Chemo-mechanical coupling model of off-shore concrete structures

M. El-Khoury[1, 2], F. Grondin[1], E. Roziere[1], R. Cortas[3], F. Hage Chehade[2]

[1] *Institut de Recherche en Génie Civil et Mécanique (GeM), UMR 6183, Centrale Nantes – Université de Nantes - CNRS, 1 rue de la Noë 44321 Nantes, France.*

[2] *Centre de Modélisation, Ecole Doctorale des Sciences et Technologie, Université Libanaise, Beyrouth, Liban.*

[3] *Centre de Recherches Scientifiques en Ingénierie (CRSI), Université Libanaise, Beyrouth, Liban.*

SUMMARY Seawater represents a complex phenomenon due to the presence of multiple ions. Previous researches aimed to estimate the resistance losses due to sulphate and chloride attacks based on probabilistic approaches. Few studies have focused on the complex chemo-mechanical modeling by coupling all the ions present in seawater and in concrete. In this study, the model proposed is based on the coupling between two codes CemPP- for the microstructure generation of the cementitious material, the evolution of the hydration and chemical reactions - and Cast3M - for the mechanical calculations and damage modeling. Results highlight the importance of considering each effect of cement paste's ion reacting with seawater and their role on the overall mechanical behaviour of the structure affected by the chemical phases present at equilibrium.

Keywords Micromechanical modeling, degradation, seawater, cement paste

I. INTRODUCTION

The offshore engineering sector is growing rapidly, supporting the use of concrete in the marine environment. In contact with seawater, concrete undergoes a degradation caused by the diffusion of aggressive ions through its porosity and their reaction with the cementitious matrix, leading to a decrease in mechanical strength. This is accompanied by the loss of cement particles and the pollution of the marine environment. To protect marine structures and reduce their degradation, it is crucial to clearly define the behaviour laws of concrete in marine environment by coupling the mechanical and chemical degradation to the hydration process. This coupling presents not only a challenge in the durability field of cementitious materials and the protection of the environment, but also significant economic and social impacts.

The experimental investigation of the micro-mechanisms associated with degradation is difficult because its evolution in real time should be tracked for long periods. Multi-scale modeling, starting from the microscopic scale, seems relevant (Rhardane, 2018). Therefore, a micromechanical model has been developed coupling the mechanical and chemical effects due to seawater attack. A code, named CemPP, based on the CEMHYD3D software from NIST (Hilloulin et al., 2016), simulates the coupling between hydration and chemical reactions at the cement paste scale. An adaptation is proposed here for the seawater problematic: brucite and thaumasite have been added. Then, the obtained chemically degraded microstructure is generated in the finite element code Cast3M to simulate the mechanical damage behaviour, loss or gain of the elastic properties subsequently defining the mechanical resistance of the structure.

II. PRESENTATION OF THE COUPLING BETWEEN HYDRATION AND SEAWATER ATTACK MODEL

The diversity of salts in seawater creates a competition between two opposing phenomena : the first leads to volumetric and expansive precipitation of ettringite and the second tends to close the surface porosity, hence limiting ionic exchanges by creating a protective surface in the case where the aluminate content is low (Guillon, 2004). An experimental study conducted by (De Weerdt et al., 2014) on ordinary concrete exposed for 10 years in a tidal zone of the Trondheim fjord shows that the seawater attack is a layered attack defined by the diffusion profiles. Seawater chemical action should be described as one of many reactions taking place simultaneously (Eglinton, 1998). Moreover, the chemical reaction time is short compared to that of diffusion; the attack of offshore concrete can then be schematized in several layers. Each zone represents ionic/chemical attack and product formation and dissolution (Table 1). To understand the effect of each phase formed / transformed on the mechanical behaviour of the structure, each layer is modeled separately as a material under hydration and one chemical reaction takes place in each layer. The simulation of the hydration-seawater attack coupling process was carried out in 3D using the CemPP code for a cement CEMI 52.5 N having 60% of C3S, 16.3% of C2S, 7.7% of C3A, 10.5% of C4AF and a fineness of 400 m^2/Kg, at the age of 72 hours. CemPP code creates a 3D microstructure of a cement paste of size 100μm^3 defined by voxels of 1μm^3. The chemical reaction time has been assumed to be very fast and the size of the microstructure being very small. A total replacement of the cement paste' phases by their reaction products is adopted as shown in table 1 (The reactor phase presented in blank is consumed and replaced by the product phase presented in hatch).

