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Service life prediction of reinforced concrete structures exposed to chloride environments – A multiscale approach

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ABSTRACT

Chloride-induced rebar corrosion is nowadays the main durability concern for reinforced concrete (RC) structures serving in chloride environments. The accurate prediction of the rate of chloride ingress into concrete and service life of RC structures can have enormous social and economic impacts. Chloride transport in concrete is a rather complicated process due to the chemical reactions between chlorides and cement matrix, i.e. chloride binding, and the complex microstructure of concrete, which is random over a wide range of length scales, from micrometres (pore) to centimetres (aggregate). This paper presents a multiscale modelling framework for estimating the chloride diffusion coefficient of concrete and service life of concrete structures that accounts for both changing microstructure due to cement hydration and chloride binding, and environmental conditions. A case study is presented to demonstrate the potential of the proposed multiscale modelling scheme for service life prediction. The multiscale simulations are validated with experimental data.

1. Introduction

Chloride-induced corrosion of reinforcing steel is one of the major causes of deterioration mechanisms in reinforced concrete (RC) structures. The entire chloride-induced corrosion process can be divided roughly into three stages, i.e. penetration of chloride ions and moisture into concrete, rust formation and expansion in surrounding concrete, and crack propagation due to continuous rust expansion. The first stage is the initiation stage, characterised by the ingress of chloride ions from concrete surface toward reinforcing steel. When the chloride content at steel surface reaches a critical or threshold value, the passivation film is broken down and the steel reinforcement starts to corrode. In most service life design codes, the first stage is considered dominant and regarded as the service life of RC structures.

Transport properties of concrete depend on the microstructure of concrete, especially the pore structure, and environmental conditions, such as degree of water saturation or relative humidity (RH), temperature and concentration of aggressive agents at concrete surface. Due to the continuing hydration of cement and physical/chemical interactions between the cement hydrates and the aggressive chemical species from the surrounding environment, the microstructure of concrete cover changes with time. Accordingly, the transport rate of species is time-dependent and depth-dependent. Most of the existing models attempt to take into account the effects of both age and environmental conditions by incorporating an ageing factor and environmental factors. DuraCrete (Brite EuRam III, 2000) is one of the frequently used models. In DuraCrete model, the apparent chloride diffusion coefficient, D_a, is given by $D_a = D_{ref} \times k_c \times k_e \times (t_{ref}/t)^n$, where D_{ref} stands for the chloride diffusion coefficient at reference time t_{ref}, k_c and k_e represent the curing factor and environmental factor, n is an ageing exponent reflecting the reduction of chloride diffusion coefficient with time and t is the exposure time. Prior to its application, values of k_c, k_e and n for various cement-based materials should be accurately determined. However, these values are still debatable up to now, although some empirical results have already been published and are used as basis for these values (Tang and Gulikers, 2007). Further studies on the determination of these parameters are required in order to predict the service life of RC structures accurately. The assessment of these empirical parameters by laboratory or in-situ tests is generally time-consuming. One way to acquire the aging factor n and curing and environmental factors k_c and k_e is by numerical simulations. In addition, in DuraCrete model D_a at different depths from the concrete cover surface is assumed to be identical, which is far from the real situation that D_a is depth-dependent.

The main purpose of this work is to present a case study of service life prediction of RC structures based on a multiscale modelling framework (Zhang, 2013 and Zhang et al. 2014). It improves our understanding of the relationship between transport properties and changing microstructure of cement-based materials induced by continuous cement hydration and chemical interactions of components of concrete with the aggressive chemical species from the environment. The inputs are mix proportions, curing age, exposure time and environmental conditions. The output is the time-dependent apparent chloride diffusivity in cement-based materials and prediction of the service life of RC structures.

2. Multiscale modelling framework

The proposed multiscale modelling scheme can be briefly described and illustrated in Figure 1. The main inputs consist of cement mineralogical composition, mixture (w/c ratio, contents and shapes of sand and coarse aggregates), age and environmental conditions (temperature, RH, etc.). With these inputs, the evolution of microstructure of cement-based materials can be generated by using computer-based cement hydration models (e.g. HYMOSTRUC3D, CEMHYD3D and µic) (Zhang et al., 2012) or experimental techniques (e.g. X-ray micro-CT) (Zhang and Jivkov, 2016). Based on the obtained microstructure, it is possible to estimate the transport properties in cement-based materials capturing the structural information at different scales. The obtained transport properties can then be used directly as input for service life prediction of RC structures.

