



Framework for reactive mass transport: Phase change modeling of concrete by a coupled mass transport and chemical equilibrium model



M.M. Jensen^{a,*}, B. Johannesson^a, M.R. Geiker^b

^a Technical University of Denmark, Department of Civil Engineering, Brovej 118, 2800 Kgs. Lyngby, Denmark

^b Department of Structural Engineering, Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway

ARTICLE INFO

Article history:

Received 3 January 2014

Received in revised form 12 May 2014

Accepted 14 May 2014

Keywords:

Chemical equilibrium modeling

Mass transport modeling

Phase change

Cement

ABSTRACT

Reactive transport modeling is applicable for a range of porous materials. Here the modeling framework is focused on cement-based materials, where ion diffusion and migration are described by the Poisson–Nernst–Planck equation system. A two phase vapor/liquid flow model, with a sorption hysteresis description is coupled to the system. The mass transport is solved by using the finite element method where the chemical equilibrium is solved explicitly by an operator splitting method. The IPHREEQC library is used as chemical equilibrium solver. The equation system, solved by IPHREEQC, is explained for aqueous, pure phase and solid solution reactions. Numerical examples, with cement-based materials, are constructed to demonstrate transient phase change modeling. A simulation of pure multi-species leaching from the material, showing deterioration of the solid phases is described and calculated. A second simulation, showing multi-species ingress with formation of new solid phases in the domain is described and calculated. It is shown that the numerical solution method is capable of solving the reactive mass transport system for the examples considered.

© 2014 Elsevier B.V. All rights reserved.

1. Introduction

Chemical phase changes as a consequence of a reactive mass transport process in porous media are well known phenomena. For example, cement-based materials show phase changes when exposed to aggressive environments, both from liquid solutions and gases. The alterations of cement-based materials are strongly related to durability and service life. The phase changes in most cement-based materials are often very slow processes due to the complex matrix of the porous network. Modeling frameworks for describing phase changes over a long period of time are useful in the sense of evaluating the long term durability of the material and as indicator for service life estimation.

Reactive mass transport modeling of cement-based materials is in many cases focused on single ionic species transport, especially chloride ingress due to its influence on reinforcement corrosion. Single ionic ingress modeling is often related to a modified diffusion coefficient. Time-dependent diffusion coefficients are used in different engineering models see e.g. Thomas and Bamforth [1], Tang and Gulikers [2]. This approach compensates for all chemical and physical changes over time in a single parameter. Other suggested diffusion coefficient dependencies are, e.g., a function

of diffusion depth Yuan et al. [3], a function of concentration Bigas [4], Tang [5], Francy and François [6].

Over the last decade multi-species transport modeling has gained acceptance, where a constant species dependent intrinsic diffusion coefficient is considered in these types of models and the transient change of the diffusion properties is a consequence of the ionic composition development. Transport models of this type are found in, e.g., Nguyen et al. [7], Truc et al. [8]. Multi-species transport modeling within porous media is often described by the Nernst–Planck equation or the Poisson–Nernst–Planck (PNP) system of equations, see e.g. Samson et al. [9], Johannesson [10], and Johannesson [11]. The multi-species transport approaches enable establishment of extended reactive transport modeling, where each ionic species is considered in chemical reactions, both in aqueous reactions and solid/liquid reactions. It has been concluded that the flexibility of the multi-species approach is a great advantage in long term simulations of cement-based materials see e.g. Marchand and Samson [12], Baroghel-Bouny et al. [13] even though the models are often associated with a range of input parameters, which can be difficult to measure separately.

A coupled reactive mass transport model within cement-based materials was proposed by Hosokawa et al. [14] based on an extended version of the Poisson–Nernst–Planck equation system coupled to a chemical model. In their work a surface complexation

* Corresponding author. Tel.: +45 45 25 17 00.

E-mail address: mmoj@byg.dtu.dk (M.M. Jensen).

model of the C–S–H phase was utilized, see Nonat and Lecoq [15], Hosokawa et al. [16]. The chemical equilibrium system of equations was solved by the PHREEQC code in which it is possible to estimate the electrical double layer composition on the C–S–H surface and thereby include binding of ionic species from the pore solution. Another model was proposed by Samson and Marchand [17], based on a Poisson–Nernst–Planck type of equation, coupled with a liquid diffusion equation in order to model non-saturated systems. A chemical model having a limited number of ions and solids was solved together with the mass transport system. Both models were solved under the assumption of instantaneous local equilibrium, which enables an operator splitting method (also known as staggered method).

The framework presented in this paper is mainly based on the work by Johannesson [10], Hosokawa et al. [14]. The model from these papers is extended with a two phase vapor/liquid model described in Johannesson and Nyman [18]. The mass transport model is coupled to the chemical equilibrium code IPHREEQC (see Parkhurst et al. [19], Charlton and Parkhurst [20]). The proposed model presented here differs from earlier work by coupling of the extended vapor/liquid transport model with the chemical equilibrium code, where all features and calculation methods are available.

The coupled model is solved numerically by the finite element method (FEM) and a brief overview of the chemical equilibrium calculation is given, based on Parkhurst et al. [19]. Precondition calculations and non-linear material parameters related to cement-based materials are shown. Numerical examples are constructed to show a numerical solution for a cement-based system, exposed to different boundary conditions. An important aspect in this framework is the capability of modifying and testing various chemical models together with a mass transport code. The constructed examples demonstrate this by combining a well known thermodynamic database CEMDATA07 (see Möschner et al. [21], Schmidt et al. [22], Möschner et al. [23], Lothenbach et al. [24], Lothenbach and Winnefeld [25]), with recent external phase descriptions, see Kulik [26].

