



A three-dimensional lattice Boltzmann method based reactive transport model to simulate changes in cement paste microstructure due to calcium leaching



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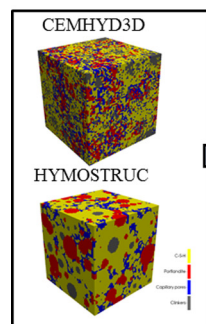
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HIGHLIGHTS

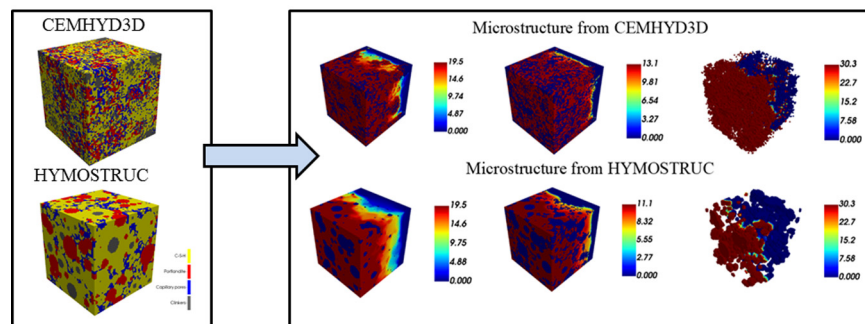
- Model to simulate changes in cement paste microstructure due to leaching is presented.
- Reactive transport model using lattice Boltzmann method and takes 3D digitized microstructure as input.
- Leaching rate is found to be directly proportional to ability to transport calcium ions.

GRAPHICAL ABSTRACT

HYDRATION MODELS



Microstructural changes and Ca concentration evolution after 800 s of leaching



ARTICLE INFO

Article history:

Received 11 September 2017

Received in revised form 19 January 2018

Accepted 22 January 2018

Available online 22 February 2018

Keywords:

Calcium leaching
Microstructure modelling
Lattice Boltzmann methods
Reactive transport modelling

ABSTRACT

In this paper, a newly developed lattice Boltzmann method based reactive transport model to simulate changes in microstructure of ordinary Portland cement paste due to calcium leaching is presented. The model takes three-dimensional digitized cement paste microstructure as input and is capable to capture an evolution of microstructure due to leaching, accounting for the dissolution of portlandite and corresponding increase in capillary porosity and the decalcification of C-S-H resulting in increase in gel porosity. The developed model has been applied to microstructures generated using two cement hydration models, CEMHYD3D and HYMOSTRUC, for three water-to-cement ratios. It was observed that the rate of leaching is directly proportional to ability of microstructure to transport calcium ions and higher fraction of percolated capillary pores result in higher rate of leaching. The model qualitatively reproduces experimentally observed changes in cement paste porosity and pore size distribution due to leaching. The quantitative validation of model at this scale is not possible by comparison of leaching obtained experiments and simulations which can be attributed to several factors including the differences in the scales of experiment and modelling study presented in this paper.

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1. Introduction

Leaching is a process in which solid phases of cement based materials dissolves because of disequilibrium created by outward transport of alkali ions by concentration gradients (diffusion) or/and pressure gradients (convection). Amongst other leachable alkali ions, leaching of calcium ions (Ca) is most important as it is a major constituent of different hydrated cement paste mineral phases such as portlandite, calcium silicate hydrates (C-S-H) and aluminates which form majority of cement paste matrix. Leaching of calcium ions results into a more porous material with lower strength and higher permeability and diffusivity [1–7]. In this paper, we refer to leaching of calcium ion as leaching.

Leaching of cement based materials in field conditions often occurs under diffusion resulting in a slow progression of leaching front with rate being only up to a few millimetres in hundred years [8,9]. Hence for most civil concrete structures with life span of few decades, leaching is not considered as an important deterioration mechanism. However, for structures which are in constant contact with water such as dams, foundations of offshore structures and bridges, water tanks, sewer pipes, or subsurface nuclear waste disposal facilities, leaching can be an important deterioration mechanism and should be taken into account in the service life evaluation.

