# A Microstructure Based Model for Chloride Penetration into Partially Saturated Concrete

*Wei-Jie Fan[1] and Xiao-Yong Wang[2]

*[1], [2] Department of architectural engineering, Kangwon National University, Chucheon 200-701, Korea*
*[2] wxbrave@kangwon.ac.kr*

## ABSTRACT

Chloride penetration is one of main reasons of steel rebar corrosion of reinforced concrete structures. For concrete structures in tidal zone, the exposure condition is wetting and drying cycles, surface zone of concrete is not fully saturated, and both diffusion and convection will affect chloride penetration profile. This paper proposed a microstructure based model for chloride penetration into partially saturated concrete. Frist, chloride diffusivity in fully saturated concrete is calculated using a hydration based model. The effects of mixing proportions and curing ages on chloride diffusivity are considered. Second, the effects of diffusion and convections on chloride penetration into partially saturated concrete are clarified. Different environment conditions, such as the ratios between wetting exposure time and dry exposure time, different initial degree of saturation of concrete, and different relative humidity in ambient environment, are considered. The analyzed results are compared with experimental results and a good agreement is found.

**Keywords:** chloride penetration; partially saturated concrete; diffusion; convection; environment conditions; microstructure based model

## 1. INTRODUCTION

In marine and coastal environments, penetration of chloride ions is one of the main mechanisms causing concrete reinforcement corrosion. Currently, most of experimental investigations about submerged penetration of chloride ions are started after the curing of concrete. (weijie fan 2015) Chloride-induced corrosion of steel bars has been identified as one of the most predominant degradation mechanisms in reinforced concrete structures. Corrosion damage in these reinforced concrete structures result in

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[1] Ph.D student
[2] Professor

cracking and spalling of the concrete. The corrosion damage in structures can also lead to future structural distress due to the loss of the strength of steel and concrete. So, service life prediction of reinforced concrete structures exposed to chloride environment is of great importance.

A large amount of work had done on service life simulation associated with chloride-induced deterioration. Diffusion as the main transport mechanism of chloride into concrete, under the assumption that the concrete cover is fully saturated.(gang lin 2009) In the wild, concrete structures in tidal zone, the exposure condition is wetting and drying cycles, surface zone of concrete is not fully saturated. So, developing a computational model of chloride ingress into nonsaturated concrete structures is necessary.

This paper proposed a microstructure based model for chloride penetration into partially saturated concrete. In this model, the interactions between the transfer of chloride and moisture are taken into account. The numerical model, in this paper, is implemented and validated by comparing numerical results with analytical solutions and experimental observations.

## 2. THEORETICAL FORMULATION

### 2.1. Moisture transport

In many papers, moisture transport in concrete is simulated using Fick's second law of diffusion, neglecting the chloride interaction with the solid phase. The moisture mass balance equation

$$\frac{\partial \theta}{\partial t} + \frac{\partial J_\theta}{\partial x} = 0 \tag{1}$$

Where $\theta$ is the moisture content in unit weight of concrete [kg/kg], and $J_\theta$ is the moisture flux [m/s] due to capillary suction and moisture diffusion.

$$J_\theta = \theta \mu = -D_\theta \frac{\partial \theta}{\partial x} \tag{2}$$

Where $D_\theta$ is the moisture diffusion coefficient [m$^2$/s].

the mean velocity of moisture($\mu$) flow is given as:

$$\mu = -\frac{D_\theta}{\theta} \frac{\partial \theta}{\partial x} \tag{3}$$

With Eq. (1), Eq. (2) becomes:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left( D_\theta \frac{\partial \theta}{\partial x} \right) \tag{4}$$

### 2.2. Heat transfer

In most field cases, chloride ion may penetrate into concrete through a combined mechanism of hydraulic advection, capillary suction, diffusion and thermal migration. Diffusion is the dominating mechanism in the case of saturated concrete, such as concrete submerged in seawater. (Xiaoyong Wang 2013)

Due to the concentration gradient between the exposed surface and the pore solution of the cement, chloride ions enter the concrete by ionic diffusion. This process is often described by Fick's 1st law of diffusion as following:

$$Jc = -Dc\frac{\partial C_f}{\partial x} + \mu C_f \tag{5}$$

Where $J_c$ is the flux of chloride ions due to diffusion (kg/m$^2$·s); $Dc$ is the effective diffusion coefficient when the concentration is expressive in kilograms per cubic meter of pore solution (m$^2$/s); $C_f$ is free chloride concentration (kg/m$^3$ of pore solution) at depth $x$ (m).

