Mechanism analysis and model calculation of chloride ion diffusion in reinforced concrete structure

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Abstract. Chloride-induced corrosion of steel in reinforced concrete structures is one of the major causes of their deterioration over time. The analysis and research on the diffusion mechanism of chloride ions in reinforced concrete structures is still insufficient, and it is necessary to calculate the path of chloride ions based on theoretical models. In this paper, the fick's second law was used to describe the free chloride concentration evolution in concrete. The Monte Carlo simulation was used to predict the cumulative distribution of corrosion initiation of reinforcing steel. The results show that the calculated results of the established model are in good agreement with the measured results.

1 Introduction

Reinforced concrete (RC) structure was very commonly used due to its easy material resource, simplified preparation and low cost[1-4]. Corrosion of reinforcing steel due to chloride ingress had been a critical issue for the durability design and construction of RC structures in marine environments. The high alkalinity of the concrete pore solution provided a protection of reinforcing steel against corrosion by forming a thin oxide layer so called passivation film. When the concentration of chloride ion on the reinforcing steel surface reached a threshold value called critical concentration, depassivation of reinforcing steel initiated and corrosion started to occur [5-7]. Chloride ingress into concrete involved several transport processes such as diffusion (i.e., the motion of chloride ion within the pore solution caused by the concentration gradient), convection (i.e., the motion of chloride ion together with the pore solution within the concrete caused by the moisture gradient), capillary absorption and migration[8-12]. In this paper, finite element model was established to calculate corrosion initiation time.

2 The difference between 1-D diffusion and 2-D diffusion

2.1 Free chloride concentration evolution

The evolution of free chloride ion concentration at point A, B and C with time were shown in Figure 1. As can be seen, the chloride ion reached point B and C in the first place due to closer distance compared to point A. And they were almost same in the first 50 years, because the free chloride ion from left side had not yet diffuse to point B. When the free chloride ion from left side reached point B, chloride concentration at point B was gradually higher than point C. The free chloride ion concentration at point A was gradually higher than point B with time, because the influence of the two-dimensional diffusion is more significant for point A.

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Corrosion initiation time at point A, B and C for different concrete cover and each bay were shown in Figure 6 and 7. As can be seen, corrosion initiated earlier at point A than B regardless of thickness of concrete cover, concrete strength and external environmental condition. Therefore taking point A to represent the reinforcing steel placed in corner square cross-section would conform to the real case better.

2.2 Corrosion initiation time at point A and B for different concrete cover

As shown in Figure 6, as the concrete cover from 50mm to 70mm, the corrosion initiation time at point A was 13.48% to 16.32% smaller than point C for C50 concrete and 15.35% to 18.26% for C60 concrete. It was found that the thicker the thickness of the concrete cover was, the more remarkable the influence of 2-D diffusion was. And the influence was more remarkable for C60 concrete.

2.3 Finite element modelling

As shown in Figure 7, from Haikou bay to Dalian bay, the corrosion initiation time at Poona A was 16.32% to 15.38% smaller for C50 concrete and 18.26% to 17.41% for C60 concrete. It was found that the higher the diffusion coefficient was, the more remarkable the influence was.
3 Durability service life calculated by Monte Carlo method

The corrosion of reinforcing steel induced by chloride was a slow and complex process, which involved many material and environmental variables. The durability service life of RC structure assessed by deterministic method didn’t conform to the real case and probabilistic limit state method. As corrosion propagated very quickly after initiation, in this paper, corrosion initiation was taken as durability limit state which the structure was able to meet its specified durability requirements with an acceptable level of safety. When the failure probability of the RC structure exceeded acceptable failure probability, durability service life of RC structure was finished.

3.1 Statistical description of influencing parameter

1) Concrete cover $c$

Randomness of thickness of concrete cover need to be considered due to the construction deviation. At present, most of the researches at home and abroad showed that the thickness of concrete cover obeyed normal distribution. Table 1 showed a summarization of statistical description of thickness of concrete cover. In this paper, truncated normal distribution (least bound was 10mm) with coefficient of variation (COV) 0.2 was taken.

| Researcher       | COV  | Probability distribution                                      |
|------------------|------|--------------------------------------------------------------|
| Vu and Stewart   | 0.25 | truncated normal distribution (least bound was 15mm)         |
| Kirkpatrick et al| 0.10 | normal distribution                                          |
| Val and Trapper  | 0.25 | truncated normal distribution (least bound was 10mm)         |
| Muigai et al     | 0.20 | truncated normal distribution (least bound was 0mm)          |
| Duan et al       | 0.20 | normal distribution                                          |
| Moradian et al   | 0.24 | normal distribution                                          |

