MODELLING REINFORCEMENT CORROSION IN CONCRETE

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Abstract

A physio-chemical model for the simulation of reinforcement corrosion in concrete structures was developed. The model allows for simulation of initiation and subsequent propagation of reinforcement corrosion. Corrosion is assumed to be initiated once a defined critical chloride threshold is reached causing the formation of anodic and cathodic regions along the reinforcement. Critical chloride thresholds, randomly distributed along the reinforcement surface, link the initiation and propagation phase of reinforcement corrosion.

To demonstrate the potential use of the developed model, a numerical example is presented, that illustrates the formation of corrosion cells as well as propagation of corrosion in a reinforced concrete structure.

Keywords: Corrosion, Concrete, Numerical simulation.

1. INTRODUCTION

Within the past decades, models as well as standards and recommendations, see e.g. [1-3], have been developed to facilitate service life prediction of reinforced concrete structures. Numerous models have been developed describing the initiation and propagation of reinforcement corrosion. Commonly, the initiation phase of reinforcement corrosion is described by the transport of aggressive substances in the concrete, either chloride ions, see e.g. [4-6], or carbon dioxide, see e.g. [7], leading to initiation of corrosion. Models dealing with the propagation of reinforcement corrosion include often the impact of environmental conditions on the corrosion behaviour; see e.g. [8-10]. To the authors’ knowledge, all of the proposed models treat either the initiation or propagation phase of reinforcement corrosion in concrete structures explicitly.

The present paper introduces a physio-chemical model, which is capable of simulating both initiation and propagation of reinforcement corrosion. To demonstrate the potential use of the model, a numerical example is presented, which illustrates the formation of corrosion cells as well as propagation of corrosion in a reinforced concrete structure exposed to chloride. Future development is to include a more detailed thermodynamic description of the elec-
trochemical reactions for the anodic and cathodic regions as well as the impact of defects, such as cracks in the concrete as well as defects along on the concrete-steel interface, on the initiation and propagation phase of the corrosion.

2. EQUATIONS USED IN NUMERICAL MODELLING

The equations describe transport properties (Sections 2.1-2.4) and reinforcement corrosion (Section 2.5).

2.1 Heat transfer

Heat transfer within the concrete domain is described by Fourier’s law as follows:

\[ \nabla \cdot (\lambda(\theta_l) \nabla T) = \frac{\partial T}{\partial t} \]

With

\[ \lambda(\theta_l) = \lambda_{\text{conc}} + \lambda_w \theta_l \]

(1)

where, \( T \) is the temperature, \( \lambda(\theta_l) \) the thermal conductivity of concrete, \( \lambda_{\text{conc}} \), and water, \( \lambda_w \), depending on the moisture content \( \theta_l \), \( \rho \) the mass density and \( C_p \) the specific heat capacity.

2.2 Moisture transport

Coupled vapour and liquid water flow, which together yields the total moisture flow, is described as follows:

\[ \frac{\partial m_{\text{v+}}}{\partial t} = C_w \frac{\partial p_c}{\partial t} = -\nabla \left( \frac{D_v(\theta_l)}{R_v T} \nabla p_{\text{v}} + K_l(\theta_l) \nabla p_c + \rho_w g \right) \]

(2)

where, \( m_{\text{v+}} \) is the sum of the water vapour and liquid water content, \( C_w \) the moisture capacity, \( p_c \) the capillary pressure, \( D_v \) the vapour diffusion coefficient, \( \theta_l \) the moisture content, \( R_v \) the gas constant of water vapour, \( T \) the temperature, \( p_v \) the vapour pressure, \( K_l \) the liquid conductivity coefficient, \( \rho_w \) the density of water, \( g \) the gravity, and \( t \) the time. Using capillary pressure as the common driving potential for vapour and liquid water transport, Eq. 2 yields Eq. 3:

\[ \frac{\partial m_{\text{v+}}}{\partial t} = C_w \frac{\partial p_c}{\partial t} = -\nabla \left( \frac{D_v(\theta_l)}{R_v T} \frac{p_{\text{v,sat}}}{p_1 R_v T} \nabla p_c + K_l(\theta_l) \nabla p_c + \rho_w g \right) \]

(3)

where \( p_{\text{v,sat}} \) is the saturation vapour pressure and \( \varphi \) is relative humidity. The derivation of the mass balance equation for isothermal moisture transport (Eqs. 2 and 3) along with the corresponding constitutive equations can be found in the literature (see e.g., [11-12]).

Furthermore, a more thorough description of the moisture transport model implemented in the present model can be found in [13] along with information on the chosen capillary pressure curve describing the moisture storage [14], vapour transport coefficient and liquid water conductivity [15-17].