By the equation of mass balance

$$\frac{\partial C}{\partial t} + \frac{\partial J_C}{\partial x} = 0 \tag{6}$$

Eqs. (3) and (4) are rewritten as

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_c\frac{\partial C_f}{\partial x}\right) - \frac{\partial(\mu C_f)}{\partial x} \tag{7}$$

Base on Freundlich isotherm, the chloride binding can be expressed as

$$C_b = \alpha C_f^{\beta} \tag{8}$$

Where $C_b$ is the bound chloride content in unit weight of concrete [kg/kg], and $a$ and $\beta$ are the parameters.

In general, If $\beta=1$, $C=C_f+\alpha C_f$

Substituting Eq. (8) into Eq. (5), the governing equation for total chloride transport becomes:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\frac{D_c}{(1+\alpha)}\frac{\partial C}{\partial x}\right) - \frac{1}{(1+\alpha)}\frac{\partial(\mu C)}{\partial x} \tag{9}$$

The initial and boundary conditions used for the analysis are shown as follows:

Wet period:          $C_f=C_s$, at x=0;

Dry period:          $J_c=0$, at x=0;

where $C_s$ is the chloride concentration of salt solution in contact with the outer surface, and  is the thickness of the member.

### 2.3. Applications of the proposed numerical model

Current models for predicting the service time of reinforcement corrosion exposed

to chloride environment are focused on chloride penetration with considering the moisture transport and the chloride transport during drying and wetting periods which frequently occur in field applications. (Xiaoyong Wang 2013)

Chloride penetration into nonsaturated concrete under combined mechanism of diffusion and convection was simulated by using the model in this paper.

Fig. 1 and Fig. 2 are the numerical results under different drying–wetting periods, (wed: exposed to 1 mol/L NaCL solution; dry: exposed to dry environment). Different drying–wetting periods are showed in table 1.

Table. 1 Different drying–wetting periods used in the numeral calculations

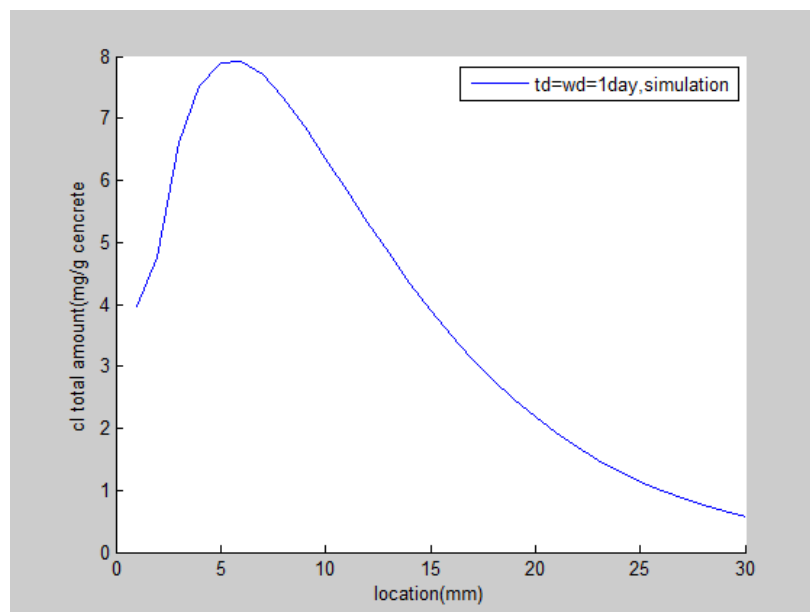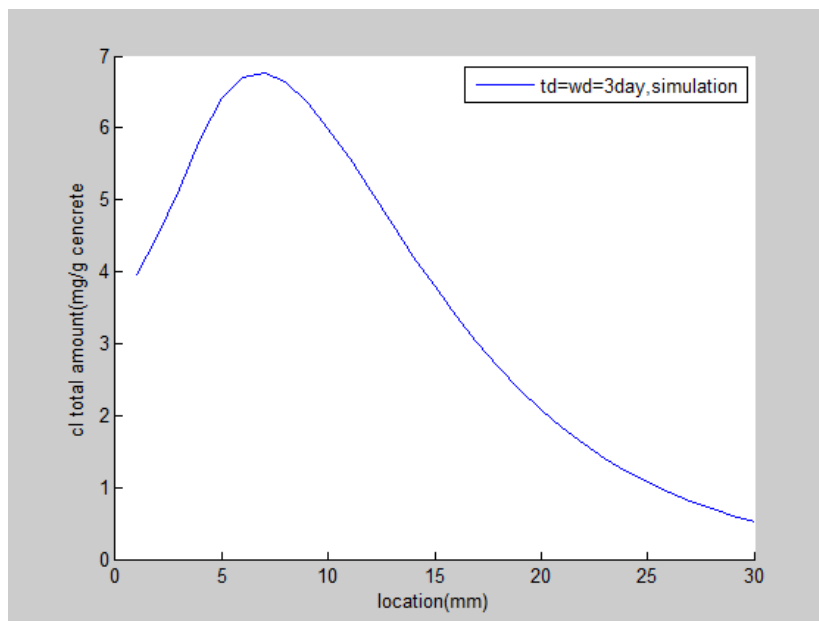|  | total time | Wed-time (in one circles) | Dry-time (in one circles) |
|---|---|---|---|
| Fig. 1 | 126 day | 1day | 1day |
| Fig. 2 | 126 day | 3day | 3day |



