Microstructural modelling to relate transport properties to chemically and mechanically induced change in microstructure (PhD)

http://www.sckcen.be/en/yop/view/115

Introduction

Microstructural models are used for investigating the evolution of the microstructure as well as for predicting transport in and mechanical properties of concrete. These models are applied to simulate interactions between particles at the microscale and make it possible to predict the hydration of cement-based materials, structural formation and the development of strength. Microstructural models allow for assessing factors that affect hydration, the probability of cracking and the effect of alkalis, gypsum and additives on the rate of hydration. Cement hydration, structural formation and the chemical evolution of cement-based materials in contact with porewater are mutually dependent phenomena. Existing microstructural models have paid relatively little attention to the modelling of the chemical evolution of cement-based materials in contact with porewater. The present research proposal intends to integrate chemical interactions between a cementitious solid phase and an aqueous phase, which are not in thermodynamic equilibrium with each other, in microstructural models.

Objectives

The main goals of the proposed Ph.D. thesis are:

- To simulate the microstructural changes of concrete due to chemical degradation processes such as carbonation, decalcification and sulphate attack, and
- To link the effect of microstructural transformations to changes in (macroscopic) transport properties (e.g. permeability or pore diffusion coefficient).

To achieve these objectives, it is intended to integrate a geochemical module into the existing model HYMOSTRUC, which has been developed at the Technical University of Delft, The Netherlands. This will allow to model chemical degradation processes as a function of invasive pore water composition for time periods beyond the period of cement hydration (i.e. the current time period of HYMOSTRUC). Research proposed as part of work package 1 will be based on the existing microstructural model HYMOSTRUC. This model for cement hydration and virtual microstructures allows simulating the degree of hydration as a function of (i) particle size distribution, (ii) chemical composition of the cement, (iii) the water/cement ratio and (iv) the reaction temperature.

The current R&D proposal plans to implement a general geochemical module in HYMOSTRUC. Together with the transport module, which was recently integrated in the HYMOSTRUC code, this will allow to couple microstructural changes with geochemical degradation processes.

Next, the new microstructural model will be used to characterize the pore structure in terms of pore size distribution, connectivity, surface area, hydraulic radius and total porosity. These properties are linked to (macroscale) transport properties by empirical or physical models. Alternatively, permeability is simulated outside HYMOSTRUC, by exporting respective geometry at the specific time and link it to a dedicated modelling tool.

Required education level of potential candidates: master in sciences, master in engineering sciences

Candidates must have a background in: Chemistry, Geology, Bio-engineering, Physics

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Multi-scale modelling of the coupled effects of chemical, mechanical and physical processes on concrete degradation (PhD)

http://www.sckcen.be/en/yop/view/117

Introduction

Predicting the performance of concrete structures is complicated by the complexity of the material, which has a heterogeneous microstructure and displays composite behaviour at a series of length scales. In particular, the overall transport and mechanical behaviour of concrete is strongly conditioned by its heterogeneous microstructure, which determines the randomness of the overall transport and mechanical variables. Permeability, diffusivity, initiation and progression of cracks within concrete are significantly controlled by this randomness. Multi-scale modelling is an approach which is followed to assess the large-scale durability of concrete. Multi-scale modelling provides a methodology to systematically incorporate detailed information about processes occurring at smaller scales into governing equations at larger scales.

Objectives

The principal objective of this research project is to develop a multi-scale modelling framework to incorporate the coupled effects of chemical, mechanical and physical processes on chemical degradation of concrete in order to assess the long-term, large-scale durability of concrete under conditions representative for a near-surface radioactive waste disposal facility based on a multi-scale modelling approach. This project essentially considers PhD research project 1 and 2 as a starting point and runs partly in parallel.

The approach to multi-scale modelling will essentially involve integration of a series of models applicable for different scales, i.e. micro-scale, meso-scale and macro-scale and in essence follows a hierarchical modelling approach. The following key steps are envisaged in realising a multi-scale model:

- Microscale modelling of unhydrated/hydrated cement paste comprising micro-porosity and solid phases of hydrated cement paste. The starting point for this task will be work package 1 but will elaborate further relations between the degree of chemical degradation, microstructural changes and permeability.
- Mesoscale modelling of hydrated cement paste, sand and voids (mortar) or mortar, aggregate, interface transition zone and voids – deriving inputs principally from microscale modelling.
- Macroscopic modelling based on the continuum approach – deriving inputs principally from mesoscale modelling. The general method that will be adopted for upscaling is the homogenization method. A detailed treatment of upscaling at the micro-meso and meso-macro levels will therefore form the central theme of this PhD research. The determination of representative elementary volumes will form a key step for all the scales considered above

A microstructural model, HYMOSTRUC, is proposed to be used at the microscopic scale. Careful consideration will be given to alternative approaches for mesoscopic scale modelling. For instance, SEM-images may be used as input for the mesoscopic scale. As far as the macroscopic modelling of concrete is concerned, a flow and reactive transport code, HP1 (Jacques et al. 2008) is proposed. This model treats the coupled physical and chemical processes at the macroscopic (continuum) scale.

Required education level of potential candidates: master in engineering sciences, master in sciences

Candidates must have a background in: Chemistry, Geology

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