NUMERICAL MODELLING OF CHLORIDE INGRESS FOR SERVICE LIFE DESIGN OF CONCRETE STRUCTURES

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Abstract:
A numerical model is presented to simulate chloride ion ingress in concrete structures exposed to variable climatological conditions. The transport mechanisms of (free) chloride ions are both diffusion through and convection by pore water. This requires an advanced model for moisture transport in both the saturated and the non-saturated area. In case that the surface of the concrete structure is in contact with liquid water, the rate of the front of the saturated area is controlled by the balance between sorption and diffusion. The chloride binding isotherm is described by a linear or Langmuir type relation. The salient practical features of the model are: multi-layer, replacement of layers, imposing a chloride profile as initial situation. The model allows to predict the effect of maintenance actions on the service life of structural concrete, as illustrated for 2 cases from practice.

1. INTRODUCTION
Exposure to a saline environment is a major threat to the durability of reinforced concrete structures. The chloride ions, present in seawater and deicing salts, penetrate the concrete. At the end of the so-called initiation phase a critical chloride content has been reached at the depth of the reinforcement and corrosion occurs at a rate depending on the availability of water and oxygen. The length of the initiation period is often used as a first approximation for the service life.

The transport of chloride ions takes place by diffusion through and convection by the pore water. Pure diffusional transport only occurs in the submerged zone of marine structures. Where cyclic wetting/drying occurs, capillary suction must be taken into account.

In this paper an advanced numerical model is presented that simulates chloride ingress in structures exposed to cyclic wetting/drying. The multi-layer model allows to incorporate the effect of maintenance, e.g. applying a coating or replacement by old contaminated by new concrete. The model has been applied to quantify the effect of maintenance actions on the service life of infrastructural structures.
2. IMPLEMENTED MODEL AND OPTIONS

2.1 General

Meijers has developed a computational model to simulate chloride ingress in concrete [1]. This model has been implemented in the module CIMCON I of the software package Femmasse. With this model a coupled system of nonlinear differential equations is solved simultaneously for variable boundary conditions to predict the evolutions of temperature, humidity, and chloride ingress in a 2D space. Although consistent results have been achieved, the model is still too complex for practical applications and cannot capture capillary suction of water satisfactorily.

In CIMCON II the model has been simplified and various very practical extensions were introduced. The limitations and simplifications of this version are: 1D space, constant temperature and maturity. The principal extensions are: ‘forced’ sorption at a wet boundary, easy generation of multi-layers with different properties, replacement of one material by another at a certain time, options for moisture diffusion models, optional inclusion of delayed or irreversible chloride binding, easy generation of variable boundary conditions and storage of material properties in an explicative material database.

In the following paragraphs details of the implemented models are given.

2.2 Moisture transport models

The principal transport mechanisms of free chloride ions in porous building materials are convection by means of a moisture flux and diffusion through the moisture caused by a concentration gradient. To obtain reliable results in the prediction of chloride ion ingress, it is therefore important that the model for moisture transport is consistent. Advanced moisture transport models exist, like that of e.g. Kiessl [2]. The practical problem with these models is that many material parameters must be defined and are often difficult to determine experimentally. One of the objectives of CIMCON II was to obtain reliable results by means of a model based on a minimum of measurable material parameters. The model presented below is an important step towards this objective.

2.2.1 Desorption isotherm

A key material property in the moisture models is the desorption isotherm \( w(h,T,\alpha) \), which describes the evaporable moisture content \( w \) as function of moisture potential \( h \), temperature \( T \), and degree of hydration \( \alpha \) (maturity). A desorption isotherm can be generated from the material database for a given concrete composition, temperature, and maturity. The desorption isotherm can be linear or piecewise linear based on the implemented mathematical model [3].

2.2.2 Moisture potential

As moisture potential the macroscopic pore humidity \( h \) is chosen. The pore humidity is in equilibrium with the environmental relative humidity as described in [4]. This choice, instead of the moisture content, is essential in cases of inhomogeneous materials and multi-layer systems. More details can be found in [1].