Fig. 1 the numerical results (td=wd=1day)

Fig. 2 the numerical results (td=wd=3day)

## 3. EXPERIMENTAL PROGRAM

### 3.1. Test method

In order to assess the validity of the proposed numerical model, comparisons of numerical results and experimental observations are conducted. The experimental results were obtained from the 126 days chloride penetration into concrete under different drying and wetting cycles.( Li CQ 2009) In the experimental test, two groups of specimens (100 mm * 100 mm * 100 mm cubes) were used to simulate chloride penetration under different cyclic drying and wetting processes. All faces, except one, were protected with epoxy paint so that chloride penetration into concrete could take place through one face only. The first group was exposed to 1 mol/L NaCL solution for 126 days, while the other one group was exposed to a series of different drying–wetting cycles, as illustrated in Fig. 3.
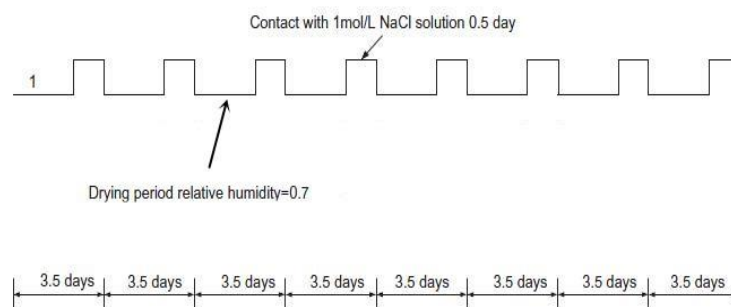


Fig. 3 Different drying-wetting periods used in the experiment

## 4. COMPARISONS WITH EXPERIMENT

In order to assess the validity of the proposed model, in this paper, comparisons of numerical results and experimental observations are conducted.

The first group was exposed to 1 mol/L NaCL solution for 126 days. The other one group was exposed to a series of different drying–wetting cycles, as illustrated in Fig. 3.

Fig. 4 is the comparisons between numerical results and experimental observations under exposing to 1 mol/L NaCL solution for 126 days.

Fig. 5 is the comparisons between numerical results and experimental observations under different drying–wetting periods (exposed to drying environment 3 days).

The analyzed results are compared with experimental results and a good agreement is found.
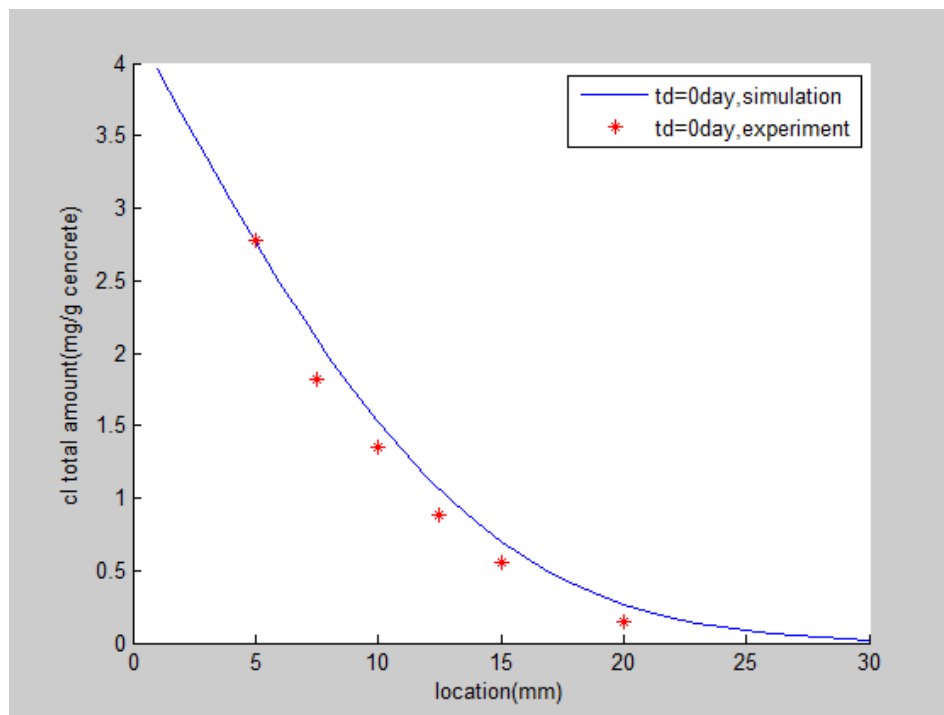


