Multiscale study of the temperature-dependent behavior of Calcium-Silicate-Hydrate

Supervisors:

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Keywords

Cement Based Materials — High-temperature response — Thermo-Hydro-Mechanical couplings — Molecular modelling/simulation — Upscaling approaches

Project Description

The improvement of concrete structures durability if of key importance to reduce to environmental footprint of the global cement production. The durability of concrete structures is closely related to the response of cement-based materials (CBM) to coupled effects of mechanical, thermal, hydric and chemical solicitations. Understanding the multi-physics mechanisms governing the behavior of CBM is crucial to predict and control the response of concrete structures over their service lifetime. Particularly, high-temperature exposure, typical of construction fires and nuclear power plants, alters the microstructure of cement paste phases and leads to the degradation of the macroscopic physical and mechanical properties. At the microscale, cement paste damage at elevated temperature is attributed to dehydration of primary cement hydration products, mainly the calcium silicate hydrates (C-S-H) gel that plays a major role in the overall strength of CBM. The thermally-induced dehydration at higher ranges of temperature involves the loss of chemically bound water in the nanopores of C-S-H. However, the underlying mechanisms of C-S-H thermal-induced damage upon heating remain poorly understood due to the complex hierarchical porous structure of C-S-H.

In a recent project of the 3SR team work, a numerical thermo-hydro-mechanical model was developed for concrete at high temperature based on phenomenological laws and neutron tomography observations [1]. This model was further improved by considering the desorption isotherms evolution at moderate temperature [2]. Yet, as the pore size

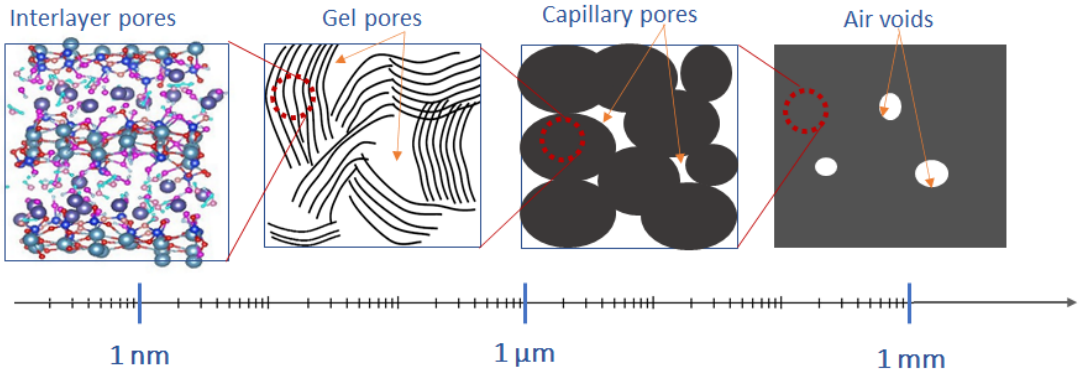

Figure 1: *Multiscale porous structure of cement paste*

approaches the nanometer scale, the liquid-vapor phase transition is strongly affected by the ultra-confinement of water near the solid surface. Therefore, the description of sorption/desorption isotherms evolution with respect to temperature, suffers from the limits of continuum approaches that consider much larger scales than that of C-S-H grains and nanopores [3]. A numerical mesoscale model of thermal dehydration, in which the physical behavior of chemically bound water in structural interlayers is handled differently than water in gel and capillary free water, is still lacking. In that context, combining molecular modeling and continuum approaches is necessary for a complete description of water behavior that is compatible with the intrinsic multiscale hierarchical nature of the C-S-H gel.

Driven by the goal of understanding the mechanisms of thermal-induced damage in CBM, we aim to develop a multiscale model of C-S-H informed by the physics of dehydration and structural features at small-scales. To characterize the effect of high temperature on the nanostructure of C-S-H, molecular modeling/simulations will be used to describe the nanostructure changes and water behavior in the confined spaces [4]. The effect of chemical composition on the thermal-induced response of C-S-H will be investigated considering a variable stoichiometry and different atomic configurations based on experimental data. To describe interactions between C-S-H atoms, we will rely on a reactive force field formalism to simulate dehydration and heating decomposition. The simulation results will be embedded into a multiscale framework and validated by experimental data in order to study and predict the Thermo-Hydro-Mechanical behavior of CBM at high-temperature.

Required skills

- Master's degree in the field of civil engineering, materials science, physics or similar.

- Experience with (or motivation to learn) molecular dynamics and modern computational physics.

- Experience with (or motivation to learn) programming and high-performance computing.

- Advanced English for scientific communication.

Duration

3 years starting from October 2023.

Application process

Please submit your application including CV, transcripts and motivation letter to Dr. Majdouline Laanaiya - majdouline.laanaiya@univ-grenoble-alpes.fr or/and Pr. Stefano Dal Pont - stefano.dalpont@3sr-grenoble.fr

References

[1] D Dauti et al. 'Modeling concrete exposed to high temperature: Impact of dehydration and retention curves on moisture migration'. In: *International Journal for Numerical and Analytical Methods in Geomechanics* 42.13 (2018), pp. 1516–1530.

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