A Coupled Transport and Chemical Model for Durability Predictions of Cement Based Materials

A Coupled Transport and Chemical Model for Durability Predictions of Cement Based Materials

The use of multi-physics numerical models to estimate different durability indicators and determine the service life of cement based materials is increasing. Service life documentation for concrete used in new infrastructure structures is required and the service life requirement for such structures is often in the range from 80-125 years. Numerical multi-physics models are valuable tools when long term predictions are of interest. The multi-physics models needs to be theoretical sound in order to meet the increasing requirements for the detail level for the simulations and increasing long term simulations. A coupled reactive mass transport model for concrete is established and different simulations of concrete exposed to different service environments are conducted. The theoretical background for the model is to a large extent based on the hybrid mixture theory, which is a modern continuum approach. The hybrid mixture theory description considers the individual phases and species, building up the whole mixture, with individual differential equations. The differential equations includes exchange terms between the phases and species accounting for the exchange of physical quantities which are essential for a stringent physical description of concrete. Balance postulates for mass, momentum and energy, together with an entropy inequality are studied within mixture theories. Special attention is paid to the criteria for the exchange terms in the studied balance postulates. A simple case of mixture theory is used to demonstrate how constitutive assumptions are used to obtain the governing equations for a specific model. The governing equation system used for the multi-physics durability model, established in this work, is an extended version of the Poisson-Nernst-Planck system of equations. The extension of the Poisson-Nernst-Planck system includes a two phase description of the moisture transport as well as chemical interactions. The vapor and liquid contents are coupled by a sorption hysteresis function and the chemical equilibrium is solved in terms of mass actions laws using the geochemical code phreeqc. The overall durability model accounts for ion diffusion, ion migration, two phase moisture transport including for hysteresis, ionic convection and chemical interactions in the pore solution and between the solid cement hydrates and the pore solution constituents. The mass transport equation system is solved using the finite element method. An operator splitting approach is utilized in order to solve the mass transport and chemical interactions sequentially. A detailed description of the continuum background of the governing equations and the numerical solution approaches used is given in this work. The durability model is tested with different input parameters and boundary conditions in order to demonstrate the applicability of the model and robustness of the algorithm established. A calculated test example shows the model response to varying vapor content at the boundary, where saturated conditions occurs in periods and leaching of ions is only allowed in this period. The effect of the sorption hysteresis function is demonstrated in this test by a comparison to a more simple numerical approach. The importance of the chemical interactions are demonstrated through different cases in terms of using different boundary conditions and chemical reaction calculation approaches. Sea-water compositions are used as multi-species boundary conditions to model natural exposure conditions of infrastructure constructions. Test examples shows that the simulation results are very sensitive to the choice of chemical reactions included in the model. It is concluded that the different numerical chemical equilibrium solution approaches used performs differently for the same initial and exposure conditions. Different numerical calcium silicate hydrate reaction approaches are studied and reactive transport modeling results using these are compared. Modeling results of ion ingress are compared with experimental results where mortar samples has been exposed to a NaCl solution or sea-water. Comparing the chloride ingress between the numerical model and the experiments at three different exposure times showed good agreement.

General information
Publication status: Published
Organisations: Department of Civil Engineering, Section for Geotechnics and Geology
Contributors: Jensen, M. M.
Number of pages: 224
Publication date: 2014

Publication information
Publisher: Technical University of Denmark, Department of Civil Engineering
Original language: English
Electronic versions:
Mads_M_nster_Jensen_Thesis.pdf