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# Numerical solution of the governing equations of diffusion/convection in a stochastic framework: application to diffusion of chloride ions into concrete

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## Résumé :

*Les phénomènes de diffusion/convection sont à l’origine de nombreuses sources de défaillances de structures. Cet article présente la méthode de résolution par couplage des phénomènes, et propose une illustration dans le cas du transport d’ions chlorures dans du béton. Les effets de (1) le modèle de climat, (2) l’entrée de chlorures induite par la convection et (3) le flux des chlorures à une et deux dimensions, sur la probabilité d’initiation de la corrosion sont étudiés avec un exemple numérique. Les résultats montrent l’importance d’inclure des modèles étendus pour la pénétration des chlorures et l’aléa afin de faire une évaluation satisfaisante de la durée de vie.*

## Abstract :

*The ingress of aggressive substances by diffusion and/or convection into construction materials can reduce significantly the life-cycle of structures until early failure. This paper presents a numerical solution of the governing equations of diffusion/convection in a stochastic framework, which is focused on the diffusion of chloride ions into concrete. The effects of: (1) the weather model, (2) the chloride ingress induced by convection and (3) the one- and two-dimensional flow of chlorides into concrete, on the probability of corrosion initiation are studied with a numerical example. The results illustrate about the importance of including comprehensive models for both chloride penetration and randomness for a satisfactory lifetime assessment.*

**Mots clefs :** diffusion, convection, entrée des chlorures, béton armé, approche stochastique

## 1 Introduction

The ingress of aggressive substances by diffusion and/or convection into construction materials can reduce significantly the life-cycle of structures until early failure. In the case of reinforced concrete (RC), it is widely known that corrosion is commonly induced by ingress of chloride ions or carbon dioxide [1, 2]. This work is devoted to chloride-induced corrosion. The mechanisms by which corrosion affects the load carrying capacity of RC structures are the loss of reinforcement section, the loss of steel-concrete bond, the concrete cracking and the delamination. Therefore, in order to ensure a given serviceability and safety level during the life-cycle of the structure, it is important to study in detail the kinematics of the diffusion of chlorides into the concrete. Chloride ingress is controlled by the complex interaction between physical and chemical processes, which have been usually simplified as a diffusion problem governed by Fick’s second law. Furthermore, most studies use a simplified solution of Fick’s law where the chloride concentration at a given time and position is estimated as a function of an error function complement [1]. The classical diffusion approach evaluates the apparent diffusion coefficient as constant in time and space, and assumes that the chloride concentration in the surrounding environment remains constant and that the concrete is saturated. Saetta et al. [3] and Martín-Pérez et al. [4] proposed a numerical formulation to solve the governing equations of Fick’s law by using a finite element approach that accounts for:

- the chloride binding capacity (i.e. interaction between chloride ions and cement paste hydration products);
- the time-variant nature and the influence of the temperature, humidity and chloride concentration in the surrounding environment;
- the change (reduction) of the chloride diffusivity of RC with concrete age;
- and the chloride flow in unsaturated concrete.

Recently, this model was updated by Val and Trapper [5], who included a probabilistic framework. Their work was aimed at computing the probability of corrosion initiation by taking into account the influence of one and two-dimensional flow of chlorides. However, it does not consider the heat flow into the concrete and the influence of the time-variant stochastic nature of humidity and temperature in the corrosion initiation. Within the context, the present paper presents a probabilistic approach that takes into consideration the stochastic nature and the effects of temperature, humidity and surface chloride concentration in the model of Saetta et al. [3].

## 2 Modeling chloride penetration

This section presents a formulation permitting to treat the problem which considers the interaction between three physical problems: (1) *chloride ingress*, (2) *moisture diffusion* and (3) *heat transfer*. Each phenomenon is represented by a partial differential equation (PDE).