2.3 Multi-ion transport

Transport of ions is described by Nernst-Planck equation taking into account transport due to diffusion, migration and convection:
\[
\frac{\partial c_i}{\partial t} = \nabla \left( D_i \nabla c_i + z_i u_{mi} F c_i \nabla \varphi - c_i u \right)
\]  \hspace{1cm} (4)

where \( c_i \) is the ionic concentration, \( D_i \) the diffusion coefficient, \( z_i \) the charge number of the ionic species, \( u_{mi} \) the ionic mobility, \( F \) Faraday’s constant, \( \varphi \) the electric potential and \( u \) the velocity of the solvent. To account for the impact of the moisture content on the diffusion of the various ions, the following relation proposed by [18] is used:

\[
D_i(S_l) = D_i^0 S_l^\beta
\]  \hspace{1cm} (5)

where \( D_i^0 \) is the free diffusion coefficient in bulk water, \( S_l \) the degree of saturation and \( \beta \) a model parameter. Chloride binding is described through an apparent diffusion coefficient for chloride ions as follows:

\[
D_{cl,bind}(S_l) = D_{cl}(S_l) \frac{1}{1 + \alpha_{bind}/\theta_l (1 + \beta_{bind}c_{cl})^2}
\]  \hspace{1cm} (6)

where \( \alpha_{bind} \) and \( \beta_{bind} \) are model parameters.

### 2.4 Oxygen transport

Transport of oxygen within the model is described by a relation proposed by [19] (please note that the diffusion of dissolved oxygen is not taken into account as the resulting limiting corrosion current (see Eq. 12), controlling the kinetics of the cathodic reaction, is negligible).

\[
D_{O_2} = 1.92 \cdot 10^{-6} \theta_{por} (1 - RH)^{2.2}
\]  \hspace{1cm} (7)

where \( \theta_{por} \) is porosity and \( RH \) the relative humidity.

### 2.5 Reinforcement corrosion

The electric potential distribution is described by Laplace’s equation and Ohm’s law is used to determine the rate of dissolution of iron within the model:

\[
\nabla^2 \varphi = 0
\]  \hspace{1cm} (8)

\[
i_{corr} = \frac{1}{\rho_{el}} \frac{\partial \varphi}{\partial n}
\]  \hspace{1cm} (9)

where \( \rho_{el} \) is the concrete resistivity and \( n \) the direction normal to the steel surface. Butler - Volmer equations are used to describe the electrochemical kinetics for the anodic and cathodic regions of the steel surfaces, respectively. Assuming that the electrochemical reactions take place at separate electrodes and polarization is high, the Butler - Volmer equations can be replaced by Tafel equations for the anodic and cathodic regions. Taking into account the effects of activation and concentration polarization [20-21] the Tafel equations can be written as follows:

\[
i_A = i_{0,A} \gamma_A \quad \text{with} \quad \gamma_A = \exp \left( \frac{\ln 10 (\varphi_A - \varphi_{0,A})}{b_A} \right)
\]  \hspace{1cm} (10)
\[ i_C = i_{0,C} \frac{1 - \gamma_C}{1 + i_{0,C} / i_{\text{Lim}} \gamma_C} \quad \text{with} \quad \gamma_C = \exp \left( -\ln 10 \frac{\phi_C - \phi_{0,C}}{b_C} \right) \quad (11) \]

where \( i_{0,A}, i_{0,C} \) is anodic and cathodic exchange current density, respectively, \( i_{\text{Lim}} \) the limiting current density, \( \phi_A, \phi_C \) the anodic and cathodic potential, respectively, \( \phi_{0,A}, \phi_{0,C} \) the anodic and cathodic equilibrium potential, respectively and \( b_A, b_C \) the anodic and cathodic Tafel constant, respectively. Combining Faraday’s law with Fick’s law, the limiting current density accounting for a lack of oxygen at the cathodic regions of the steel surface can be given as follows:

\[ i_{\text{Lim}} = \frac{zFD_{O_2}}{\delta} c_{O_2} \quad (12) \]

where \( \delta \) is the diffusion layer thickness and \( c_{O_2} \) the oxygen concentration. To account for the impact of temperature on Eq. 10 and 11, the Tafel constants, \( b_A \) and \( b_C \), are described as follows [20]:

\[ b_A = \frac{RT}{F(1 - \alpha_A)} \quad \text{and} \quad b_C = \frac{RT}{F(1 - \alpha_C)} \quad (13) \]

where \( \alpha_A, \alpha_C \) is the anodic and cathodic charge transfer coefficient, respectively.

To describe the moisture dependence of the concrete resistivity a power law is used in the present model:

\[ \rho_{el} = \sqrt{\frac{1/\theta - a}{b}} \quad (14) \]

where \( a, b \) and \( c \) are modelling parameters.