TABLE 1. Phases replacements used in CemPP to generate the chemically degraded microstructures.

	Phases \ Layer	I	II	III	IV	V	VI	Hydrated
Reactors	Calcium hydroxide			■		■	■	■
	CSH	■	■		■	■	■	■
	Hydrated C3A	■	■	■	■			■
Products	Brucite	■						
	Calcite		■					
	Thaumasite			■				
	Gypsum				■			
	Ettringite					■		
	Friedel Salt						■	

III. MECHANICAL DAMAGE MODEL

2D chemically modified microstructures, extracted from the 3D microstructures obtained before, are meshed in the finite element code Cast3M. Mechanical properties (Young's modulus, Poisson's ratio, strength, fracture energy) of all cement paste's phases are considered intrinsic for the following damage model based on the work of (Rhardane, 2018) where these values are summarized. The damage model is based on a micro-plane approach (Fichant et al., 1997; Fichant et al., 1999). A uniaxial load is applied as incremental horizontal displacements on one of the sides of the 2D section while the opposite side is fixed. The stress field (σ) and the scalar damage value (D) are evaluated by the following relations:

$$\sigma = (1 - D)C^0 : \varepsilon^e \quad (1)$$

$$\dot{D} = \frac{\kappa_0(1 + B_T\varepsilon_{eq})}{\varepsilon_{eq}^2}\exp[-B_T(\varepsilon_{eq} - \kappa_0)] \quad (2)$$

Where C^0 is the initial stiffness tensor, ε_{eq} the equivalent strain (= $(\langle\varepsilon^e\rangle_+ : \langle\varepsilon^e\rangle_+)^{1/2}$), κ_0 the damage threshold and B_T a slope parameter for the strain-stress curve. This approach allows coupling chemical and mechanical effects without introducing a chemo-mechanical coupling parameter that needs calibration tests in the behaviour law as done in macroscopic models. Since this model works at the microscopic scale, phenomena are distinguished and damage is evaluated according to the phase's mechanical properties and volume fractions variations reacting with seawater.

IV. RESULTS AND DISCUSSION

The objective of the study is to give at first an evaluation of effective residual elastic properties of cement pastes attacked by seawater in order to give an elastic behaviour law used at the upper scales (mortar and concrete). Figure 1 presents a 2D section of each layer extracted from the 3D microstructures generated in CemPP at the age of 28 days. The color variation between the hydrated layer and the six attacked layers highlights the phase's changes in the microstructure. Figure 2 shows elastic parameters (Young's modulus and Poisson's ratio) variations as a function of the specimen's age. We can note that layer III, which no longer contains CSH, registers the smallest Young's modulus and the largest Poisson's ratio subsequently leading to a significant drop in the layer's resistance compared to the others. It can also be concluded that chemical attack reduces the Poisson's ratio of all layers. The formation of calcite increases the rigidity of the area and closes the porosity on the surface; which reduces ionic exchanges. The brucite rich layer acts as a protective layer, its Young's modulus remains similar to that of the intact layer, but its Poisson's ratio is lower than that of the hydrated layer.

