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Simulation of chloride migration in reinforced concrete

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ABSTRACT

In a large extent, durability and service life of reinforced concrete structures is influenced by penetration of deicing salts or seawater salts to the steel reinforcement. The steel corrosion is induced by a raising chloride concentration and possibly can lead to concrete cover spalling due to volumetric changes of oxides formed at the steel surface. Therefore, a critical concentration of chlorides is monitored and investigated by numerical simulations in service life assessments.

This contribution is devoted to modeling and numerical solution of the diffusionconvection problem applied to chloride migration in concrete. The theoretical background is reviewed with some of the numerical consequences and strategies that need to be used for a successful problem solution. The solution is implemented into an in-house opensource FEM software accounting for non-constant electric field and chloride binding existing in a real reinforced concrete element. The three stage approach is applied and demonstrated on an example of a reinforced concrete beam. First, an increased concentration of chlorides in the cover layer of the beam is simulated with pure diffusion over a long time period (10 years). Second, the two-dimensional distribution of an externally applied electric field is calculated in the beam. Third, an electrochemical extraction process in which the migration of ions is accelerated by an application of the electric field is simulated. The short time (2 days) treatment leads to rapid decrease of chloride concentration in the concrete cover but leaves elevated concentrations in deeper areas of the beam cross section as a direct consequence of the real action of two-dimensional and non-constant electric field. © 2017 Elsevier Inc. All rights reserved.

1. Introduction

The durability of reinforced concrete structures is very much related to the transport of water and ionic species in a porous microstructure of concrete. Major factor influencing the service life of a structure is the state of the load-bearing steel reinforcement and its possible corrosion. Depending on exposure conditions, concrete type, geometrical configuration and other structural and environmental parameters, the corrosion is initiated usually after several tens of years in normal conditions but can be significantly shorten (to years) if the concrete cover is not sufficient, carbonated or salt exposure is high as in the case of e.g. sea shore structures. Due to volumetric expansion of corrosion products, the corrosion process ultimatively leads to spalling of the concrete cover and further ingress of harmful species to the reinforcement. One of the most common and most deteriorating mechanisms causing steel damage is chloride induced corrosion. Critical chloride

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concentration level at which a considerable corrosion damage starts is about 0.2 - 0.4% Cl⁻ per cement weight and it was studied by many researchers in the past (e.g. [1,2]).

Concrete, as a heterogeneous composite, is in a real situation characterized with fully or partially saturated pores. Water in pores allows ionic species (chlorides and other ions) to be dissolved and transported in the concrete due to different mechanisms. One of them is the ionic diffusion. It presents a relatively slow process governed by water saturation level (e.g. [3,4]), concentration gradient (e.g. [5]), porosity and pore tortuosity of the material (e.g. [6]). Convection of ions appears in the case of water flow (which is more pronounced in cracked concrete) or in the case of application of an external electric field which governs the flux of charged ions (e.g. [7,8]). An external electric field is used for performing accelerated penetration tests on concrete specimens as well as for repairing a real structure [9,10]. In the later case the method is called electrochemical chloride extraction (ECE) and has been successfully used for mitigation of chloride attack on e.g. concrete bridges [11].

Although the topic of electromigration and ECE has been widely covered in the literature from the experimental point of view [12–16] as well as from theoretical point of view [7,8,17,18], contributions respecting the real rebar configuration in a reinforced concrete structure and the real electric potential gradient distribution are rather rare. The potential gradient is widely assumed to be constant [7] or the variation of the potential gradient is derived only from the multi-ionic species transport [8] or a simple domain geometry is solved to simulate experimental results [18]. In contrast, application of the ECE treatment to the reinforced concrete element leads to an uneven distribution of chloride concentration which is caused by a non-constant electric potential gradient [19].

Therefore, the purpose of this paper is twofold. First, the theory for chloride migration in concrete is presented and implemented in an open-source finite element code and typical situations such as chloride penetration and extraction on a reinforced concrete beam with real reinforcement arrangement are calculated using experimental characteristics obtained in the previous research [20,21]. The uneven distribution of an electric potential around the rebars is calculated based on the Gauss law of electrostatics and used for extraction of chlorides in a numerical example.

2. Diffusion and convection of ions in concrete

2.1. Ionic transport in saturated environment

In this paper, transport of ions in saturated environment is assumed to be governed by three main driving forces. First, the classical diffusion based on Fick's law leads to the ion flux density in the form

$$\boldsymbol{j}_d = -D\nabla \varrho_c \tag{1}$$

where *D* is the diffusion coefficient (m^2/s) and ϱ_c is the partial density of chlorides (kg/m^3) . Generally, in the flux density (1) the diffusion coefficient should be replaced by a second order tensor but with respect to the assumption of isotropy, a single coefficient is sufficient. In reality, the *D* is a function of different variables such as concrete age, porosity, degree of hydration, aggregate size, temperature, humidity and local chloride concentration (e.g. [6,22]).

It is more common to use concentration instead of the partial density of chlorides. The concentration, *c*, is the ratio of the weight of chlorides in an unit volume and total weight of the unit volume. Therefore, it has the form

$$c = \frac{\varrho_c}{\varrho} \tag{2}$$

where ϱ is the total density of concrete (kg/m³). With assumption of constant total density, the diffusion flux density can be rewritten into the form

$$\boldsymbol{j}_d = -D\varrho \,\nabla \boldsymbol{c} \;. \tag{3}$$

The second part of the ion flux density is driven by the intensity of applied electric field. The flux density is expressed by the Nernst–Planck equation

$$\boldsymbol{j}_{e} = \frac{DFz\varrho_{c}}{RT}\boldsymbol{E} = -\frac{DFz\varrho_{c}}{RT}\nabla\phi = -\frac{DFz\varrho_{c}}{RT}\nabla\phi$$
(4)

where *D* is the diffusion coefficient (m²/s), F = 96, 487 C/mol is the Faraday constant, *z* is the valence of ions, ρ_c is the partial density of ions (kg/m³) R = 8.314 J/K/mol is the molar gas constant, *T* is the temperature (K), *E* is the intensity of electric field (V/m), ϕ is the electric potential (V). The diffusion coefficient, *D*, is sometimes called the migration coefficient. More details can be found in [23].

Finally, ion convection can be caused by the net water flow. The ion flux density has the form

$$\boldsymbol{j}_{c} = \varrho_{c} \boldsymbol{v} = \varrho c \boldsymbol{v} . \tag{5}$$

Another possible driving force, the ion chemical activity, is sometimes assumed in the literature [7,24] and the flux density has the form

$$\mathbf{j}_{chem} = -Dc\nabla(ln\gamma) \ . \tag{6}$$

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