Due to slow rate of leaching, experimental studies are often carried out under accelerated conditions using either aggressive low pH solutions such as deionized water [10–14], ammonium nitrate solution [1,3,4,13,15–21] and ammonium chloride solution [22] or accelerating transport of ions by applying an electric field [23,24] or pressurized flow [25]. Due to different leaching mechanisms for different experimental setups, leaching rates obtained from different experiments varies substantially. For instance, leaching rates in experiments with ammonium nitrate are 10 times higher than in experiments using deionized water [13]. Similarly, leaching depth is proportional to the square-root of time in diffusion-controlled leaching experiments, but directly proportional to time in experiments in which an electric field is used [26]. Thus, while these experiments allow for comparative studies between different types of cement-based materials, their results can hardly be used to predict the extent of leaching and service life in field conditions. Moreover, leaching leads to formation of several distinct altered zones [1,10] and transport properties, such as diffusivity and permeability measured on leached sample, are representative for this zoned material and cannot serve as input for reactive transport models [12,21,27–32] use to predict leaching progression. Such models rather need expression to relate geochemical changes (e.g. change in porosity, change in portlandite content, etc.) during leaching to evolving transport properties. In literature, some models use the relationship derived for hydrating cement pastes as input [28], or modification to these models [12,21,32], or utilizing effective media theories [31], the latter too being hard to parameterize experimentally. One of the output of the three dimensional model presented in this study is an evolved microstructure after leaching which can serve as input to numerically compute the in properties due to leaching.

The existing approaches for simulation of evolution of cement paste microstructure due to leaching are either based on dissolution of mineral phases randomly from cement paste microstructure using stochastic rules which ignores influence of local concentration gradient in cement paste microstructure on dissolution [19,33–36] or more recently reactive transport models of Gaitero et al. [37] and Ukrainczyk and Koenders [38] which suffers from several simplifications. Gaitero et al. and Ukrainczyk and Koenders [38] presented reactive transport models which simulate ion transport by the Nernst-Planck or the diffusion equation,

respectively, and leaching of a mineral phases through a resolved microstructure. Both models are three dimensional. The simulation domain was 10 μm cube with 0.25 μm resolution and 50 μm cube with 1 μm resolution for Gaitero et al. and Ukrainczyk and Koenders, respectively. Both models used HYMOSTRUC [39,40] to generate initial microstructure. Solid phases considered by Gaitero et al. considered in the simulations were, clinkers inner-product C-S-H, outer product C-S-H and overlapping C-S-H. For describing C-S-H reaction, they assumed that C-S-H consist of leachable portlandite and non-leachable C-S-H with Ca/Si equal to one limiting the geochemical model to portlandite dissolution. They accounted for the increase in diffusivity of the C-S-H phase through a linear relationship with respect to porosity. Ukrainczyk and Koenders considered only C-S-H dissolution in presence of deionized water considering transport of only Ca ions. Although these models demonstrate the potential of a microstructural reactive transport model for leaching, there is a lack of a robust framework to simulate leaching through microstructure of reasonable size accounting for both portlandite and C-S-H dissolution.

In this study, we present a three-dimensional microstructural reactive transport model to simulate the evolution of an ordinary Portland cement paste microstructure with a reasonable size of simulation domain during calcium leaching. The model is able to capture changes in cement paste pore structure and development of new capillary pores due to dissolution of portlandite and increase in porosity of C-S-H due to leaching. The model considers transport of ions through diffusion equation which is solved using lattice Boltzmann method. The reaction model is based on thermodynamic equilibrium approach and implemented as look up table which speeds up simulations. The developed model is applied to simulate leaching through digitized cement paste microstructure generated using both HYMOSTRUC (modified version with includes portlandite nucleation and growth [41]) and CEMHYD3D with three different water-cement (w/c) ratio viz., 0.25, 0.4 and 0.5. It should be noted that while the developed model is applied to virtual microstructures, it can also take tomographic images of hydrated cement paste directly as input. This model has been implemented in an newly developed open-source lattice Boltzmann method based framework *Yantra* (version 0.5) [42,43]. Remainder of the paper is organized as follows. Section 2 provides details on assumption involved in model development, governing equations and details on numerical model with relevant implementation details. Simulation results are discussed in detail in Section 3 and conclusions based on simulations are given in Section 4.

2. Model description and implementation aspects

2.1. Governing equations

The formulation of the boundary value problem for simulating calcium leaching through cement paste microstructure is presented in this section. Following assumptions are made

- Only portlandite and C-S-H phases are affected by leaching and minor hydration products are treated as C-S-H phases.
- Diffusion of ion occurs only through capillary pores domain (Ω_{CP}) and a porous C-S-H phase domain (Ω_{CSH}). Unhydrated cement paste and portlandite are non-diffusive.
- Influence of ion activity and electro-kinetic charges on diffusion is neglected. All species have the same diffusion coefficient.

With these assumptions, calcium leaching through cement paste microstructure can be described with a reaction-diffusion process as,

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