To link corrosion initiation, i.e. the formation of anodic regions at the reinforcement surface, and subsequent propagation of reinforcement corrosion a conditional statement is defined along the reinforcement surface. Since the present model is dealing with chloride-induced corrosion the conditional statement comprises the definition of a critical chloride threshold for elements along the reinforcement surface, which might be defined as follows:

\[ BC_{\text{Steel}} = \begin{cases} i_A & \text{for } c_{cl} \geq c_{crit} \\ i_C & \text{for } c_{cl} < c_{crit} \end{cases} \quad (15) \]

where \( BC_{\text{steel}} \) defines the boundary condition along the steel surface, \( c_{cl} \) is the chloride concentration along the reinforcement and \( c_{crit} \) the critical chloride threshold defined along the reinforcement elements. Within the literature varying chloride threshold values can be found, ranging from 0 to around 0.4 % of weight cement [22], mainly influenced by the defects [23-24] present along the reinforcement as well as the electrochemical potential [22]. In the present model, the critical chloride threshold is varied randomly, ranging from 0 to 0.4 % of weight cement, along the reinforcement surface to represent an actual structure with defects present at the concrete steel interface. Also, possible impacts due to corrosion induced damages are not considered.
3. NUMERICAL EXAMPLE

3.1 Geometry and boundary conditions

To illustrate the potential use of the presented model, a simple beam geometry is modelled, see Fig. 1. The applied boundary conditions, i.e. annual variations of relative humidity, temperature, chloride concentration and oxygen concentration at the concrete surface, are given in Fig. 2.

![Figure 1: Model geometry with environmental boundary conditions and model domains.](image1)

![Figure 2: Environmental boundary conditions applied in the model, annual variation of a) relative humidity, b) temperature and c) chloride ions. The oxygen concentration is assumed to be constant at the concrete surface.](image2)

3.2 Material properties

An overview of the most important material properties, for the present numerical example, is given in Fig. 3 and 4. Information on the transport and material properties, i.e. transport coefficients, moisture storage and microstructure is shown in Fig. 3. Oxygen and chloride transport coefficients are presented in Fig.4 along with the electrochemical properties of the steel and concrete.

![Figure 3: Material properties overview.](image3)

![Figure 4: Transport coefficients and electrochemical properties.](image4)
3.3 Results and discussion

Results of the numerical model are given in Fig. 5 for selected times (in all plots the colours relate to the following times: black - 18.6 years, blue - 21.8 years, red - 24.8 years and green - 37.3 years). Fig. 5 a) illustrates the potential distribution and Fig. 5 c) the chloride concentration together with the defined critical chloride threshold along the reinforcement surface for selected times. From the results presented it can be clearly seen how anodic areas are forming along the reinforcement at different times as the critical chloride threshold is reached.

Fig. 5 b) illustrates the corrosion current density along the reinforcement for the selected times. Finally, the accumulated cross sectional reduction for the worst area of the reinforcement is given for the complete simulation time, i.e. 100 years, in Fig 5 d). It can be seen that within the initial 21 years, no cross sectional reduction is happening, as no corrosion has been initiated yet. After, initiation of corrosion an increase in the cross sectional reduction can be seen, which is mainly influenced by the environmental conditions, i.e. the moisture content and oxygen availability at the reinforcement surface. To illustrate the impact of the annual variations on the cross sectional reduction the subplot in Fig 5 d) gives the results obtained between 30 and 32 years of simulation. The impact of the environmental boundary conditions can be clearly seen in the subplot of Fig. 5 d) as the cross sectional reduction is varying within
the selected simulation time. Finally, a significantly reduced corrosion rate can be seen for the last 30 years, since all of the reinforcement is acting anodic and very slow micro cell corrosion is governing the cross sectional reduction now.

Figure 5: Results from numerical simulation along the reinforcement surface for selected times (black - 18.6 years, blue - 21.8 years, red - 24.8 years and green - 37.3 years), a) potential distribution, b) corrosion current density, c) critical chloride threshold and chloride concentration and d) cross sectional reduction over 100 years of simulation time.

4. CONCLUSIONS

A numerical model was described which allows for simulation of initiation and propagation of reinforcement corrosion in concrete structures. Corrosion is assumed to be initiated once a defined critical chloride threshold is reached causing the formation of anodic and cathodic regions along the reinforcement. Critical chloride thresholds, randomly distributed along the reinforcement surface, link the initiation and propagation phase of reinforcement corrosion. To demonstrate the potential use of the model, an example was given illustrating the impact of environmental boundary conditions on the initiation and propagation of reinforcement corrosion.

Future development is to include a more detailed thermodynamic description of the electrochemical reactions for the anodic and cathodic regions as well as the impact of defects, such as cracks in the concrete as well as defects along on the concrete-steel interface, on the initiation and propagation phase of the corrosion.
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