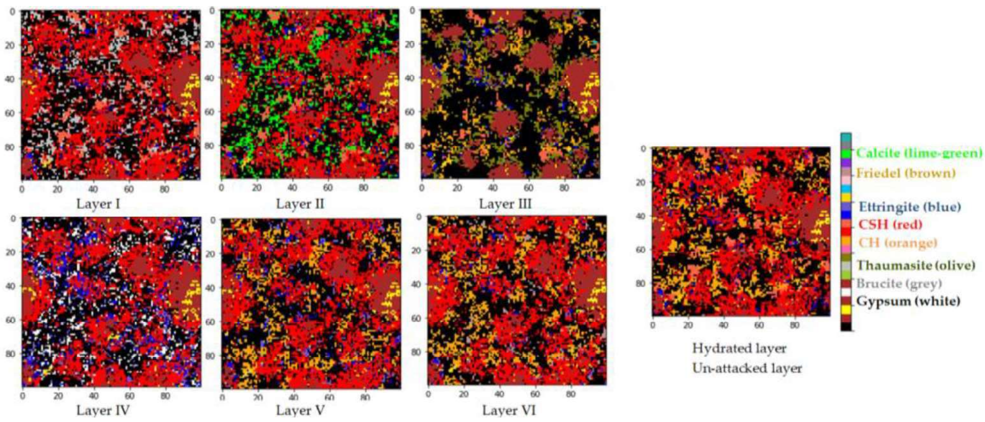

FIGURE 1. 2D section of each layer extracted from the 3D microstructures generated at the age of 28 days

Ettringite formation, described as expansive, and the chloride ions action leading to Friedel's salt formation maintain the Young's modulus similar to that of the hydrated layer. But the gypsum formation increases it.

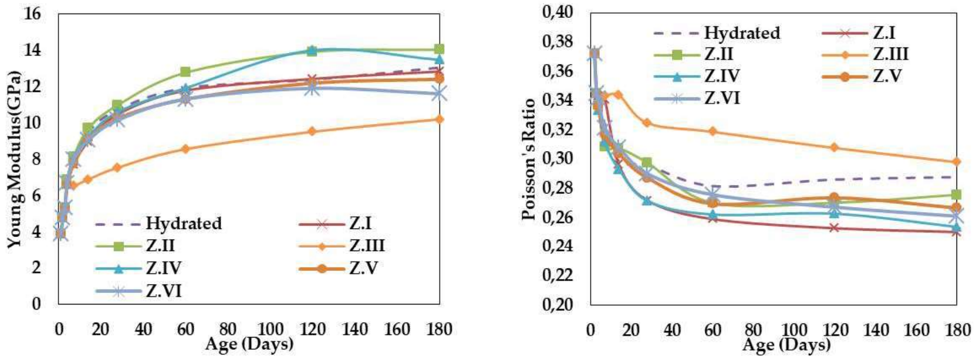

Figure 2. **(a)Young's modulus and (b) Poisson coefficient variation**

VI. CONCLUSIONS AND PERSPECTIVES

A new model has been developed for the analysis of the behaviour of cementitious materials in seawater. The first approach presented in this work aims to determine the effective elastic properties of cement pastes after the sea attack. It will be used in a next work at the mortar and concrete scales as input data for the cement paste's matrix. The results show that the overall behaviour of a structure is influenced by the chemically modified phases and it is thus possible to define the maximum permissible load as a function of the structure's age and therefore of its chemical degradation level. Consequently, this methodology highlights the importance of examining all the ions present in seawater since each ion participates in either a gain or a loss of elastic properties, affecting the overall behaviour of the offshore structures.

REFERENCES

Eglinton, M. (1998) 'Resistance of concrete to destructive agencies', in Hewlett, P. C. (ed.) *Lea's Chemistry of Cement and Concrete - Fourth Edition*. Elsevier Ltd., 299–342.

Fichant, S., La Borderie, C. and Pijaudier-cabot, G. (1999) 'Isotropic and anisotropic descriptions of damage in concrete structures', *Mechanics of cohesive frictional materials*, 4, 339–359.

Fichant, S., Pijaudier-cabot, G. and La Borderie, C. (1997) 'Continuum damage modelling: Approximation of crack induced anisotropy', *Mechanics Research Communications*, 24(2), 109–114.

Guillon, E. (2004) *Durabilité des matériaux cimentaires: modélisation de l'influence des équilibres physico-chimiques sur la microstructure et les propriétés mécaniques résiduelles*. ENS Cachan.

Hilloulin, B. *et al.* (2016) 'Mechanical regains due to self-healing in cementitious materials: Experimental measurements and micro-mechanical model', *Cement and Concrete Research*,80,21–32.

Rhardane, A. (2018) *Élaboration d'une approche micromécanique pour modéliser l'endommagement des matériaux cimentaires sous fluage et cycles de gel-dégel*. Centrale Nantes.

De Weerdt, K., Justnes, H. and Geiker, M. R. (2014) 'Changes in the phase assemblage of concrete exposed to sea water', *Cement and Concrete Composites*, 47, 53–63.