MESO-SCALE SIMULATION OF CHLORIDE INGRESS IN CRACKED CONCRETE

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Abstract

A three-dimensional meso-scale lattice model for simulating chloride diffusion in uncracked and cracked concrete is presented. Both the fracture and the chloride diffusion simulations consider concrete as a three-phase composite, consisting of coarse aggregates, mortar matrix and the interface. Based on Fick’s second law, a discrete formulation using the lattice approach is proposed. Different phases are assigned with different properties (tensile strength, diffusion coefficient) in order to simulate the fracture and ingress behaviour. Also, a temperature dependent diffusion coefficient is taken into account. The effects of temperature and concrete heterogeneity on the chloride penetration are evaluated and discussed. In order to model the influence of cracking on chloride ingress, a relation between the crack width and the diffusion coefficient is adopted. Also in the case of cracked concrete, the effect of temperature is evaluated and discussed. This study shows that concrete temperature and composition have a marked effect on chloride ingress in concrete. In cracked concrete, although these factors also have an influence, the most significant is the effect of cracking. It is concluded that the lattice model can be successfully applied to model chloride diffusion in uncracked and cracked concrete on the meso-scale.

1. INTRODUCTION

Reinforced concrete infrastructures around the world are increasingly deteriorating. The most important cause for this is chloride induced corrosion of reinforcing steel. Chlorides from the environment can penetrate through the concrete cover and can cause the breakdown of the passive layer which forms around the rebars in concrete, and the corrosion process begins. Therefore, the time to corrosion initiation essentially depends on the speed of chloride penetration through the concrete cover.

Since it is still common to define the service life of a reinforced concrete structure as a time needed for the initiation of the corrosion process, it is necessary for an engineer to be able to predict this time. Besides the material (concrete composition), environmental (chloride exposure) and execution (curing) parameters, cracking can also have a marked influence on
this process. Reinforced concrete structures are never crack-free: cracking can occur due to mechanical or thermal loading, shrinkage, and other causes. Since this would further complicate the service life design process, it is usually omitted.

The influence of cracking on the chloride penetration has just recently become a focus of attention in the research community. A significant number of experimental studies has tried to quantify the effect of cracking on the diffusion of chloride ions in concrete (for an overview, see [1]). Some numerical models have also been proposed recently (e.g. [1-4]). Most of the models have focused on the macro-scale behaviour, i.e. concrete was modelled as a homogeneous material. On the other hand, a 2D model based on the truss-network approach proposed in [5] considered concrete as an assembly of coarse aggregates, mortar matrix, and the interface.

The presence of coarse aggregates in the matrix has two opposite effects on chloride penetration [6]. Firstly, since aggregates are, in general, non-permeable, their presence in the matrix increases tortuosity of the pores. Therefore, chloride ions have to move around the aggregate particles. Secondly, an interface which forms between the matrix and the aggregate is in general more porous, and therefore permeable, than the matrix itself. Consequently, penetration of chloride ions is faster in the interface.

In this paper, a 3D meso-scale lattice model which couples the diffusion of chloride ions and concrete cracking is proposed. Procedures for simulating both fracture and chloride ingress are presented.

2. METHOD

2.1 Fracture model

Lattice models have long been used for simulating fracture processes in concrete [7]. A continuum is treated as an assembly of truss or beam elements. In the model, all elements are linear elastic. When loading (or a prescribed displacement) is applied, a crack is formed by removing the element which has the highest stress/strength ratio. These steps are repeated until the system fails, or a pre-described value of either load or displacement has been reached. Realistic cracking patterns are therefore achieved. The model has been successfully used in fracture modelling of concrete on both the macro and meso-scale, fibre-reinforced concrete, and so on. Details on the underlying equations for the 3D analysis, element matrices, and implementation can be found in [8]. The only difference is that, in the current analysis, cross sectional areas of individual elements were determined using the so-called Voronoi scaling method [9]. The node arrangement was regular, and individual Voronoi cells were shaped as truncated octahedrons. The effects of domain boundaries on the Voronoi scaling were neglected.

2.1 Chloride diffusion model

The proposed model treats concrete as an assembly of one-dimensional “pipe” elements, through which chloride diffusion takes place. An assembly of these elements in 3 spatial dimensions enables the simulation of chloride penetration in 3D. The cross sectional area of each element is calculated using the Voronoi scaling approach, same as in the fracture model. In the present work, chloride diffusion is assumed to be the only parameter governing chloride transport. The model is, therefore, suitable for water saturated conditions only.