2) Surface chloride ion concentration $C_s$

Randomness of surface chloride ion concentration need to be considered due to rainfall, wind direction and force. Table 2 showed a summarization of statistical description of surface chloride ion concentration. In this paper, lognormal distribution was taken. For atmospheric zone and splash and tidal zone, the influence of the external environment was obvious. In consideration of different environment conditions, COV were respectively taken as 0.3 and 0.1. For submerged zone, the environment condition was stable, COV was taken as 0.1. Mean value of surface chloride ion concentration were respectively taken as 39.6 kg/m$^3$, 88.75 kg/m$^3$ and 123.36 kg/m$^3$ for atmospheric zone, splash and tidal zone and submerged zone.

| Researcher       | COV  | Probability distribution |
|------------------|------|--------------------------|
| Marques et al    | 0.10 | normal distribution      |
| Val              | 0.30 | normal distribution      |
| Val and Trapper  | 0.20 | normal distribution      |
3) Initial diffusion coefficient \( D_0 \)

Randomness of initial diffusion coefficient need to be considered due to deviation of material, match ratio, agitation, pour and curing. Table 3 showed a summarization of statistical description of initial diffusion coefficient. Lognormal distribution with COV 0.2 was taken.

| Researcher     | COV   | Probability distribution |
|----------------|-------|--------------------------|
| Vu and Stewart | 0.50  | lognormal distribution   |
| Duan et al     | 0.30  | lognormal distribution   |
| Moradian et al | 0.16  | normal distribution      |
| Kwon et al     | 0.08  | normal distribution      |
| Muigai         | 0.21  | gamma distribution       |

4) Critical concentration \( C_r \)

For atmospheric zone and splash and tidal zone that oxygen can easily reach the surface of the steel, uniform distribution with range 0.1%-0.25% (free chlorine ion as a percentage of weight of binder) was taken as critical content.

3.2 Kriging modeling

Monte Carlo method which was a statistic repeated sampling method was used to determine the corrosion initiation time distribution. The minimum sampling times was usually determined by the following equation:

\[
N \geq 100 / P_f \quad (1)
\]

Where N was minimum sampling times, \( P_f \) was the acceptable failure probability. In this paper, acceptable failure probability was taken as 10%, therefore minimum sampling times \( N=1000 \).

If each sample were calculated by finite element model, it would consume huge time. In this paper, Kriging model was used to estimate corrosion initiation time which can be set up with a small size train sample. Central composite design (CCD) method was used to establish the train sample. According to central composite design, 5 levels (\( \pm 1 \), \( \pm \alpha \) and 0) should be selected for each variable, which shown in Figure 4, where x and y axes respectively represented a variable. It contained 3 parts: factorial design (2n points at corner), a center point and 2n axial points, where n was the number of variables. So size of train sample was 25 for 4 variables.

![Central composite design for two variables schematic diagram](image)

There were three characteristics of Kriging model: 1) if the input point was one of the train sample points, the estimation was entirely accurate; 2) the nearer from the train sample points the input point was, the more accurate the estimation was; 3) if the input point was outside the scope of train sample points, it would produce larger deviation.
3.3 Precision testing

An example was used to verify the prediction precision of Kriging model in the whole space experiment. A C50 RC structure exposure to tidal/ splash zone located at Haikou bay was simulated. The mean of thickness of concrete cover was 50mm. With the distributions of \( C_s, C_r, D_0, \) and \( c \), train sample was established. Kriging model was constructed based on the toolbox “DACE” of MATLAB software. Corrosion initiation time calculated by finite element model called real value, and corrosion initiation time predicted by Kriging model called estimated value. As shown in Table 4, the estimated value and the real value to matched pretty well.

| The error       | Mean absolute error | Maximum absolute error | Mean relative error | Maximum relative error | Mean square error |
|-----------------|---------------------|------------------------|---------------------|------------------------|------------------|
| Point B         | 1.07 years          | 4.49 years             | 1.24%               | 3.65%                  | 1.50 years       |
| Point A         | 1.14 years          | 5.33 years             | 1.43%               | 3.11%                  | 1.66 years       |

4 Conclusion

In this paper, The influences of the variability on boundary chloride concentration, thickness of concrete cover, and chloride diffusion coefficient on cumulative distribution of corrosion initiation of reinforcing steel were studied thoroughly.

1. The corrosion initiation time for reinforcing steel placed in corner of square cross-section was lesser because of 2-D diffusion, especially for thicker concrete cover, higher concrete strength, and higher diffusion coefficient.
2. The influence of COV of surface chloride ion concentration on durability service life was not obvious. Increasing thickness of concrete cover and concrete strength would significantly improve the durability service life.
3. For different external environment and exposed zone, the durability service lives were largely different. The higher the ambient temperature, the worse the durability of the structure.

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