2. Methods

2.1. Reactive mass transport

Mass transport in the porous system of a cement-based material is in this model described by an extended version of the PNP system of equations. The equation system describing the mass transport is based on the work of Johannesson [10] with the exception that chemical interactions are taken into account in the solution procedure as described in Hosokawa et al. [14]. The transport of the individual ionic species in the pore solution is described by individual transport equations. The governing mass transport equation in use is

$$\varepsilon^l \frac{\partial c_i^l}{\partial t} + c_i^l \frac{\partial \varepsilon^l}{\partial t} = \nabla \cdot (D_i^l(\varepsilon^l) \varepsilon^l \nabla c_i^l + D_i^l c_i^l \nabla \varepsilon^l - A_i^l c_i^l z_i \varepsilon^l \nabla \Phi) + v^{ls} \varepsilon^l \nabla c_i^l + v^{ls} c_i^l \nabla \varepsilon^l + q_i; \quad i = 1, 2, \dots, m \quad (1)$$

where c_i^l is the concentration of the i th ion in the liquid phase l , ε^l is the volume saturation of the liquid phase in the pore system, $D_i^l(\varepsilon^l)$ is the diffusion coefficient for the i th ion, A_i^l is the ionic mobility, z_i is the valence state of the i th ion, Φ is the total electrical potential of the liquid, v^{ls} is the liquid velocity with respect to the solid s and q_i is a source/sink term accounting for chemical equilibrium. The numerical solution of chemical equilibrium is introduced in the transport equation as an operator splitting approach, by assuming an instantaneous local chemical equilibrium state after each mass transport step performed. The operator

splitting approach for reactive transport models is simply to determine a transient solution for the mass transport part and use these results as input for the chemical equilibrium calculation. This solution is then used as a set of initial values for the next transport calculation. Through this approach chemical equilibrium is solved for each discrete element in the spatial domain at all considered time steps.

The electrical potential of the solution considered is determined by the Gauss law, see Johannesson [10], this is the Poisson part of the PNP equation system. The Poisson equation is coupled to the diffusion Eq. (1) by the electrical potential Φ . The Poisson equation is given as

$$\xi_d \xi_0 \nabla^2 \Phi = F \sum_{i=1}^m c_i z_i \quad (2)$$

where ξ_d is the relative dielectricity coefficient, ξ_0 is the dielectricity coefficient of vacuum and F is the Faraday's constant.

The liquid transport for non-saturated porous materials is described by a two phase model proposed by Nyman et al. [27], Johannesson and Nyman [18]. The proposed model uses the saturation degree as driving potential for moisture transport. The two phase model enables a detailed transient description of changing boundary conditions, e.g. tidal zone modeling. The governing equation for the liquid transport is given as

$$\rho_w \frac{\partial \varepsilon^l}{\partial t} = \nabla \cdot (D_\varepsilon^l(\varepsilon^l) \nabla \varepsilon^l) + R(\varepsilon^{l,eq}(\phi_v) - \varepsilon^l) \quad (3)$$

where ρ_w is the water density, $D_\varepsilon^l(\varepsilon^l)$ is the transport coefficient for the liquid phase, R is a penalty number and $\varepsilon^{l,eq}(\phi_v)$ is the liquid volume fraction equilibrium function. The function $\varepsilon^{l,eq}(\phi_v)$ is a history dependent function, describing the sorption hysteresis. An individual function is established for each spatial element in the numerical discretization, based on a third order polynomials. The function is established between a set of initially defined adsorption and desorption boundary isotherms, see Johannesson and Nyman [18], Nyman et al. [27] for details.

The governing equation for the vapor phase transport, which is coupled to (3) is given by

$$\rho_{vs}(\varepsilon_p - \varepsilon^l) \frac{\partial \phi_v}{\partial t} - \rho_{vs} \phi_v \frac{\partial \varepsilon^l}{\partial t} = \nabla \cdot (D_\phi \nabla \phi_v) - R(\varepsilon^{l,eq}(\phi_v) - \varepsilon^l) \quad (4)$$

where ρ_{vs} is the vapor saturation density, ε_p is the porosity of the system, ϕ_v is the relative humidity and D_ϕ is the diffusion coefficient for the vapor phase. It is seen that the penalty function in Eq. (4) has opposite sign compared to Eq. (3) in order to establish an equilibrium between the vapor and liquid phase, based on the volume fraction equilibrium function $\varepsilon^{l,eq}(\phi_v)$.

2.2. Numerical calculation method

The mass transport equations are solved by the FEM, where weak formulations of Eqs. (1)–(4) are established and discretized by Galerkins method, see Ottosen and Petersson [28]. The transient system is solved by a single parameter implicit time integration scheme, given as

$$\mathbf{a}_{n+1} = (\mathbf{C} + \Delta t \theta \mathbf{K})^{-1} [(\mathbf{C} + \Delta t(1 - \theta)\mathbf{K})\mathbf{a}_n + \mathbf{f}_n + \theta(\mathbf{f}_{n+1} - \mathbf{f}_n)] \quad (5)$$

where \mathbf{a}_{n+1} is the solution at the time step $n + 1$, \mathbf{C} is the global damping matrix, Δt is the time stepping length, θ is the time stepping parameter, \mathbf{K} is the global stiffness matrix, \mathbf{f} is the load vector and \mathbf{a}_n the initial values for the time step. The numerical solution is improved, due to the non-linearities introduced, by a modified version of the Newton–Raphson scheme, see Ottosen and Ristinmaa [29]. The residual ψ of the solution is given by

Download English Version:

<https://daneshyari.com/en/article/7960378>

Download Persian Version:

<https://daneshyari.com/article/7960378>

[Daneshyari.com](https://daneshyari.com)