The governing equation for the chloride ingress simulation is the Fick’s second law:
\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \]  

(1)

Here, \( C \) is the chloride content, \( D \) the chloride diffusion coefficient, and \( x \) the spatial coordinate. Using the standard Galerkin procedure, the following system of linear equations arises (in matrix form):

\[ M \dot{C} + KC = f \]  

(2)

Here, \( M \) is the element mass matrix, \( K \) the element diffusion matrix, and \( f \) the forcing vector. The dot over \( C \) indicates a time derivative. If the forcing vector is discarded (i.e. no flux boundary conditions are applied), element matrices have the following form:

\[ M = \frac{[2 \quad 1]}{6\omega}, \quad K = \frac{[1 \quad -1]}{1} \frac{[1 \quad -1]}{1} \]  

(3)

Here, \( l \) is the element length, \( A \) element cross sectional area, and \( D \) its diffusion coefficient. Depending on the analysis, \( \omega \) takes values of 1, 2 or 3 for one, two, and three-dimensional cases, respectively [10]. Using the Crank-Nicholson procedure, the system of linear equations is discretized in time, and the following equation results:

\[ (M + \frac{1}{2}\Delta t \cdot K)C^n = (M - \frac{1}{2}\Delta t \cdot K)C^{n-1} \]  

(4)

This equation is then solved for each discrete time step (\( \Delta t \)) and chloride profiles are obtained.

The diffusion coefficient of chloride ions in concrete shows a strong dependence on temperature. In order to take that into account, a following approach is taken:

\[ D = D_{\text{ref}} \cdot \exp \left[ \frac{U}{R} \left( \frac{1}{T_{\text{ref}}} - \frac{1}{T} \right) \right] \]  

(5)

Here \( D_{\text{ref}} \) is the chloride diffusion coefficient at the reference temperature, \( U \) the activation energy of the chloride diffusion process (44.6 kJ/mol for \( w/c=0.5 \)), \( R \) the universal gas constant (8.314 J/(mol K)), \( T_{\text{ref}} \) the referent temperature (296 K), and \( T \) the concrete temperature. Due to the size of the analysed specimen, it is reasonable to assume that the temperature in it is constant and equal to the ambient temperature.

In order to take the effect of cracking into account, the diffusion coefficient of chloride ions was taken as dependent on the crack opening. In order to include that in the model, diffusion coefficient of every cracked single element was modified. The following bilinear relation was used, as proposed by Djerbi et al. [11], obtained from steady-state migration tests:

\[ D_{cr} (m^2/s) = 2 \cdot 10^{-11} w - 4 \cdot 10^{-10}, \text{ for } 30 \mu m \leq w < 80 \mu m \]  

\[ D_{cr} (m^2/s) = 14 \cdot 10^{-10}, \text{ for } w \geq 80 \mu m \]  

(6)

This implies that the diffusion coefficient in the crack is independent on the material effects, even if the tortuosity and roughness are different. Every cracked element was assigned with a diffusion coefficient depending on the level of damage (crack width). In this manner, chloride diffusion through the crack is simulated. It has to be noted that the chloride diffusion
coefficient of cracked elements was taken as temperature independent; in other words, equation (5) was only applied to the uncracked elements.

3. RESULTS AND DISCUSSION

3.1 General details

In the current approach, a computer generated concrete meso-structure is used [12]. As a basis, a concrete cube of 150x150x150 mm$^3$ is used. A slice of 10x10x50 mm$^3$ is cut from the cube and used in both the fracture and chloride penetration simulations (Figure 1). A lattice was projected on top of the meso-structure, with each of the voxels corresponding to a certain node. Different material properties were assigned to different elements (coarse aggregate, interface, and mortar matrix), depending on the nodes they connect.

![Figure 1. Generated concrete cube, a slice cut from it, and the corresponding lattice](image)

3.2 Fracture simulation

In order to induce cracking, the lattice is subjected to uniaxial tension in the longitudinal direction. This causes a through crack, as the splitting test used in [11]. In order to implement material heterogeneity, different mechanical properties were assigned to the aggregate, matrix and interface elements respectively (Table 1). This way, realistic material behaviour is simulated. Cracks generally occur at the weak interface, propagating around the aggregate particles and through the matrix.

<table>
<thead>
<tr>
<th>Phase</th>
<th>E (GPa)</th>
<th>$f_t$ (MPa)</th>
<th>$D_{ref}$ (m$^2$/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>75</td>
<td>16.25</td>
<td>1·10$^{-16}$</td>
</tr>
<tr>
<td>Mortar</td>
<td>30</td>
<td>6.25</td>
<td>1·10$^{-12}$</td>
</tr>
<tr>
<td>Interface</td>
<td>15</td>
<td>3.125</td>
<td>5·10$^{-12}$</td>
</tr>
</tbody>
</table>
Figure 2. Load-displacement curve for the specimen, together with the total crack width used in the chloride diffusion analysis. Note: Diffusion coefficients of elements are modified according to the local (element) crack width.

