

MULTISCALE MODELLING SCHEME FOR PREDICTING SERVICE LIFE OF REINFORCED CONCRETE STRUCTURES – A CASE STUDY

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Abstract: Service life prediction with respect to chloride-induced corrosion of reinforcing steel is one of main concerns in the design or cost-efficient repair of reinforced concrete structures exposed to marine environments. This paper presents a multiscale modelling scheme for estimating the chloride diffusivity in cementitious materials and the service life of concrete structures that accounts for both changing microstructure of the concrete 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 simulation results are compared with those obtained using the DuraCrete model. The comparison indicates the predicted service life based on DuraCrete model is generally substantially shorter than that estimated using the approach in this study.

Keywords: Cement paste, Mortar, Concrete, Microstructure, Chloride diffusivity.

1. INTRODUCTION

Chloride-induced corrosion of steel reinforcement is one of the major causes of deterioration mechanisms in reinforced concrete 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, characterized by the ingress of chloride ions from the concrete surface toward the reinforcing steel. When the chloride content at the 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.

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, concentration of aggressive agents at the 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 considering an ageing factor and environmental factors. DuraCrete [1] is one of the frequently used models. In the DuraCrete model, the apparent chloride diffusion coefficient, D_a , is given by

$$D_a = D_{ref} k_c k_e \left(\frac{t_{ref}}{t} \right)^n \quad (1)$$

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 the chloride diffusivity with time, t is the exposure time. Values for k_c , k_e and n for various cement-based materials should be accurately determined in advance. However, these values are still debatable, although some empirical results have already been published and are used as basis for these values [2]. Further studies on the determination of these parameters are required to predict the service life of structures accurately. The assessment of these empirical parameters by laboratory or in-situ tests is generally time-consuming. One way to capture the aging factor n and curing and environmental factors k_c and k_e is by numerical simulation. Additionally, in the DuraCrete model D_a at different depths from the surface of concrete cover are identical. The spatial variation of D_a is not taken into account.

The main purpose of this work is to present a case study of service life prediction of reinforced concrete structures based on a multiscale modelling scheme [3]. It improves our understanding of the relationship between transport properties and changing microstructure of cement-based materials induced by continuous hydration of cement and physical/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 under saturated or non-saturated conditions and prediction of the service life of concrete structures.

2. DEFINITION OF SCALES

The heterogeneity of concrete manifests itself at different length scales. To develop an appropriate multiscale modelling scheme for fluid and ion transport in concrete, it is essential to consider the spatial scales involved and how the physical processes and characteristics of the system associate with the corresponding scale. In general, the length scales in concrete systems may vary from a nano-level in the order of 10^{-9} m to a macro-level on the order of 10^0 m for some regional applications. A scale hierarchy related to fluid and ion transport in concrete is defined, which consists of five elementary levels, i.e. nano-, sub-micro-, micro-, meso- and macro-scale [4,5].

A characteristic length scale of 10^{-9} m is generally considered the smallest length scale for characterizing the complex microstructure of cementitious materials. It is the scale of gel pores in the calcium silicate hydrate (C-S-H) solid gel formed at early ages by the hydration of two calcium silicates (C_3S and C_2S) in cement. The next scale, i.e. the sub-micro-scale, refers to the capillary pore, which manifests itself at a characteristic length scale of 10^{-7} m. At this scale, fluids are considered to be composed of a large number of molecules that collide with each other and move. The characteristic length scale of approximately 10^{-4} m refers to cement paste and the interfacial transition zone (ITZ), which are composite materials consisting of capillary pores, hydration products and anhydrous cement grains. Meso-scale refers to mortar and concrete, which is of the

order of 10^{-3} to 10^{-1} m. At this scale, the porous cement paste matrix, sand particle inclusions and ITZ between inclusions and matrix form the mortar and concrete. The meso-scale is a continuum scale in which the standard continuum modelling approach for fluid and ion transport in porous media can be applied. The macro-scale is of the order of 10^{-1} m or larger. With respect to transport properties in concrete at the macro-scale, continuum theory-based approaches, like finite element method or finite volume method, have been profusely employed for simulations.

The upscaling from the micro-scale to meso-scale is a crucial issue for modelling of fluid and ion transport in concrete across a range of scales. The scales of interest in this study are the micro-scale and the meso-scale. The link between micro- and meso-scale is of primary interest.