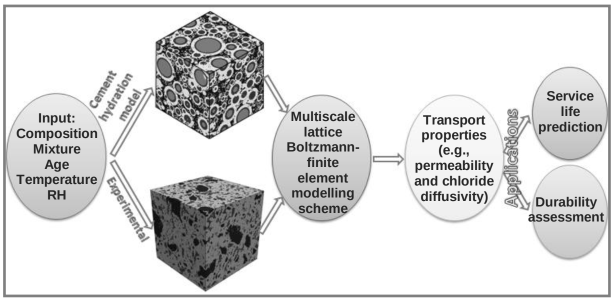

Figure 1. Schematic illustration of multiscale modelling framework for service life prediction.

Figure 2 shows the 3D microstructure of ordinary Portland cement concrete at multiple length scales, i.e., cement paste, mortar and concrete. Among them, the microstructure of hydrating cement paste is generally considered as a composite consisting of pores, hydration products and anhydrous cement grains. It can be modelled by HYMOSTRUC3D or acquired by high-resolution X-ray micro-CT along with a series of image processing and analysis. For more details, the reader is referred to (Zhang et al., 2012) and (Zhang and Jivkov, 2016). Here, the simulated microstructure is used as an example.

Mortar is simulated as a three-phase material consisting of sand, cement paste and interfacial transition zone (ITZ) between them. The spherical sand particles are placed in a three-dimensional periodic computational volume filled with cement paste in order of size from largest to smallest and no particles overlap. The region within 32 µm from aggregate-paste interface is defined as the ITZ, the 3D microstructure of which can be directly extracted from the ribbon paste simulated by using the HYMOSTRUC3D model. More details about the microstructure of ITZ can be found in (Zhang et al., 2014). The ITZ surrounding each sand particle is allowed to overlap each other and freely intersect the aggregate particles. Five sieve ranges for the sands varying from 0.125 mm to 4 mm are considered (see Table 1). The mesostructure of mortar is subsequently digitized into voxels. The ITZ thickness of 32 µm is chosen as the resolution (one voxel size on a side). Thus, for a typical mortar with size of 8 mm on a side, the system volume contains 250×250×250 voxels. An example of the digitized mesostructure of mortar can be seen in Figure 2. The volume fraction of sands in the mortar is 25.8%.

Concrete is simulated as a composite of coarse aggregate, mortar and ITZ between them. The thickness and microstructure of the ITZ in concrete is considered to be similar to that in mortar. The coarse aggregates are assumed to be spherical. The mesostructure of concrete is generated following a similar procedure as mortar by replacing sand with coarse aggregate and bulk paste with mortar. The rib size of cubic volume is 100 mm. The diameter of the used aggregates ranges from 4 mm to 16 mm. The total mass of coarse aggregates in concrete is 2653 g. Among them, 36% are in the sieve ranging from 4 to 8 mm and the size of the remaining 64% varies from 8 to 16 mm. The corresponding volume fraction of coarse aggregates in the concrete is approximately 30%. The simulated mesostructure of concrete is then digitized. An example is illustrated in Figure 2.

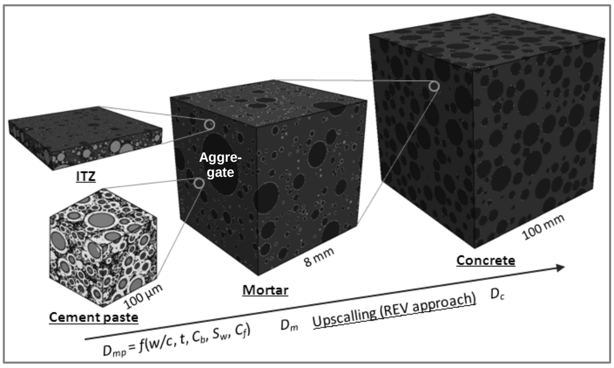

Figure 2. 3D microstructure of concrete at multiple length scales.

Table 1. Sieve ranges for sands in mortar

Sieve range (mm)	[2, 4)	[1, 2)	[0.5, 1)	[0.25, 0.5)	[0.125, 0.25)
Mass percentage (%)	27.0	25.2	19.2	15.3	11.6