2.2.3 Diffusion process

The driving force in the diffusion process is the gradient of the moisture potential. The governing equation is:
where \( q_w \) is the moisture flux in \([\text{kg/m}^2\text{s}]\); \( \lambda \) is the moisture permeability coefficient in \([\text{kg/ms}]\) and \( x \) is the coordinate in 1D \([\text{m}]\). The related diffusion equation reads:

\[
\frac{\partial w}{\partial t} = -\frac{\partial w}{\partial x} = C \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial h}{\partial x} \right)
\]

where \( w \) is the moisture content in \([\text{kg/m}^3]\); \( t \) is time in \([\text{s}]\); \( C \) is the moisture capacity \([\text{kg/m}^3]\).

As can be seen in Eq. 2, moisture capacity \( C \) is the derivative of the desorption isotherm with respect to moisture potential \( h \). It should be noted that moisture permeability coefficient \( \lambda \) depends generally strongly on moisture potential \( h \). This relation, however, is not always known from experimental results. In literature more data is available for diffusion coefficient \( D \) with unit \([\text{m}^2/\text{s}]\). If it is assumed that the following relation holds:

\[
\frac{\partial h}{\partial w} = \left( \frac{\partial w}{\partial h} \right)^{-1} = \frac{1}{C}
\]

then Eq.1 can be rewritten as:

\[
q_w = -\lambda \frac{\partial h}{\partial x} = -\lambda \frac{\partial h}{\partial w} \frac{\partial w}{\partial x} = -\frac{\lambda}{C} \frac{\partial w}{\partial x} = -D \frac{\partial w}{\partial x}
\]

from which the following relation is obtained:

\[
\lambda = DC
\]

The substitution of this relation in Eq.2 results in:

\[
C \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left( CD \frac{\partial h}{\partial x} \right)
\]

Eq.6 can be simplified if moisture capacity \( C \) is a constant, i.e. if the desorption isotherm is a linear function of moisture potential \( h \). The equation can be reduced to:

\[
\frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial h}{\partial x} \right)
\]

which is a “classical” diffusion equation used by many authors. Because moisture capacity \( C \) is generally not a constant, Eq.6 is used as diffusion equation in CIMCON II. Diffusion coefficient \( D \) depends also strongly on moisture potential \( h \). In CIMCON II two options have been implemented to describe this relation: Bazant’s model [5] and Mensi’s model [6].

### 2.2.4 Boundary conditions

Between the surface of concrete and the surrounding air generally an interface is defined to describe the resistance for evaporation. Meijers showed that the use of such moisture interface elements results in poor results [1]. That is why in CIMCON II only the moisture potential can be prescribed on the boundary as well as a no-flux condition to simulate symmetry. A large variety of functions for the prescribed moisture potential can defined by the user.
A difficulty is still the definition of moisture potential $h$ at RH 100 % and a wet surface. Such a situation occurs e.g. in a simple sorption test (Fig. 1). According to the presented model a moisture potential $h = 1$ must be applied at surface A and B, and in the simulation the sorption process starts equally from both sides (gravity effects neglected). This behaviour is generally not observed; the sorption from side B is far more dominant. To overcome this difficulty an option is made to apply a so-called “forced” sorption boundary condition. The details of this condition are explained below.

![Figure 1. Schematical representation of a sorption experiment in a closed container.](image)

### 2.2.5 The “forced” sorption boundary condition

As a first approximation the assumption has been made that moisture sorption takes place as a sharp wet front. For that purpose the problem domain is subdivided in a saturated and in a non saturated area, as can be seen in Fig.2.

![Figure 2. Subdivision of the problem domain in a saturated and a non saturated area.](image)

The moisture flux in the saturated area is defined as:

$$ q_w = -\lambda_s \frac{\Delta P}{x} $$

(8)

where $q_w$ is the moisture flux in [kg/m²s]; $\lambda_s$ the saturated moisture permeability coefficient in [kg/m²s]; $\Delta P$ the macroscopic capillary suction force [m] (height of water column) and $x$ the distance between the wet boundary and the sharp wet front [m].
It should be noted here that sign of $\Delta P$ is always negative (suction). The basic equation with respect to the moisture balance for an infinitesimal small time step $dt$ reads:

$$q_w \, dt = w_f \, dx$$

(9)

where $w_f = w_s - w_i$ is the amount of moisture to obtain saturation [kg/m$^3$] (Fig.2), in which $w_i$ is the initial moisture content [kg/m$^3$] and $w_s$ is the moisture content at saturation [kg/m$^3$].

