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MODELING OF CHLORIDE MIGRATION IN CONCRETE

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Abstract: *In many cases, reinforced concrete structures are influenced by penetration of deteriorating salts that cause corrosion of the steel reinforcement. From a micro-structural point of view, concrete is a heterogeneous composite with tortuous pore microstructure with partially or fully saturated pores. Water in pores allows salt ions to be dissolved and transported towards reinforcement. Different mechanisms such as diffusion or convection take place. The ion convection can be caused by electromotive force acting on charged particles and is caused by an electrical potential gradient. This contribution is devoted to modeling of the diffusion-convection problem applied to chloride migration in concrete. The influence of an external electric field is studied and problems of chloride penetration and extraction are solved. It is shown in the paper that the electric field accelerates the chloride migration by multiple times compared to natural diffusion and can be used as an efficient treatment for rehabilitation of reinforced concrete structures affected by chloride attack.*

Keywords: Reinforced concrete, Chlorides, Electromigration, Diffusion, Convection.

1. Introduction

Durability issues of reinforced concrete structures are widely connected with the transport of deteriorating salts within the porous system of concrete. Serious problems of steel corrosion that can be encountered at many engineering structures such as bridge decks and columns lead to the reduction of loading capacity and ultimately to the their failure. As an indicator, critical chloride concentration at the reinforcement is used as a measure to find the onset of steel corrosion. The critical chloride level is in the order of 0.2 – 0.4 % of Cl^- per cement weight and can be found in the literature (e.g. Angst, 2009; Ann, 2007). Once the corrosion starts it leads to concrete cracking and spalling of the concrete cover. The transport of salts in concrete obeys different mechanisms including diffusion and convection as the most prominent.

Repair technologies of affected structures are mostly destructive but a few non-destructive techniques like electrochemical chloride extraction (ECE) exist. The technique utilizes accelerated motion of chloride ions in electric field which is superior to diffusion. The extraction of the chlorides only takes days on a regular structure compared to diffusion of that usually takes years in which ions slowly travel to the reinforcement. The ECE method is successfully used for mitigation of chloride attack on various structures including concrete bridges.

2. Transport to ions in concrete

In this paper, transport of ions in saturated environment is assumed to be governed by three main driving forces. First, the concentration gradient governs the ion flux density (Fick's law) as

$$\mathbf{j}_d = -D\rho\nabla c \qquad (1)$$

where D is the diffusion coefficient (m^2/s), ρ is the total density of concrete (kg/m^3) and c is the concentration, i.e. ratio of the weight of chlorides in an unit volume and total weight of the unit volume.

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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 (Oh, 2007; Xi, 2007). 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 as

$$\mathbf{j}_e = \frac{DFzc\rho}{RT}\mathbf{E} = -\frac{DFzc\rho}{RT}\nabla\Phi \tag{2}$$

where D is the diffusion (migration) coffcient (m^2/s), F=96.487 C/mol is the Faraday constant, z is the valence of ions, R = 8.314 J/K/mol is the molar gas constant, T is the temperature (K), $\mathbf{E}$ is the intensity of electric field (V/m), Φ is the electric potential (V). More details can be found in (Černý, 2002). Finally, ion transport can be driven by water convection in which case the ion flux density is

$$\mathbf{j}_c = \rho c\mathbf{v}\,. \tag{3}$$

Overall, the total flux density of ions has the form

$$\mathbf{j}_c + \mathbf{j}_d + \mathbf{j}_e = \rho\left(-D\nabla c - \frac{DFzc}{RT}\nabla\Phi + c\mathbf{v}\right). \tag{4}$$

The mass balance equation for ions has the form

$$\frac{\partial c}{\partial t} = div\rho\left(D\nabla c + \frac{DFzc}{RT}\nabla\Phi - c\mathbf{v}\right). \tag{5}$$

An electric field can be applied to accelerate the extraction of ions from concrete in repair applications because pure diffusion would be very slow. In these applications, the electric field is given and it can be assumed to be constant in time. Therefore, the last two terms in the balance equation could be aggregated into a single term as

$$c\hat{\mathbf{v}} = \frac{DFzc}{RT}\nabla\Phi - c\mathbf{v}\,. \tag{6}$$

Special attention must be devoted to the gradient of the electric potential, In many papers on the ion penetration or extraction, the gradient of the electric potential is assumed to be constant which is generally not true, especially in the case of reinforced structures with sparse reinforcing bars that serve as counter electrodes. In contrary, the electric potential has to satisfy the Gauss law of electrostatics in the form

$$\varepsilon_r\varepsilon_o div\mathbf{E} = \varepsilon_r\varepsilon_o\Delta\Phi = \varphi \tag{7}$$

where φ is the density of charge (C/m^3), ε_r is the relative permitivity (-) and ε_o = 8.854·10^{-12} F/m is the permitivity of the vacuum. Equation (7) has to be solved for an appropriate domain and boundary conditions first. The electric potential obtained is then used in calculation of the flux density (6). With the help of (6) one can rewrite the mass balance equation (5) as

$$\frac{\partial c}{\partial t} = divD\nabla c + div(c\hat{\mathbf{v}}). \tag{8}$$