Figure 3. Side-view of the cracked specimen (displacements have been scaled for visibility).

3.3 Chloride ingress simulation

A prescribed chloride content of $5 \times 10^{-3}$ g/cm$^3$ of concrete was applied at the bottom of the specimen. Material heterogeneity with respect to chloride diffusion was implemented by assigning different chloride diffusion coefficients to the aggregate, matrix, and interface elements, respectively (Table 1). Consequently, coarse aggregate particles are considered as virtually impermeable inclusions in the mortar matrix, surrounded by a highly permeable interface. The twofold nature of aggregate inclusions with respect to chloride transport [6] is thus represented in the analysis. For the cracked case, equation 6 was used to modify the diffusion coefficients of cracked elements, depending on the crack width, but independent of their initial diffusion coefficients (i.e. independent of the material effects) [11]. The local crack width of an element was defined as a difference between the distance of its end nodes before and after the cracking.

Two different cases were analysed: uncracked and cracked. For the analysis of temperature effects, both the uncracked and the cracked case are tested for different temperatures: laboratory conditions (23°C), cold conditions (3°C) and hot conditions (40°C).

The effects of temperature on the maximum penetration depth of the uncracked specimen are shown in Figure 4. Here, penetration depth is defined as the depth at which the maximum chloride content is $1 \times 10^{-3}$ g/cm$^3$. 
The effects of temperature are coupled with the effect that the concrete meso-structure, i.e. the inclusion of impermeable concrete aggregates, has on the chloride penetration. Since the aggregates are impermeable, they obstruct the chloride diffusion process, even at higher temperature. Also, their presence causes a significant difference between the maximum chloride content and the average chloride content at a certain depth (Figure 4):
Since chloride penetration is much faster in cracked concrete, in the case of cracked specimen, temperature has a somewhat different effect on the maximum chloride penetration depth (Figure 7):

![Figure 7. The effect of temperature on maximum chloride penetration depth into a cracked specimen](image)

Figure 7. The effect of temperature on maximum chloride penetration depth into a cracked specimen

![Figure 8. Chloride penetration profile in cracked concrete-side view (23°C after 20 hours)](image)

Figure 8. Chloride penetration profile in cracked concrete-side view (23°C after 20 hours)

The increase in concrete temperature, which increases the diffusivity of concrete, seems to lead to lower maximum penetration depth. Instead of increasing the maximum penetration depth, this increase in diffusivity caused some of the chloride ions to penetrate perpendicular to the crack instead of penetrating further through the crack. Similar findings were reported by [13]: while monitoring the water uptake in fractured brick specimens by using X-ray radiography, they discovered that if the uptake capacity of the crack is too low to fill both matrix and the crack, a large part of the inflow gets sucked up by the matrix. In the case of chloride ions, therefore, this phenomenon might be caused by the increase in the “uptake” capacity of the matrix. In the analysed case, the cause was the temperature increase. It could also be caused by increased porosity: the higher the concrete porosity (and diffusivity), the more of the chloride ions from the crack would be imbibed by the matrix.

4. CONCLUSIONS

In the paper, the application of the 3 dimensional lattice model for simulating chloride diffusion on the meso-scale is presented. A procedure for simulating chloride diffusion of cracked concrete specimens, i.e. coupling with the fracture mechanics model, is also proposed, based on the crack-width dependent diffusion coefficient. Also, effects of the temperature on chloride ingress in both uncracked and cracked specimens have been included. For the uncracked case, simulation results indicate that the composite structure of concrete has a marked effect on chloride penetration profiles. The presence of coarse and impermeable aggregates and the highly porous interface in the matrix causes deviations of the chloride profile from the ideal (Fickian) behaviour: maximum chloride concentrations are significantly higher than the average concentrations at a certain depth. Temperature effects can increase chloride penetration significantly, causing the change in diffusion coefficients; high temperature increases maximum penetration depth significantly, while low temperature
decreases it. This implies that concrete in warmer regions is much more susceptible to chloride induced corrosion than concrete in mild and colder regions. For the cracked case, the effect of concrete heterogeneity was less pronounced: the (through) crack presents a main pathway for chloride ingress. This ingress is significantly faster than that in the uncracked case. Also, the effect of temperature is different than in the uncracked case: it causes a slowdown in the chloride penetration through the crack by causing the increased influx of chloride ions in the surrounding concrete.

It can be concluded that the lattice model can be successfully used to model chloride diffusion in composite cement based materials. Future work will include validation of the model and determination of input parameters. Also, other transport mechanisms, such as capillary suction, will be taken into account. Effects of chloride binding and time need to be evaluated as well.

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