The substitution of Eq. 8 in Eq. 10 and the integration in time results, after some algebraic manipulations, in:

$$x = \sqrt{\frac{-2\lambda_s \Delta P}{w_f}} \, t$$

(10)

The results from a sorption test are the penetration coefficient $B$ [m/s$^{0.5}$], the sorption coefficient $S$ [kg/m$^2 \cdot s^{0.5}$], and the amount of moisture to obtain saturation $w_f$ [kg/m$^3$]. The relation between $S$ and $B$ is given by:

$$S = Bw_f$$

(11)

The penetration equation for sorption conditions reads:

$$x = B\sqrt{t}$$

(12)

Comparing Eq.10 with Eq.12 and considering the relation given by Eq.11, Eq. 8 can be rewritten in terms of measured material data as:

$$q_w = \frac{B^2w_f}{2x} = \frac{BS}{2x}$$

(13)

Eq. 13 has been generalised for multilayer systems in CIMCON II.

So far the diffusion process which takes place in the non saturated area at the wet front and at the opposite boundary is not considered (Fig.2). As sorption proceeds the moisture flux is slowed down and the sharp wet front is smoothened by the diffusion process. The penetration depth can even become constant if the moisture flux caused by sorption balances the moisture flux caused by diffusion.

2.2.6 Numerical procedure

Because the spatial and time discretisation for the finite element method is performed in a standard manner it is not further explained here. The point of interest is the method in which the “forced” sorption boundary condition is realised. In a time step $\Delta t$ first the diffusion equation is solved for the entire problem domain (saturated and non saturated area) taking into account imposed boundary conditions (at the wet surface $h = 1$). After this step the elements are “(re)filled” until saturation in a sequential manner from the wet border. In the (re)fill procedure the length of the time step and flux equations are considered.

2.3 Chloride ion ingress model

It is assumed that chloride ions have no influence on moisture transport and moisture storage properties. Based on this assumption it was decided (from a computational efficiency point of view) to solve the chloride ion ingress problem in a staggered way. This means that
in a time increment first the moisture transport problem is solved and next that of the chloride ion ingress.

The basics of the chloride ingress model of program CIMCON I have also been implemented in program CIMCON II. Only some elementary equations are given here. The interested reader is referred to [1] for more details.

The total chloride content \( C_{\text{tot}} \) (kg Cl/m\(^3\) concrete) is related to the free chloride content \( C_{\text{free}} \) (kg Cl/m\(^3\) pore water) and the bound chloride content \( C_{\text{bound}} \) (kg Cl/kg cement gel) by:

\[
C_{\text{tot}} = \frac{W}{\rho_w} C_{\text{free}} + \xi_1 C_{\text{bound}} \quad (14)
\]

where \( W \) is the evaporable water content, \( \rho_w \) the density of water and \( \xi_1 \) the cement gel content (kg/m\(^3\)), calculated from \( 1.25 \alpha \) times the cement content.

In both CIMCON versions chloride binding can be described by a linear or Langmuir type relation. In the case of a linear adsorption isotherm, the bound chloride is related to the free chloride ions by:

\[
C_{\text{bound}} = \frac{C_{\text{free}}}{\xi_2} \quad (15)
\]

Equations (14) and (15) are then combined into:

\[
C_{\text{tot}} = C_{\text{free}} \left( \frac{W}{\rho_w} + \frac{\xi_1}{\xi_2} \right) \quad (16)
\]

As mentioned previously, in CIMCON II new options for delayed or irreversible binding are available.

### 2.4 Validation tests

Validation tests were first performed for moisture transport by pure diffusion at constant surface potential. The mathematical solution of the profile is reproduced exactly by the model. The results of capillary suction tests could be reproduced well too.

In validation runs of chloride ingress in submerged concrete, it was observed that setting the chloride diffusivity \( k_1 \) in the model equal to 0.9 to 1.0 times the effective diffusion coefficient (obtained from profile fitting) led to good agreement.

