Proposal of post-doc subject (CEA DPC/SECR/LECBA)
Modelling and simulation of the long-term behavior of cementitious materials with low-clinker content

Context

The objective of the European project EnDurCrete is to develop and study sustainable and low cost concrete formulations for enhancing the service life and durability of reinforced concrete structures subjected to severe loading conditions over a long period. The concept is based on the use of low clinker cements, high-value industrial by-products, new nanoparticles and hybrid systems. Significant improvements of performance are sought mainly on mechanical and durability properties, but also regarding the self-healing and self-control capabilities of materials. As part of this project, the CEA/LECBA is responsible for studying and modeling the mechanical behavior and diffusive properties of new materials based on CEM II and CEM VI cements during their hydration and at long term. Furthermore, numerical simulations on representative elementary volumes (REVs) and on structural elements will allow validating the models and investigating the effects of degradation due in particular to carbonation.

Program

Concerning the analytical part, it is envisaged to implement upscaling methods similarly to previous works (see e.g. [1], [2]) to obtain macroscopic estimations of the physical parameters (elastic moduli and diffusion coefficient) at the scale of the cement paste, mortar and concrete. The estimations are based on a simplified description of the microstructure of the materials associated with a precise characterization of the different phases at the scale considered (from about one hundred micrometers for cement pastes to about ten centimeters for concrete), then on the application of effective medium homogenization schemes. The models developed will also rely on the calculations of mineralogical assemblages obtained during the hydration and degradation of the various cements at the University of Science and Technology of Norway (NTNU), as well as on the experimental data of characterization of the mechanical and diffusive properties collected during the project. Particular attention will be paid to investigating and highlighting the main advantages of the new materials with regard to the resistance to chemical attacks (decalcification, carbonation) and (micro)cracking.

In a second step, 3D numerical simulations will be performed at the mesoscopic scale on REV mortars and concretes in order to validate the analytical models. The 3D samples will be built using specific tools integrated in the Salome CAD code (www.salome-platform.org), allowing users to randomly distribute particles with defined shape (spheres, polyhedrons) and size into a cube and generating the corresponding meshes [3], [4]. They can also be obtained experimentally by tomography. These simulations will in particular make it possible to study the effects of the shape and the spatial distribution of the inclusions on the macroscopic mechanical and diffusive properties, and to investigate the aspects related to the initiation and the propagation of the microcracking. In addition, the behavior of materials exposed to atmospheric carbonation will be analyzed. Simulations will thus be performed first in 1D with a simplified model on a supposedly homogeneous material to determine the overall response of a concrete sample subjected to the exposure of CO_2-enriched air at different relative humidities. Then, the behavior of representative 3D samples of a concrete structure exposed to the atmosphere and comprising aggregates and steel reinforcements, will also be simulated. In this case the kinetics of carbonation will be analyzed and their impact on the formation of expansive corrosion products and the initiation of microcracking in the vicinity of the reinforcement will be modeled in a simplified way. Again, the experimental data gathered in the project will be used to identify mechanical and diffusive parameters and to validate the models.

The post-doctorate position, which is funded over two years, takes part in the European Endurcrete project. As such, the candidate will participate in the various meetings and exchanges planned with the other 15 partners.

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References

[1] B. Bary and S. Bejaoui, "Assessment of diffusive and mechanical properties of hardened cement pastes using a multi-coated sphere assemblage model," *Cement and Concrete Research*, vol. 36, no. 2, pp. 245–258, Feb. 2006.
[2] O. Bernard, F. J. Ulm, and E. Lemarchand, "A multiscale micromechanics-hydration model for the early-age elastic properties of cement-based materials," *Cement and Concrete Research*, vol. 33, no. 9, pp. 1293–1309, 2003.
[3] B. Bary, C. Bourcier, and T. Helfer, "Analytical and 3D numerical analysis of the thermoviscoelastic behavior of concrete-like materials including interfaces," *Advances in Engineering Software*, vol. 112, pp. 16–30, 2017.
[4] T. T. H. Nguyen, B. Bary, and T. de Larrard, "Coupled carbonation-rust formation-damage modeling and simulation of steel corrosion in 3D mesoscale reinforced concrete," *Cement and Concrete Research*, vol. 74, pp. 95–107, Aug. 2015.