3. MULTISCALE MODELLING SCHEME

3.1 Overview

The proposed multiscale modelling scheme is briefly described and illustrated in Figure 1. The main input consists of cement mineralogical composition, mixture (w/c, contents and shapes of sand and coarse aggregates), age and environmental conditions (temperature, RH, etc.). With these inputs, the evolution of the microstructure of cement-based materials can be generated by using computer-based cement hydration models (e.g. HYMOSTRUC3D, CEMHYD3D, μ ic and so on) [6] or experimental techniques (e.g. X-ray micro-CT) [7]. 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 in cement-based materials can be used directly as input for service life predictions of reinforced concrete structures.

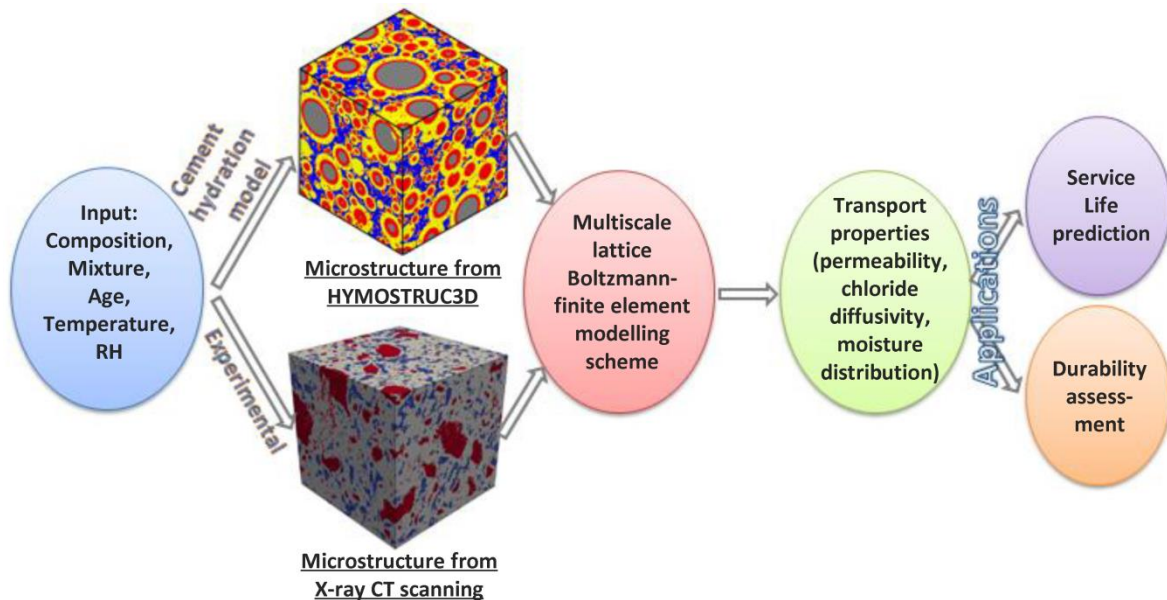


Figure 1: Schematic illustration of service life prediction of reinforced concrete structures using multiscale modelling scheme

3.2 3D structures: cement paste, mortar and concrete

As introduced in Section 2, 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 after a series of image processing and analysis. For more details, the reader is referred to [6] and [7].

Mortar is simulated as a three-phase material consisting of sand, matrix paste and ITZ. 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 20 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 HYMOSTRUC3D. More details about the microstructure of ITZ can be found in [4,5]. 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. The obtained mesostructure of mortar is subsequently digitized into voxels. The ITZ thickness of 20 μm is chosen as the resolution (one voxel size on a side). Thus, for a typical mortar with size of 5 mm on a side, the system volume is $250 \times 250 \times 250$ voxels. An example of the digitized mesostructure of mortar is shown in Figure 2. The total mass of sands in the mortar is 1.397 g with a corresponding volume fraction of 58%.

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.