### 3. PRACTICAL APPLICATIONS

Phenomenological models for chloride penetration as developed within the Duracrete-project [7] are nowadays applied to predict the service life of chloride loaded concrete structures. In these models it is assumed that the surface chloride content is constant during the entire service life and that chloride transport takes place by pure diffusion. There are, however, many practical situations where these assumptions are not met. For instance, land structures may experience a prolonged period of drying before loaded with chlorides from deicing salts during frost periods. A pronounced convection zone will then develop in the chloride profiles of such structures due to capillary suction of chloride containing water. Maintenance actions like the application of a coating or hydrophobing agent will lead to a
variation with time of the surface chloride content. The numerical model described here is able to predict chloride penetration in such cases. Two examples are presented in this section.

3.1 Application of a hydrophobing agent

The effect of the application of a hydrophobing agent on the service life of a tunnel floor in the Netherlands has been modelled with Cimcon I. To find suitable boundary conditions for chloride in the numerical model, the results from an experimental investigation performed in the Netherlands [8] were used. In this investigation deicing salts were periodically applied to slag cement concrete stored outside. The effect of various hydrophobing agents on the chloride profile was studied. In comparison with untreated concrete, the surface chloride content was found to be reduced by a factor 2. This effect remained unchanged for at least 5 years. In practice a surface treatment with a hydrophobing agent needs to be repeated approximately every 10 years.

Based on these results the surface chloride content was assumed to half that of the untreated concrete ($C_{su}$) during the first 5 years, to increase linearly to $C_{su}$ in the next 5 years and then to remain constant. Any effect of the hydrophobing agent on the chloride diffusivity in the outermost layer was ignored in the simulations. The end of the initiation phase, where the critical chloride content is reached at the depth of the outer reinforcement, was taken as the end of the service life. Simulations were run for untreated and hydrophobed concrete. The concrete was assumed to be submerged, as agreed between contractor and principal. Chloride transport was therefore pure diffusional. It was found that the service life of the concrete floor was increased by 40 years. This increment is 4 times the lifetime, assumed for the hydrophobing agent.

3.2 Choice of most suitable maintenance actions based on simulations

The second case concerns 3 concrete bridges, located in the Persian Gulf. A small portion of the outer area of the box girders of the bridges shows salt scaling. Chloride penetration was found to be severe in these areas (Fig. 3). Currently, the following repair procedure is executed: cleaning with sweet water, filling cavities and surface finishing with epoxy resin, followed by the application of an epoxy coating. The question was raised if this procedure is sufficient to prevent rebar corrosion in the next 50 years. An alternative procedure, that was considered, is to remove the outer 20 mm of the salt infiltrated concrete, to replace it with sprayed concrete and seal it with a watertight epoxy coating.

With CIMCON II it is now possible to decide on the basis of simulations which repair procedure is most suitable. The alternative procedure was simulated as follows:

- a 2-layer model was applied, in which the outermost 20 mm consists of non chloride contaminated concrete and the underlying layer is the existing concrete, in which the chloride profile from Fig. 3 for a depth of 20 mm and more was introduced,
- the chloride boundary condition was set at no flux, representing the watertight epoxy coating.

For the current repair procedure the chloride profile of Fig. 3 is taken as the starting situation and the chloride boundary condition was again set at no flux.
Figure 3. Average chloride profiles of scaling and non-scaling areas of the box girders after 20 years of service. Note: \( m_c \) = cement weight.

In the Figures 4 and 5 the evolution with time of the total chloride profile is shown after execution of respectively the current and alternative repair method. In the first case the profiles are levelling off with time by unidirectional inward diffusion. In the latter case the first 20 mm with high chloride levels are replaced by sprayed concrete with low chloride content, after which the profile in the existing concrete levels off by diffusion in 2 directions: into the sprayed concrete and deeper into the existing concrete. The alternative repair method thus leads to a much stronger reduction of the chloride levels.

Figure 4. Evolution with time of chloride profile in scaled area after current repair method (sealing with epoxy coating).
Figure 5. Evolution with time of chloride profile in scaled area after alternative repair method. New, sprayed concrete is present in the first 20 mm.

4. CONCLUSIONS

The numerical model, implemented in CIMCON II, allows to describe chloride ingress in concrete structures much closer to reality than the currently available phenomenological models. The effect of maintenance actions like replacing chloride contaminated concrete by new concrete or the application of a coating or hydrophobing agent, on the service life of the structure can now be incorporated.

REFERENCES