As mentioned above, according to the multiscale modelling framework (see Figure 1) it is possible to investigate the transport properties in cement-based materials in a quantitative manner capturing the structural characteristics at each scale. The time-dependent chloride diffusivity in cement-based materials as a consequence of continuous cement hydration and chloride binding can be estimated. Other influencing factors, such as w/c ratio, chloride concentration, ITZ, and content and shape of aggregate on chloride diffusivity in cement-based materials can be taken into account as well. Moreover, the multiscale modelling scheme is capable of simulating the moisture distribution in cement-based materials and quantitatively analysing the effect of the degree of water saturation or humidity on transport properties in cement-based materials. For ease of application, the apparent chloride diffusivity of concrete, D_a, can be expressed as a function of different variables

$$D_a = D_{ref} f_1(w/c) f_2(t) f_3(C_b) f_4(S_w) f_5(C_f) f_6(ITZ) f_7(\emptyset_A) \quad (1)$$

where D_{ref} is defined as the chloride diffusivity at a reference condition, i.e. at reference w/c ratio, reference time, reference saturation degree, reference chloride concentration, reference aggregate content. $f_1(w/c)$ represents the effect of w/c ratio of the specimen, $f_2(t)$ denotes the effect of age of the specimen, which reflects the microstructure evolution of the specimen due to cement hydration with time, $f_3(C_b)$ stands for the dependence of chloride diffusivity on chloride binding, $f_4(S_w)$ indicates the effect of water saturation degree on the chloride diffusivity, $f_5(C_f)$ accounts for the influence of free chloride concentration on the chloride diffusivity, $f_6(ITZ)$ and $f_7(\phi_A)$ represent the influences of the ITZ and aggregate content on the chloride diffusivity, respectively. The effect of individual factors on the chloride diffusivity in concrete can be found in previous works (Zhang et al., 2012; Zhang et al., 2014).

3. Service life prediction – A case study

To demonstrate the potential of the proposed multiscale modelling framework to predict the service life of RC structures subjected to chloride environment, a case study is shown. The estimated apparent chloride diffusivity in concrete, D_a, taking into the various factors as expressed in Equation 1, is considered as an input variable for simulating the chloride ingress in concrete using non-linear finite element method. Ionic diffusion is assumed to be the sole mechanism of chloride transport. The governing equation for the chloride diffusion process in concrete can be written as $\partial C_f/\partial t = \nabla(D_a \nabla C_f)$. A typical RC member with size of 150×90×90 mm^3 is extracted from the bridge pier submerged in seawater and divided into three-dimensional elements with eight nodes. The three-dimensional finite element model of the RC member is shown in Figure 3. The assumptions for the finite element simulation are given as: (1) the used cement is Portland cement CEM I 42.5 N. After 28 days of curing, the mould is removed and the concrete structure is exposed to seawater; (2) the concrete is homogeneous and fully saturated; (3) the cover depth is assumed equal to 50 mm; (4) the initial chloride content, C_0, in concrete is considered zero; (5) only the left surface of the structure is exposed to chloride environment. Due to the concentration difference, chlorides move from the surface towards the steel reinforcement along the *x*-direction. Here, the surface chloride content, C_s, is assumed to be constant and equal to 0.5 mol/l; (6) over the past three decades, a number of global efforts have been made to determine an appropriate threshold for the critical chloride content, C_{cr}, which is normally defined as the corresponding chloride content at the steel surface to corrosion initiation. However, no general agreement on the value of C_{cr} has been achieved. As an example, C_{cr} is assumed equal to 0.2 mol/l. The input data used in the finite element simulation are summarised in Table 2.

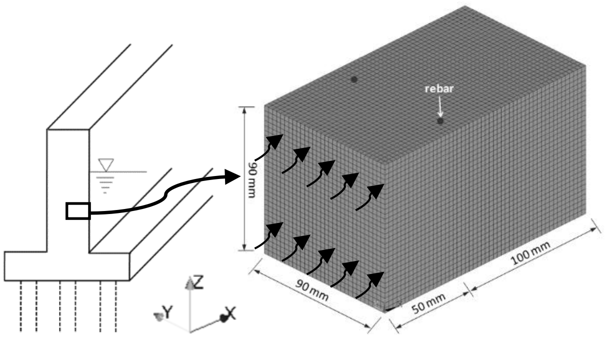

Figure 3. 3D finite element model of RC member.

Table 2. Input data used in the finite element simulation

Mixture		Parameters	
Cement type	CEM I 42.5 N	S_w (%)	100
W/c ratio	0.5	Cover (mm)	50
Sand (%)	25.8	C_o (mol/l)	0
Gravel (%)	42.0	C_s (mol/l)	0.5
Curing condition	Standard	C_{cr} (mol/l)	0.2
Curing Age (days)	28	D_e (m^2/s)	4×10^{-12}

Based on the given assumptions and initial boundary conditions, the transient diffusion equation for chloride can be solved at each time step to acquire the free chloride concentration at various depths in the RC member. Prior to each next time step, the apparent chloride diffusion coefficients at different depths are updated by incorporating the effects of age $f_2(t)$, chloride binding $f_3(C_b)$ and chloride concentration $f_5(C_f)$. Figure 4 depicts the penetration of chloride ions into RC member at an exposure time of 20 years and 100 years, respectively. Figure 5 shows the predicted chloride profiles in the RC member after various exposure time, which can be used to evaluate the corrosion initiation time. It can be seen that chloride ions move from the concrete surface along the diffusion direction and reach the steel reinforcement. The chloride concentration near the steel reinforcement increases with increasing exposure time. At a certain time (t = 65 years), the free chloride concentration at the steel surface reaches the critical chloride concentration, i.e. C_{cr} = 0.2 mol/l, which means that at this time depassivation of the embedded steel reinforcement is assumed to occur and the process of corrosion begins. According to the definition given in the previous section, the end of service life of this RC structure is estimated as 65 years.

