

Structure and dynamics of water in ordinary Portland and low CO₂ cements

Cement is the single most used material in the world, but despite many centuries of intensive usage and an ever-increasing worldwide demand, many physico-chemical fundamental questions regarding the cement setting process remain elusive. During this process different hydrates nucleate and grow, of which calcium silicate hydrates (C-S-H) is the most important binding phase. C-S-H is indeed the key compound controlling the final cement properties, such as strength and durability. Although a large deal of research effort has been devoted to the study of C-S-H, its poorly crystalline character has made it inherently difficult to fully characterize it. Moreover, the presence of aluminates phases both in ordinary Portland cement and in new low-CO₂ emissions cement formulations result in Al-substituted C-A-S-H. Whereas much effort has been put in understanding the atomic structure of these phases, both the structure and diffusion of water through their pores remain poorly understood. Understanding water organization in the C-S-H phase is not only important for the setting behavior, but also because water plays a key role in the dissolution-recrystallization and carbonation processes which are the main cause of the loss of cement strength. Moreover, water diffusion in C-S-H nanopores is important to understand the exchange of other ions in pollutant removal or in the context of nuclear waste storage.

In this Ph.D. project, the atomic structure of C-(A)-S-H, and the structure and dynamics of water in the different pores of these materials will be studied using a combination of neutron scattering techniques, including neutron pair distribution function analyses and inelastic neutron scattering, with synchrotron X-ray scattering and laboratory-based methods such as water adsorption isotherms, infrared spectroscopy or thermogravimetric and calorimetric analyses. We are looking for a motivated candidate with a background in physics, materials science, or chemistry, with fluency in English, and a strong motivation to work in an international environment.