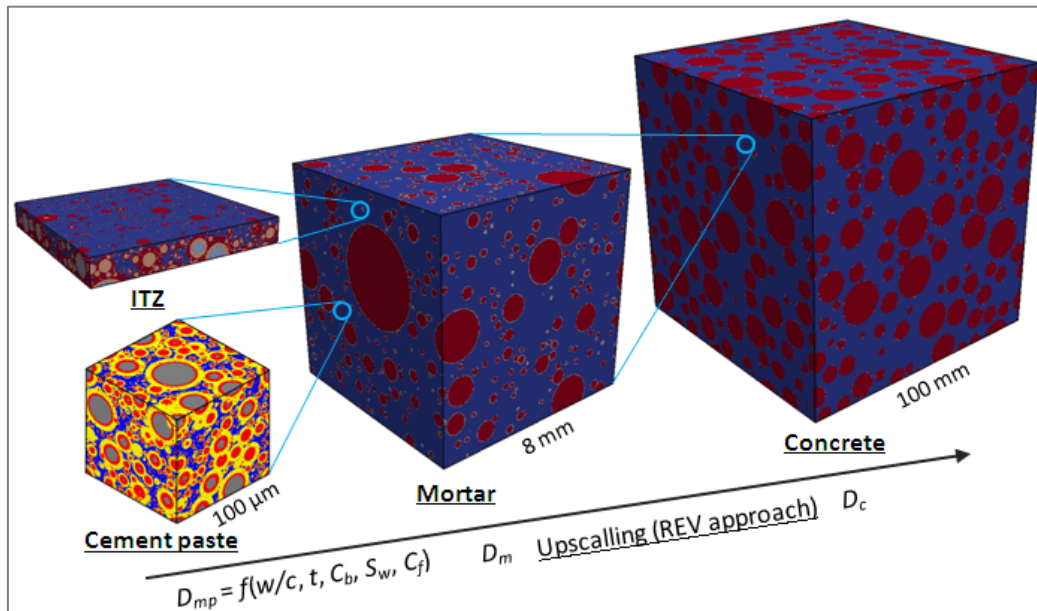


Figure 2: Multiscale modelling scheme for chloride diffusivity of concrete

3.3 Chloride diffusivity in concrete

As shown above, according to the multiscale modelling scheme (as shown in Figure 2) 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, aggregate content and aggregate shape 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 D_a is generally expressed as a function of different variables

$$D_a = D_{ref} f_1(w/c) f_2(t) f_3(C_b) f_4(S_w) f_5(C_f) f_6(ITZ) f_7(\phi_A) \quad (2)$$

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 [3-9].

4. SERVICE LIFE PREDICTION – A CASE STUDY

4.1 Input

To demonstrate the potential of the proposed multiscale modelling scheme to predict the service life of reinforced concrete structures subjected to chloride attack, a case study is shown. The estimated apparent chloride diffusivity in concrete, D_a , taking into the various factors as expressed in Equation 2, is considered as an input variable for simulating the chloride ingress in concrete using 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 reinforced concrete member with size of $150 \times 90 \times 90 \text{ mm}^3$ 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 reinforced concrete member is shown in Figure 3. The assumptions for the finite element simulation are given as follows.

- 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.
- The concrete is homogeneous and fully saturated.
- The cover depth is assumed equal to 50 mm.
- The initial chloride content, C_0 , in concrete is considered zero.
- 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

rebars along the x -direction. Here, the surface chloride content, C_s , is assumed to be constant and equal to 0.5 mol/l.

- Over the past three decades, a number of research efforts have been made to determine an appropriate threshold for the critical chloride content, C_{cr} . 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 summarized in Table 1.

