Towards multi-scale modelling of physico-chemical degradation processes in concrete structures

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Several physico-chemical processes such as chloride induced corrosion, calcium leaching, carbonation, sulphate attack, etc. lead to degradation of concrete structures. Physico-chemical processes initiates dissolution/precipitation processes within concrete at pore-scale which leads to significant changes in its pore structure and in turn affects its physical and mechanical properties. Physics based models for prediction of extent of these degradation mechanisms will therefore require time dependent constitutive relations which would be very difficult to parametrize if not impossible for such complex Multiphysics processes. Therefore, a "*bottom-up*" modelling approach starting with modelling of these processes and upscaling these models to structural scale can be a "*potential game changer*". Such models would allow us to improve service life predictions, connect accelerated laboratory tests to field conditions and can act as a virtual laboratory which can be used to quickly optimize and test new mixes.

In this presentation I would provide an overview of my research activities focusing towards development of multiscale approaches for physico-chemical degradation processes in concrete structures. I start by introducing current models to describe pore-structure of concrete at different scales of cement system which serves as starting point for multi-scale model. Following this I introduce a lattice Boltzmann method-based Multiphysics modelling framework developed to capture physico-chemical processes at different scales in concrete. Finally, three example cases are presented to show current advances made in development of "bottom-up" modelling approaches for degradation processes of concrete structures. First example is upscaling of chloride ion diffusivity by coupling models at different scales (molecular and pore scales). Second example presented is development of models for calcium leaching at different spatial scales and discussions on insights obtained from these models. Final example is microstructural modelling of coupled dissolution/precipitation processes due to combined leaching and carbonation considering changes in porosity at nanoscale.