### 2.1 Governing equations

According to Martín-Pérez et al [4], the governing equations can be expressed in the following general form:

$$\zeta \frac{\partial \psi}{\partial t} = \underbrace{\text{div } J}_{\text{diffusion}} + \underbrace{\text{div } J'}_{\text{convection}} \quad (1)$$

where  $\psi$  represents the studied parameter,  $t$  is the time and the correspondence between  $\zeta$ ,  $J$ ,  $J'$  and the terms for the physical problem is presented in Table 1.

Table 1: Correspondence between Eq. 1 and governing differential equations.

Physical problem	$\psi$	$\zeta$	$J$	$J'$	$q_\psi^s$
Chloride ingress	$C_{fc}$	1	$D_c^* \vec{\nabla} C_{fc}$	$C_{fc} D_h^* \vec{\nabla} h$	$q_h^s$
Moisture diffusion	$h$	$\partial w_e / \partial h$	$D_h \vec{\nabla} h$	0	0
Heat transfer	$T$	$\rho_c c_q$	$\lambda \vec{\nabla} T$	0	0

For *chloride ingress*,  $C_{fc}$  is the concentration of free chlorides,  $h$  is the relative humidity and  $D_c^*$  and  $D_h^*$  represent the apparent chloride and humidity diffusion coefficients, respectively:

$$D_c^* = \frac{D_{c,ref} f_1(T) f_2(t) f_3(h)}{1 + (1/w_e) (\partial C_{bc} / \partial C_{fc})} \quad (2)$$

$$D_h^* = \frac{D_{h,ref} g_1(h) g_2(T) g_3(t_e)}{1 + (1/w_e) (\partial C_{bc} / \partial C_{fc})} \quad (3)$$

where  $D_{c,ref}$  and  $D_{h,ref}$  are reference diffusion coefficients measured to standard conditions [3],  $w_e$  is the evaporable water content, and  $f_i$  and  $g_i$  are correction functions to account for the effects of temperature, relative humidity, aging and degree of hydration of concrete. These functions are detailed in [2]. The term  $\partial C_{bc} / \partial C_{fc}$  represents the binding capacity of the cementitious system which relates the free and bound chlorides concentration at equilibrium [6]. Langmuir and Freundlich isotherms are the most used to estimate the binding capacity [7, 8]. Glass and Buenfeld found that chloride binding is estimated more accurately by Langmuir isotherm [8], consequently, such isotherm is used in this work.

For *moisture diffusion*, the humidity diffusion coefficient  $D_h$  is estimated by accounting for the influence of the parameters presented in [2] –i.e.,  $D_h = D_{h,ref} g_1(h) g_2(T) g_3(t_e)$ . The term  $\partial w_e / \partial h$  (Table 1) represents the moisture capacity which relates the amount of free water,  $w_e$ , and the pore relative humidity,  $h$ . For a given temperature this relationship has been determined experimentally by adsorption isotherms. According to the Brunauer-Skalny-Bodor (BSB) model [9], the adsorption isotherm depends on temperature, water/cement ratio,  $w/c$ , and the degree of the hydration attained in the concrete,  $t_e$ . Xi et al. [10] developed experimentally expressions for such parameters. This work adopts the BSB model to represent the moisture capacity.

Finally, for *heat transfer* (see Table 1)  $\rho_c$  is the density of the concrete,  $c_q$  is the concrete specific heat capacity,  $\lambda$  is the thermal conductivity of concrete and  $T$  is the temperature inside the concrete matrix after time  $t$ .

### 2.2 Boundary conditions

The boundary conditions at the surface consider the flux of  $\psi$  crossing the concrete surface,  $q_\psi^s$  (Robin boundary condition) [3]:

$$q_\psi^s = \underbrace{B_\psi (\psi^s - \psi_{env})}_{\text{diffusion}} + \underbrace{\psi_{env} q_\psi^s}_{\text{convection}} \quad (4)$$

where  $B_\psi$  is the surface transfer coefficient,  $\psi^s$  is the value of  $\psi$  at the exposed surface and  $\psi_{env}$  represents the value of  $\psi$  in the surrounding environment. The correspondence between Eq. 4 and the physical problems is also presented in Table 1.