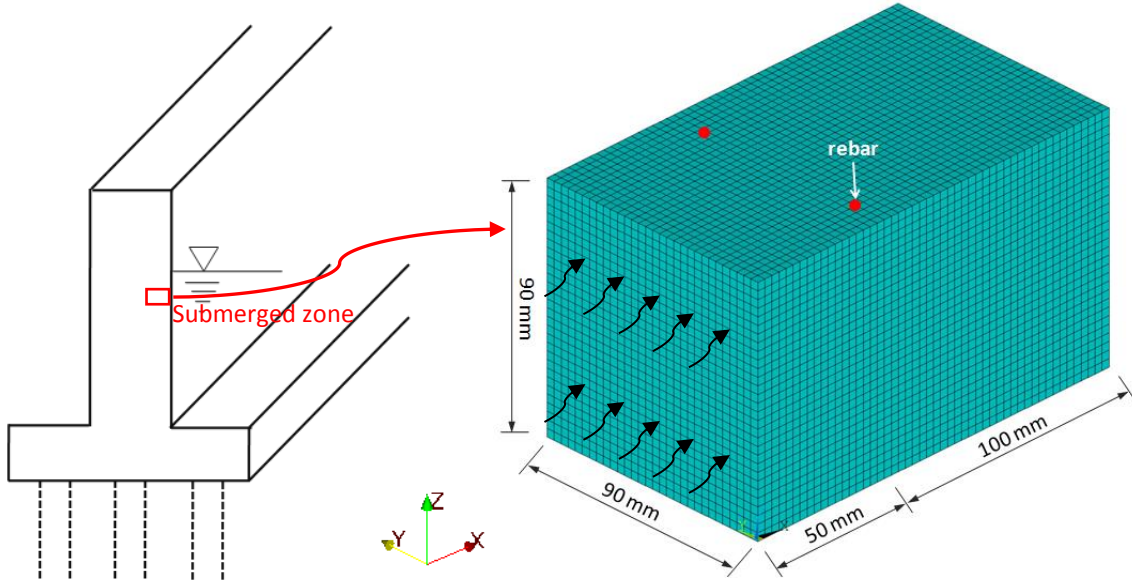


Figure 3: Three-dimensional finite element model for reinforced concrete member

Table 1 : 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 depth (mm)	50
Sand content (%)	25.8	C_0 (mol/l)	0
Gravel content (%)	42	C_s (mol/l)	0.5
Curing condition	Standard	C_{cr} (mol/l)	0.2
Curing age (days)	28	D_e (m ² /s)	4.0×10^{-12}

4.2 Output

Based on the given assumptions, initial and boundary conditions, the transient diffusion equation for chloride is solved at each time step to acquire the free chloride concentration at various depths in the reinforced concrete 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 shows the predicted chloride profiles in the reinforced concrete member after various exposure times, 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 rebars. The chloride concentration near the steel rebars increases with increasing exposure time. At a certain time ($t = 65$ years), the free chloride concentration at the rebar 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 rebar 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 reinforced concrete structure is estimated as 65 years, as illustrated in Figure 4.

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 4. These findings indicate that the cover depth plays a significant role in the service life of reinforced concrete structures.

