Multiscale modelling of chloride transport in cementitious materials

PhD candidate: Khalil Ferjaoui

To reduce the CO_2 footprint of construction materials, concrete producers blend their cement with Supplementary Cementitious Materials (SCMs). And even though such blended systems are eco-friendlier than the Ordinary Portland Cement (OPC), they are required to respect standards. In this context, understanding and predicting the durability of blended concrete is important for optimizing the design of new cementitious materials. Even though chloride ingress is one of the most common problems for reinforced concrete, the quantification of the link between ionic transport and the microstructure is still a challenge. Modelling transport in cementitious materials by Fickian processes usually fails to predict experimental results and particularly those of blended systems. Chloride ingress is thought to be influenced, at the nanoscale, by the adsorption of ions on the hydrates surface due to the formation of an Electrical Double Layer (EDL). Therefore, a multiscale approach will be adapted to model the phenomena arising at different scales. The method for the calculation of ionic diffusivities will couple the Metropolis Monte Carlo algorithm (MC) to the Poisson Nernst-Planck (PNP) equation. First, the Monte Carlo is applied to the Grand Canonical ensemble to determine the ions distributions in the pores as a function of the pore radius. Once the densities of all ionic species are determined, the PNP system is resolved with the Finite Element Method (FEM) and effective diffusion coefficients are calculated as a function of the pore size. The contribution of the microstructure on the transport is to be investigated by developing a consistent microstructural model of the C-S-H, the main hydration product.