## 2.3 Numerical solution

The flow of chlorides into the concrete is estimated by solving simultaneously the system of equations described by Eq. 1 and Table 1. This study uses the methodology proposed in [4], which combines a finite element formulation with finite difference to estimate the spatial and temporal variation of  $C_{fc}$ ,  $h$  and  $T$ . The finite element formulation uses three types of elements: (1) four-node linear rectangular, (2) bilinear one-dimensional semi-infinite and (3) bilinear two-dimensional semi-infinite. Semi-infinite elements are used to represent the existence of material beyond the unexposed bounds. For finite difference, the Crank-Nicolson method is the adopted scheme.

Figure 1 depicts the procedure to estimate the profiles of chlorides,  $C_{fc}(x; t_i)$ , humidity,  $h(x; t_i)$ , and temperature,  $T(x; t_i)$ , for the flux in one dimension –i.e.,  $x$ . For the first iteration ( $i = 1$ ), by taking into consideration the initial temperature into the concrete,  $T(x; t = 0) = T_{ini}$ , the temperature profile is obtained from the chloride ingress equation. The humidity profile is determined from the moisture diffusion equation by using the initial humidity into the concrete,  $h(x; t = 0) = h_{ini}$ , and the temperature profile estimated previously –i.e.  $T(x; t_1)$ . Finally, the chloride profile is computed from the heat transfer relationship, by accounting for the initial chloride concentration into the concrete,  $C_{fc}(x; t = 0) = C_{fc,ini}$ , and the profiles of temperature and humidity before determined. For the next iteration ( $i = 2$ ), the profiles obtained from  $i = i - 1$  are established as the new initial conditions. An iterative procedure is implemented to find the profiles of humidity and chlorides because the diffusion coefficients and isotherms also depend on the actual profiles of humidity and chloride concentration.

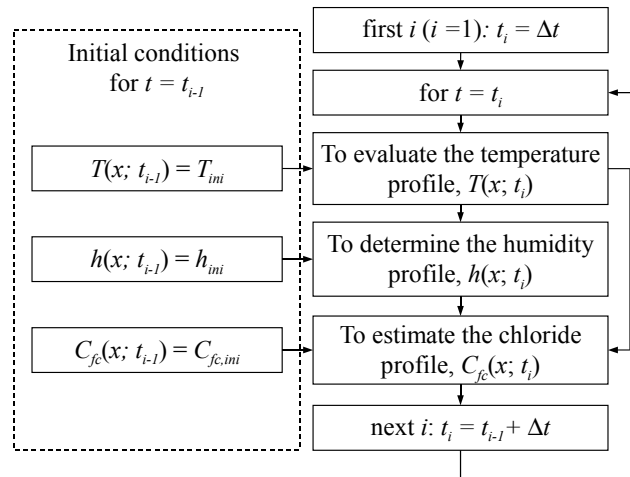


Figure 1: Algorithm of solution of the system of PDEs

## 3 Stochastic approach

There is significant uncertainty related to environmental conditions, material properties, cover and model parameters. Therefore, to give appropriate estimations of chloride ingress into concrete, the model exposed in section 2 is introduced into a stochastic framework. This section describes the adopted probabilistic approach to this problem.