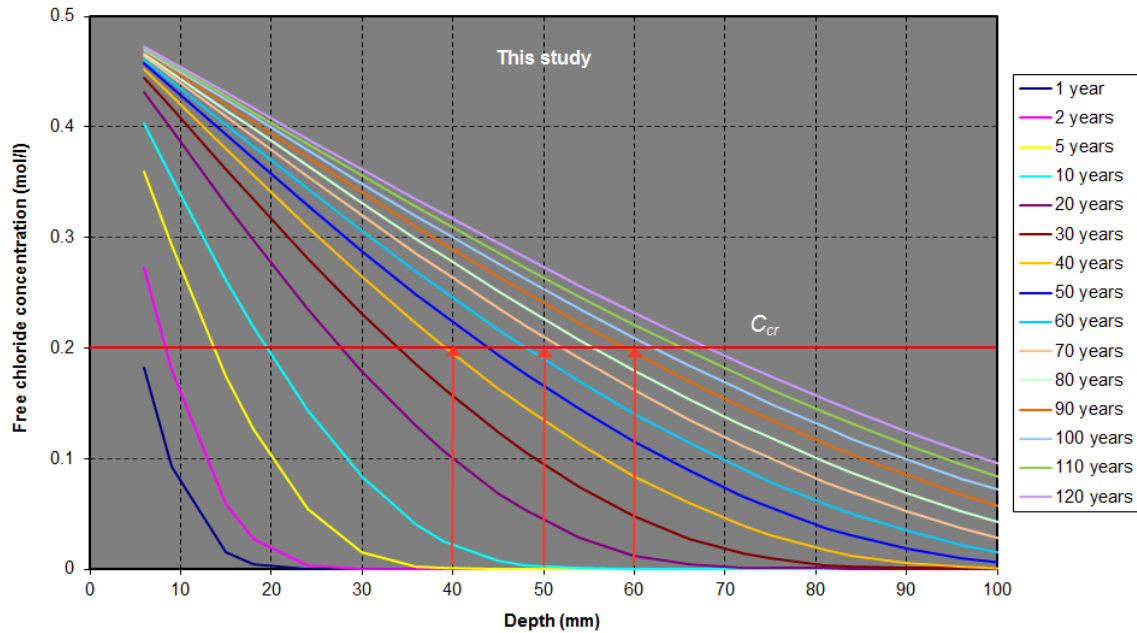


Figure 4: Predicted chloride profiles in the reinforced concrete member

For comparison, the DuraCrete model is also used to predict the chloride ingress in the reinforced concrete member. The assumptions, initial and boundary conditions used in the DuraCrete model are the same as those in the above simulations. The concrete age at the start of exposure t_{ref} is 28 days. The measured chloride diffusion coefficient of $w/c = 0.5$ concrete at curing age of 28 days with the rapid chloride migration (RCM) method is used, i.e. $D_{ref} = 1.32 \times 10^{-11}$ m²/s. Other input parameters for the submerged zone, such as curing factor k_c , environmental k_e and aging factor n are specified as those given in the DuraCrete guidelines [1]: $k_c = 0.79$; $k_e = 1.32$; $n = 0.30$. Based on these input data, the time-dependent apparent diffusion coefficient in concrete can be calculated according to Equation 1 and directly utilized to predict the chloride profiles in the reinforced concrete member after different periods of exposure, as shown in Figure 5.

It can be seen that the chloride concentration at the surface of steel rebars (depth = 50 mm) reaches the threshold chloride concentration at $t = 23$ years. Thus, the service life of reinforced concrete member is determined as 23 years. For cover depths of 40 and 60 mm, the service lives are estimated as 13 and 38 years respectively, which are much shorter than the predicted service life obtained from the multiscale modelling scheme in this study.

Figure 6 displays the predicted profiles after 5, 20, 50 and 100 years of exposure by 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.

The difference between them may be attributed to the following aspects:

- The input parameter used in the DuraCrete model is not chloride diffusion coefficient but chloride migration coefficient of concrete measured by RCM test, which is usually higher than the chloride diffusion coefficient. In this study the chloride diffusion coefficient obtained from multiscale modelling scheme is used, which is lower than the migration diffusion coefficient.
- After a certain period of exposure the chloride concentrations at different depths are different, as a result of which the bound chloride at different depths should be different. As a consequence, the time-dependent chloride diffusion coefficients are not identical at different depths, but depth-dependent. However, in the DuraCrete model the chloride diffusion coefficients at different depths are assumed identical, as a result of which the chloride concentrations at some depths may be overestimated.
- The chloride diffusion coefficient decreases with increasing chloride concentration. However, this factor is not taken into account in the DuraCrete model, which may cause the chloride concentration being overestimated and the predicted service life being underestimated. In this study, the time-, depth- and concentration-dependent chloride diffusion coefficient are implemented by storing the obtained results at the end of each time step and updating the diffusion properties of each element in the 3D model of the concrete member for the next time step of analysis.
- In the multiscale modelling scheme, some simplifications are made. For instance, the thickness of ITZ is fixed as 20 μm and the aggregates are considered as spheres, whereas in reality the ITZ thickness may be a function of the aggregate size and the aggregates are generally irregularly shaped. Therefore, the estimated chloride diffusivity may be a little different with the experimental results.