Fig. 4 Comparisons between numerical results and experimental observations under exposing to 1 mol/L NaCL solution for 126 days (drying days=0)
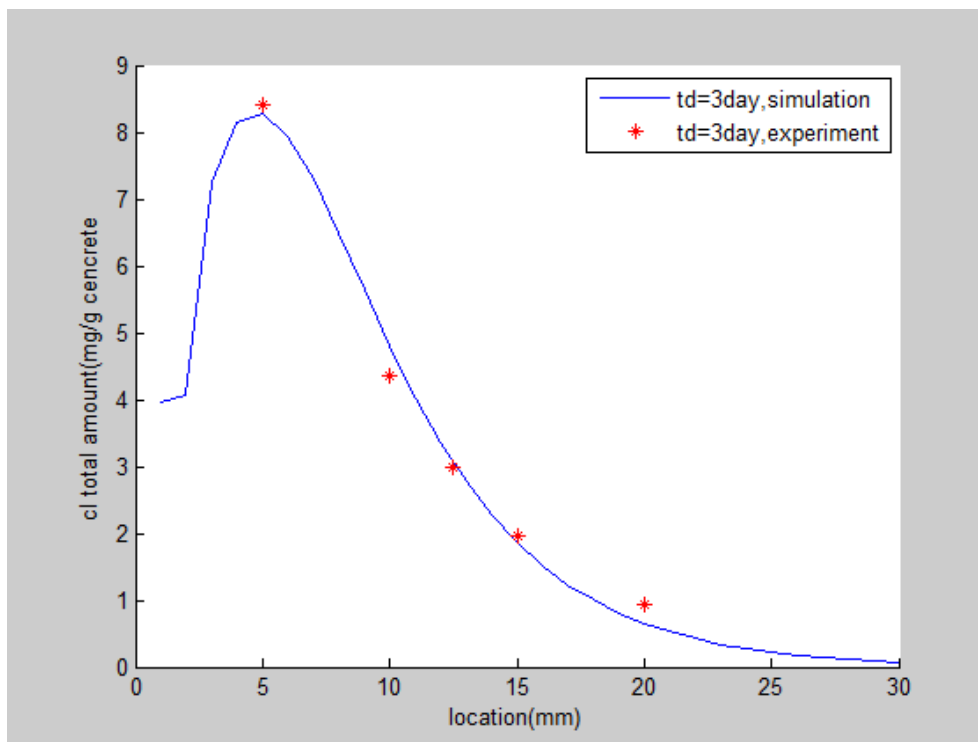
Fig. 5 Comparisons between numerical results and experimental observations under drying–wetting periods(drying days=3)


## 3. CONCLUSIONS

An integrated finite element-based numerical model has been developed in this paper for predicting chloride incursions of reinforced concrete structures exposed to chloride environments. This paper proposed a microstructure model for chloride penetration into partially saturated concrete. Frist, chloride diffusivity in fully saturated concrete is calculated using a hydration based model. The effects of mixing proportions and curing ages on chloride diffusivity are considered. The analyzed results are compared with experimental results and a good agreement is found. The present study and analysis enable the following conclusions to be drawn:

(1) At the same time, chlorine ion diffusion under wet and dry cycles more intense than the case of under saturation.

(2) The numerical results under different drying–wetting periods have obvious differences. This shows the need for an evaluation of chloride incursions of reinforced concrete structures exposed to drying and wetting cycles on the basis of wet-dry time allocation. The numerical results under different drying–wetting periods


**Acknowledgement**

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