Nanoscale Modeling of Smart Nano-Engineered Cementitious Composites

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Summary

There is an urgent need for new sustainable cement technology that can minimize the environmental and economic impact of cement production and use in civil engineering. This reduces energy consumption and greenhouse gas emission as well as the sensing capacity for structure health monitoring. The aim is to help achieving sustainable and smart constructions and infrastructures within through the improvement of civil engineering material mechanical and environmental performances.
Recently, a new field has emerged in materials science called nanoscale modelling. It allows linking our understanding of a few elementary mechanisms (usually at the microscopic scale) with the behaviors observed at the macroscopic scale. This offers a unique opportunity to bring these advances in developing and studying a green, smart and sustainable cementitious material, which can be a potential substitute of conventional construction materials.

To improve the traditional behavior of cement, it is essential to explore the properties of the nanogranular-binding phase of the cement, called the Calcium–Silicate–Hydrate (C–S–H). While C–S–H gel has reached significant level of understanding under a number of varying conditions, cement nanoscience is looking for the future by studying the effects of the ingress of foreign nanomaterials into the C–S–H nanostructure.

Combining nanoscale tools with the high performance of computer simulation methods, the following PhD project is proposed.

We aim, first, to study deeply the new generation of nano-engineered cementitious composites (NECC) by incorporating to calcium silicates hydrates (C-S-H) nanostructure different kind and geometries of nanoparticles (nano-oxides, nano-montmorillonite clays and carbon buckyballs) as well as other nanotubes of carbon and calcite whiskers. We project to study essentially the open questions of the dispersion, the density, the interfacial shear strength between nanomaterials with C-S-H and how they can fill the pores, affect the degree of hydration and can reduce the compressive strength.

We focus in the second objective on modeling the self-heating abilities of the nano-engineered concrete that is ultra-resistant to humidity changes at high temperatures. We aim then to analyze how the addition of various kinds of nanomaterials improves the degree of hydrophobicity of NECC surfaces.

In the third objective, we focus on the role of conductive nanomaterials (like carbon nanotubes) on the anti-crack abilities, and functional properties of NECC: The flexural and compressive strengths, electrical conductivity and piezoresistivity under different compressive loading conditions will be investigated. This project will give a big step to the development of the self-sensing capability of the nano-modified cementitious materials.

The last objective concerns analysis of the environmental and economic impact of this innovation in the civil engineering construction and health monitoring.