To investigate the effect of cover depth of concrete on the service life, different cover depths of 40, 50, and 60 mm are considered. Other conditions are similar to those used in the previous simulations. This results in a service life of 41, 65, and 91 years, respectively, as shown in Figure 5. These findings indicate that the cover depth plays a significant role in the service life of RC structures.

For comparison, the DuraCrete model is also used to predict the chloride ingress in the RC member. The assumptions and initial boundary conditions are set to be the same as those in the above simulations. Figure 6 shows the predicted profiles after 5, 20, 50 and 100 years of exposure using the method in this study and the DuraCrete model, respectively. The chloride concentrations at different depths obtained from the DuraCrete model are obviously higher than those estimated using the multiscale modelling scheme in this study.

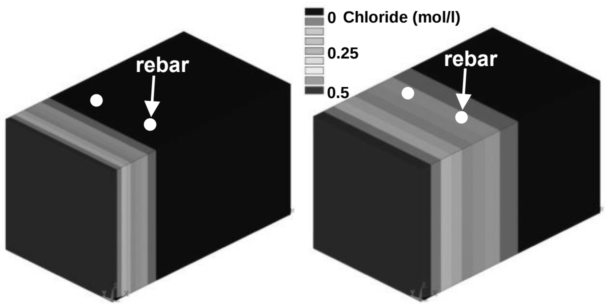

Figure 4. Penetration of chloride into RC member at various exposure time: (a) t = 20 years; (b) t = 100 years.

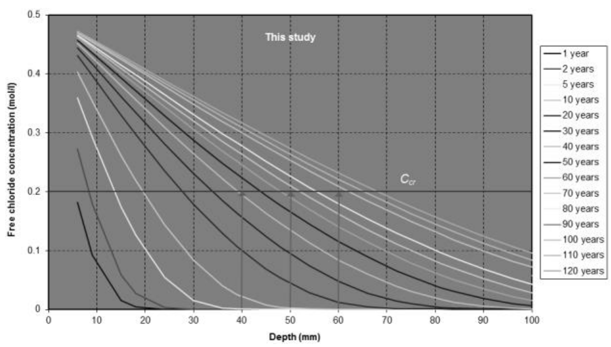

Figure 5. Predicted chloride profiles in RC member.

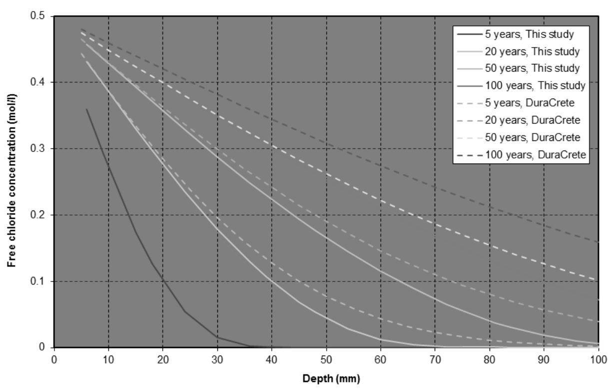

Figure 6. A comparison of the predicted chloride profiles.

4. Conclusions

A comprehensive multiscale modelling approach for predicting the chloride diffusivity in cement-based materials and service life of reinforced concrete (RC) structures has been presented. From the finding of the present study, the following conclusions can be drawn:

- Chloride diffusivity in concrete is not only time-dependent but depth-dependent. Environmental conditions affect chloride diffusivity in concrete as well. To accurately predict the service life of RC structures both microstructural features and environmental conditions should be taken into account.
- Cover depth of concrete has a significant influence on the predicted service life. For cover depths of 40, 50, and 60 mm, service lives are found to be 41, 65, and 91 years, respectively
- The proposed multiscale modelling framework provides a better insight into the transport phenomena in cement-based materials, and offers guidance and reference to engineers and researchers for predicting the service life and assessing the durability of reinforced concrete structures, and to designers for designing structures to meet their expected service life.

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