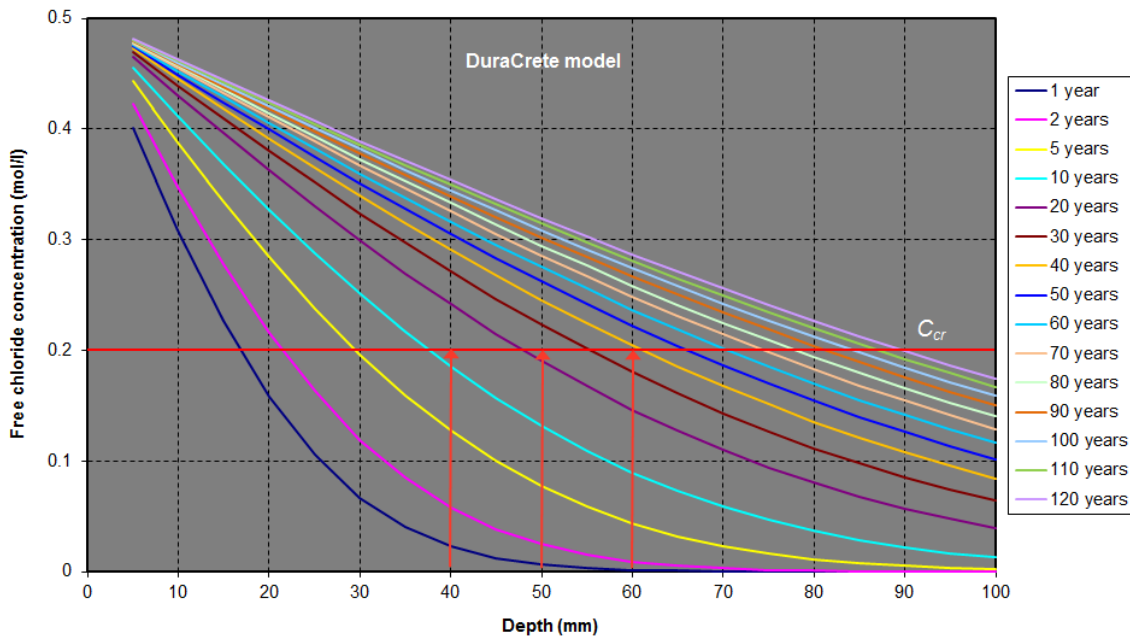


Figure 5: Predicted chloride profiles in the reinforced concrete member using DuraCrete model

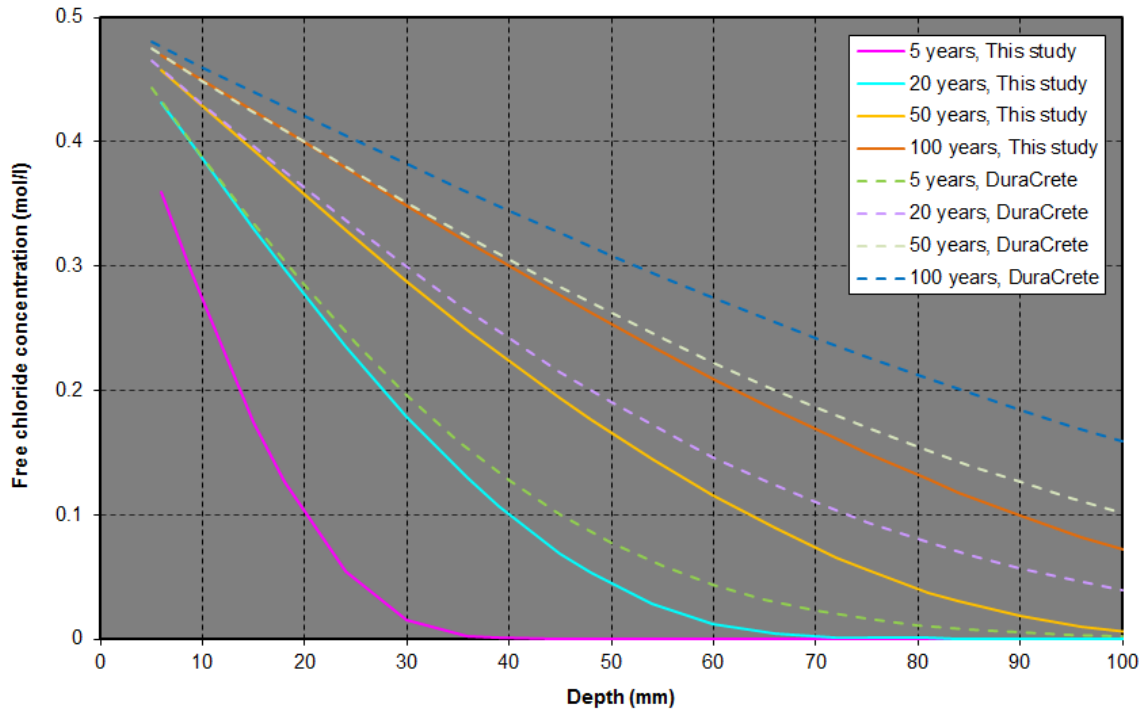


Figure 6: Comparison of the predicted chloride profiles in the reinforced concrete member by using the method in this study and DuraCrete model

5. CONCLUSIONS

A comprehensive multiscale modelling approach for predicting the chloride diffusivity in cement-based materials and service life of reinforced concrete 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 also depth-dependent. Environmental conditions affect chloride diffusivity in concrete as well. To accurately predict service life of reinforced concrete 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 scheme 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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