

Dynamics of water nanoconfined in cement by atomistic simulations

SYLVIA M. MUTISYA¹, JAMES M. DE ALMEIDA²,
CAETANO R. MIRANDA^{2,*}

¹NMA, Universidade Federal do ABC, Santo André, SP,
09210-580, Brazil

²DFMT, Instituto de Física, Universidade de São Paulo, São
Paulo, SP, 05508-090, Brazil

*cmiranda@if.usp.br

Cement paste is a complex, heterogeneous and porous material with outstanding mechanical properties that make it a suitable binder for construction applications. Water within the pores of cement plays a crucial role in durability of concrete structures. By combining molecular dynamics simulations with Nuclear Magnetic Resonance (NMR) modeling, we study the dynamical properties of water nanoconfined in the main binding phase comprising of calcium silicate hydrates (C-S-H). We explore the influence of the C-S-H surface, progressive confinement and connected pores to water dynamics within the interlayer, gel pores (1-5 nm) and in the vicinity of a C-S-H globule particle (Fig.1). Water within the first hydration layer of C-S-H surface exhibit slow dynamics indicated by small self-diffusion coefficient, long rotational correlation time and short T_2 relaxation time. The properties of water in the proximity of C-S-H surface does not change significantly altering the pore model from infinite planar pores to C-S-H globule particle. Additionally, the water dynamics in the C-S-H edge-edge environment resemble the one observed at C-S-H planar surfaces. Interpore exchange analysis using NMR T_2 - T_2 relaxation revealed that there is exchange between small and large gel pores and at short times, the adsorption/desorption of water from a 1 nm pore may be limited only to the edges.

Fig.1: a) Defected tobermorite C-S-H model b) Interlayer and gel pores. c) Connected pore d) globule disk-like particle.

