8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

NUMERICAL MODEL OF CALCIUM LEACHING IN CEMENTITIOUS MATERIALS, CONSIDERING THE PROCESS KINETICS AND ADVECTIVE CALCIUM TRANSPORT

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Key Words: *Concrete Structures, Durability, Calcium Leaching, Computing Methods.*

ABSTRACT

Calcium leaching is of importance during assessment of durability of concrete structures exposed to direct contact with deionised water. Usually thermodynamic equilibrium of the calcium ions in pore solution and the solid calcium in material skeleton, as well as purely diffusive calcium transport, are assumed in modelling of the process, e.g. [1, 2].

A novel mathematical model of calcium leaching in isothermal cementitious materials, considering additionally, as compared to [1, 2], the process kinetics and advective transport of calcium ions, is derived here by means of mechanics of multi-phase porous media. This is an extension of the chemo-hygro-thermo-mechanical model of concrete, previously proposed by the Authors in [3]. The new model consists of the three mass balance equations of water, moist air and calcium dissolved in water, and the linear momentum conservation equation for the multi-phase medium. Chemical degradation of the material strength properties due to calcium leaching is taken into account. Constitutive relationships describing transport and strength properties of chemically degraded cementitious materials are presented. Convective-type boundary conditions, better describing physical phenomena during calcium leaching in real conditions than Dirichlet's BCs, used in [1, 2], are formulated. More details about the model can be found in [4].

Calcium leaching process is modelled by considering thermodynamic imbalance of the calcium in solid and liquid phases, what allows for description of the process kinetics and avoiding numerical problems reported in [5]. The model is used for calculation of calcium mass sources in concrete elements exposed to various boundary conditions, with liquid calcium concentration changing at different rates, including very fast processes. The results obtained show some differences in comparison to the traditional leaching models, based on the thermodynamic equilibrium assumption. The differences are significant for relatively fast processes, while for slower ones they are negligible.

Discretization of the equations in space domain is performed by means of Finite element Method, while in time domain a Finite Differences scheme is applied. The obtained nonlinear equation set is solved with a Newton-Raphson procedure. A number of numerical examples concerning leaching of 1-D and 2-D concrete structures exposed to various boundary conditions is solved and discussed. They show numerical robustness

of the non-equilibrium model of concrete leaching as compared to the traditional model based on thermodynamic equilibrium assumption, what allows analysing processes with very fast decrease of calcium concentration. One can also state that the faster leaching process is, the more distant from the equilibrium state is calcium contained in the material skeleton and ions in pore solution, what influences the leaching process rate. Significant differences of the results concerning calcium leaching obtained with Dirichlet's and Robin's boundary conditions are observed. The latter boundary conditions describe much better the phenomenon's physics in real situations and they result in much slower progress of the calcium leaching process. Concrete elements exposed to direct contact with deionised water from more than one direction, like for example columns or structure corners, are jeopardized by much faster progress of chemical degradation than 1-D structures, due to easier outflow of calcium ions from the leaching zone where calcium concentration is elevated. The numerical model presented allows for analyses of durability of concrete structure in various conditions, also those which were before impossible for modelling, like for example leaching due to existing water pressure gradient.

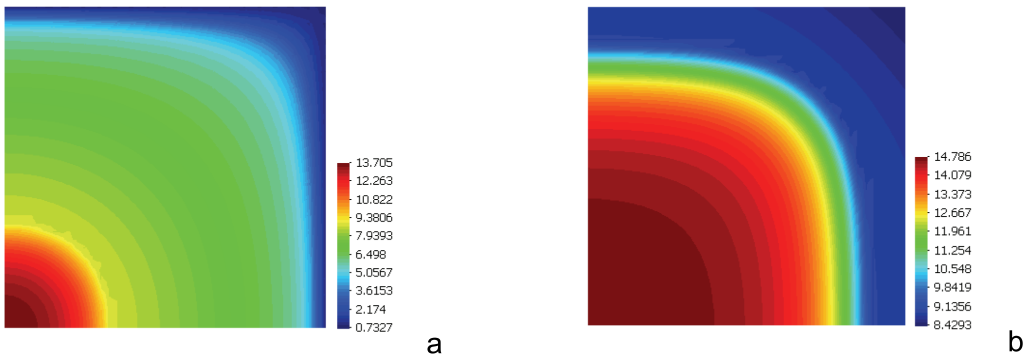

Figure 1. Comparison of the solid calcium concentration in a square (4cm x 4cm) concrete specimen after 20,000 days of contact with the water containing 1 mol/m^3 of calcium ions, modelled with different boundary conditions: a) Dirichlet's BCs, b) Robin's BCs.

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