined using a self-consistent scheme. This homogenization method is completed with the use of a mechanical percolation law based on probabilistic considerations. The solid phases of the paste (anhydrous and all hydrates) are thus subdivided into percolated and unpercolated phases. Another originality of the proposed model is that the unpercolated phases are not ignored, as is usually the case, but only the shear modulus is reduced to zero (bulk modulus unchanged). It can be seen in this paper that this approach allows us to reproduce the evolution of the Young’s modulus at early age for pastes with different W/C ratios.

At the second stage of homogenization, the Mori-Tanaka scheme is used with the paste as the matrix and the sand as elastic inclusions. For the last level, the same is done with mortar as the matrix and aggregates as inclusions. The results of elastic properties prediction obtained at these two stages are validated on the three levels (paste, mortar, concrete).

The micromechanical model is applied to fit evolution laws relating mechanical properties to hydration degree in order to a numerical implementation. This allows successfully modeling the early age behavior of massive reinforced concrete structures. Indeed, strains, forces and crack pattern are globally well reproduced.

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