The term $divD\nabla c$ represents the diffusion and the term $div(c\hat{\mathbf{v}})$ represents the convection. The convection term can be further modified into the form

$$\frac{\partial c}{\partial t} = divD\nabla c + \hat{\mathbf{v}}^T\nabla c \tag{9}$$

because the mass balance equation for water is described by $div\mathbf{v} = 0$ and the charge density is zero. The mass balance equation (9) is defined on a domain Ω with boundary Γ which is split into two disjoint parts Γ_D and Γ_N. The concentration is prescribed on Γ_D (Dirichlet boundary condition) while ion flux density is prescribed on the part Γ_N (Neumann boundary condition). The problem is solved in time interval (0, t_{max}). Because of the time dependent problem, initial condition has to be defined. The boundary and initial conditions can be written in the form

$$\forall\mathbf{x}\in\Gamma_D, t\in(0,t_{\max}) : c(\mathbf{x},t) = c_D(\mathbf{x},t) \tag{10}$$

$$\forall \mathbf{x} \in \Gamma_N, t \in (0, t_{\max}) : \mathbf{n}^{\mathrm{T}} \mathbf{j}(\mathbf{x},t) = j_N(\mathbf{x},t) \tag{11}$$

$$\forall \mathbf{x} \in \Omega) : c(\mathbf{x},0) = c_0(\mathbf{x}) \tag{12}$$

where c_D is the prescribed concentration, **n** is the unit normal vector to Γ_{N}, j_N is the prescribed ion flux density in the normal direction to the boundary Γ_{N} and c_0 is the initial concentration. The problem (9-12) was solved by the finite element method based on the Galerkin-Petrov approach.

3. Numerical example

As an example, chloride extraction process accelerated by an electric field from a cantilever bridge deck with a barrier was modeled with the help of numerical approach described above. Scheme of the bridge deck part with the vertical barrier is shown as a blue domain in Fig. 1a. Prior to extraction part of the domain (white line in Fig. 1a) was exposed to 10 years of chloride diffusion. The chloride concentration distribution after this exposure on the deck and barrier is shown in Fig. 1b. For this simulation, the diffusion coefficient of concrete was assumed as $7.4 \cdot 10^{-12}$ m^2/s. For the extraction process, the electric field was created by the application of voltage of 20 V to the reinforcement while 0 V was assumed on the top deck and the top and left cornice surface. Distribution of the electric potential was obtained from equation (7) where the permitivity of concrete is $39.843 \cdot 10^{-12}$ F/m and the permitivity of the air is $8.854 \cdot 10^{-12}$ F/m. It should be emphasized that the mesh is larger than the deck with cornice itself because the electric potential is distributed also in their vicinity (green domain in Fig. 1a). The distribution of the electric potential is depicted in Fig. 2.

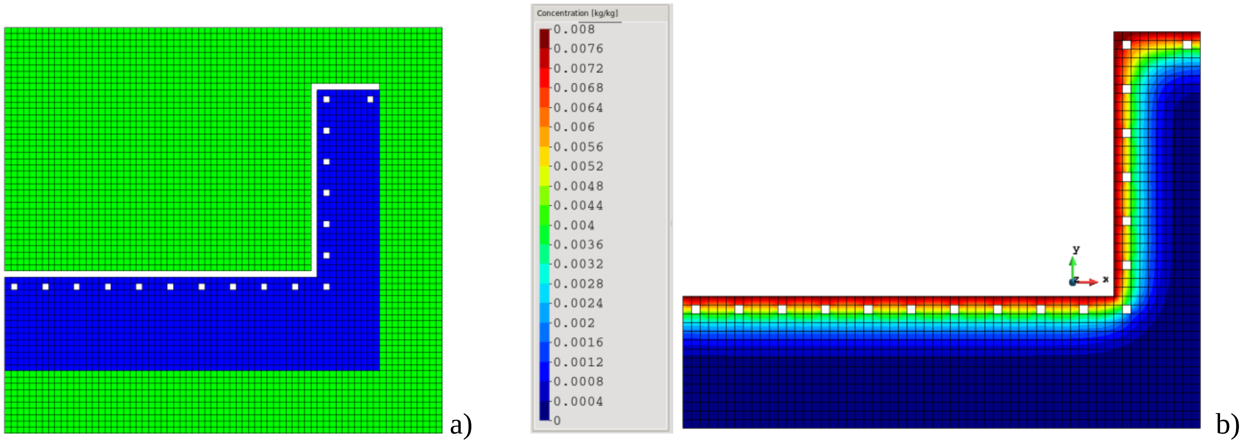

Fig. 1: a) FE mesh; b) Distribution of the chloride concentration after 10 years of exposure.

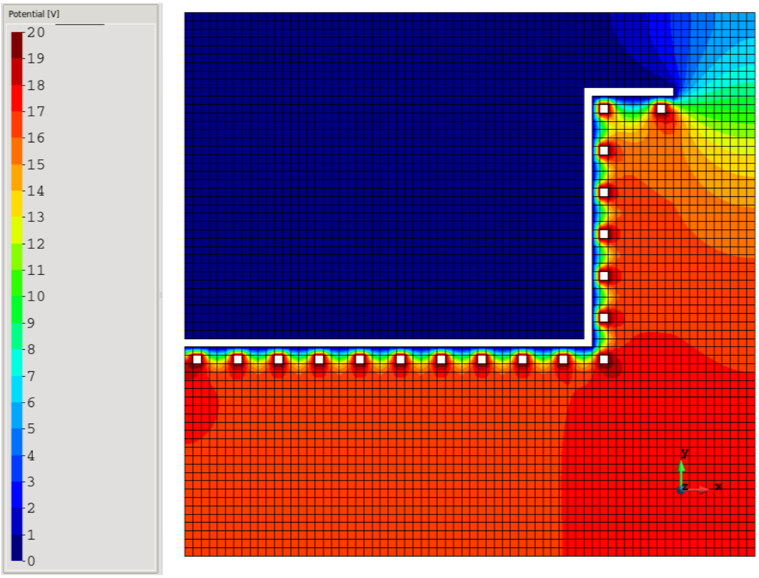

Fig. 2: Distribution of the electric potential.

The extraction process was prescribed by imposing Dirichlet boundary condition (zero Cl concentration to the deck and barrier top surface) lasting for 48 hours. Concentration from Fig. 1a was assumed as an initial condition. Fig. 3 shows distribution of the chloride concentration in two times 8.2 and 48 hours after the start of extraction. It can be seen in Fig. 3 that the process is highly efficient and after 48 hours leads to zero surface concentration and 80 % reduction of original concentration at the reinforcement layer. It can also be seen that still high chloride concentrations remain behind the reinforcement and are not extracted. The reason lies in the distribution of the electric field (Fig. 3) that does not allow the development of a higher potential gradient in this region. Thus, the extraction is only effective for the chlorides located in front and partially between the reinforcement bars. Chlorides located behind the reinforcement either stay there or need to be extracted later after their diffusion to upper concrete layers.

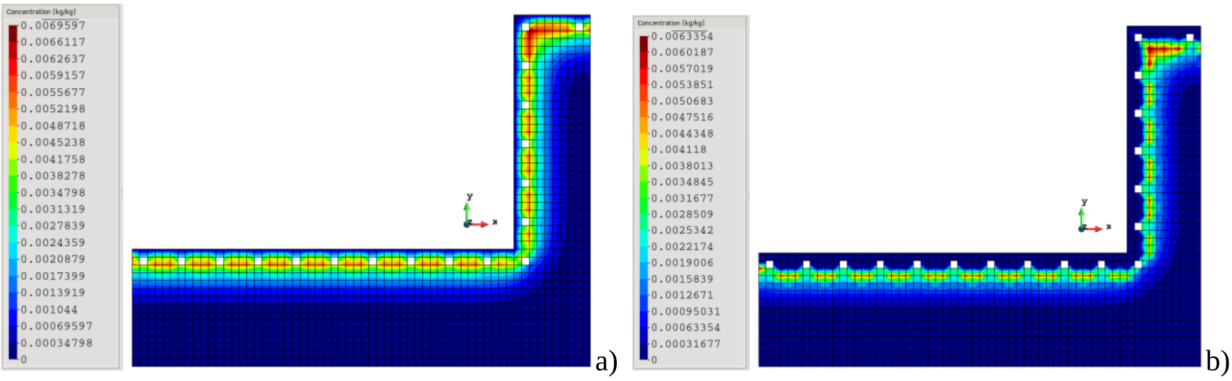

Fig. 3: Chloride concentration after extraction in time of: a) 8.2 hours; b) 48 hours).

4. Conclusions

The paper shows a numerical framework for the solution of convection-diffusion process applied to a practical example of chloride penetration and extraction on a bridge deck with vertical barrier. The framework is based on the finite element solution of the extended Nernst-Planck equation. The electric potential is described by the Gauss law of electrostatics and gives uneven distribution within the reinforced concrete structure. Electrochemical chloride extraction process is solved in the example to show the efficiency of the repair technology applied to a real structure and to show the effect of uneven potential gradient distribution. Although, the extraction was found to be very efficient between the deck surface and the reinforcement, caution must be paid to the regions between and behind the reinforcement where the potential gradient is small leading to decreased efficiency of the method.

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References

Angst, U., Elsener, B. and Larsen, C.K. (2009) Vennesland, Critical chloride content in reinforced concrete a review, Cement and Concrete Research 39 (12), 1122-1138.

Ann, K.Y. and Song, H.-W. (2007) Chloride threshold level for corrosion of steel in concrete, Corrosion Science 49 (11), 4113-4133.

Oh, B.H. and Jang, S.Y. (2007) Effects of material and environmental parameters on chloride penetration profiles in concrete structures, Cement and Concrete Research 37 (1), 47-53.

Xi, Y. and Bazant, Z. (1999) Modeling chloride penetration in saturated concrete, J. Mater. Civ. Eng. 11 (1), 51-57.

Černý, R. and Rovnaníková, P. (2002) Transport Processes in Concrete, Spon Press, London, New York, ISBN 0-415-24264-9.