### 3.1 Modeling of weather: humidity and temperature

To make a good estimation of the time to corrosion initiation, it is important to implement a model that reproduces realistically the temperature and the humidity during the period of analysis. In this context, stochastic process models were used to represent the random nature of the weather parameters. Taking into account the simplicity of the implementation and the computational time, Karhunen-Loève expansion is appropriate to represent the weather variables, as the process autocorrelation is known by the weather conditions. Let  $\kappa(t, \theta)$  be a random process, which is function of the time  $t$  defined over the domain  $\mathbf{D}$ , with  $\theta$  belonging to the space

of random events  $\Omega$ ,  $\kappa(t, \theta)$  can thus be expanded as follows [11]:

$$\kappa(t, \theta) \simeq \bar{\kappa}(t) + \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i} \xi_i(\theta) f_i(t) \quad (5)$$

where  $\bar{\kappa}(t)$  is the mean of the process,  $\xi_i(\theta)$  is a set of normal random variables,  $n_{KL}$  is the number of terms of the truncated discretization,  $f_i(t)$  are a complete set of deterministic orthogonal functions and  $\lambda_i$  are the eigenvalues of the covariance function  $C(t_1, t_2)$ . Since closed-form solutions for  $f_i(t)$  and  $\lambda_i$  are obtained for an exponential and triangular covariances [11], this paper assumes that the processes of temperature and humidity have an exponential covariance. To account for the seasonal variations of temperature and humidity, it is supposed that the mean of the process,  $\bar{\kappa}(t)$ , follows a sinusoidal trend:

$$\bar{\kappa}(t) = \frac{\phi_{max} + \phi_{min}}{2} + \frac{\phi_{max} - \phi_{min}}{2} \sin(2\pi t) \quad (6)$$

where  $\phi_{max}$  is the maximum temperature or humidity,  $\phi_{min}$  is the minimum temperature or humidity and  $t$  is expressed in years. Figure 2a shows the deterministic time-variant trend and a stochastic realization for the temperature. It is important to notice that there are extreme values for the stochastic realization. Since during real exposure there are temperatures/humidities higher or lower than the seasonal trend, it is can be claimed that this approach leads to more realistic assessments.

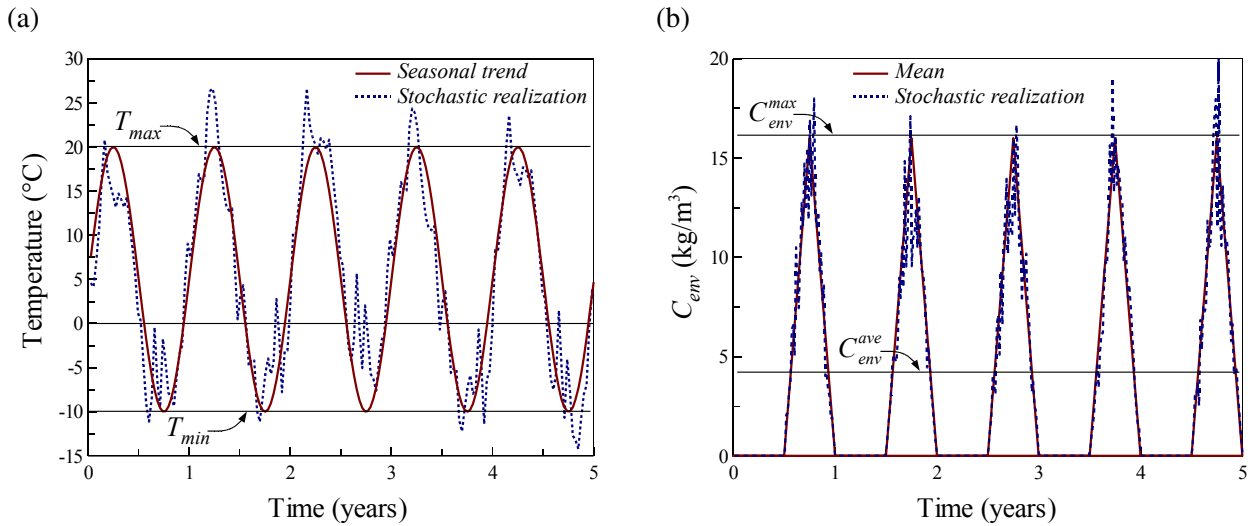


Figure 2: Stochastic realizations of: (a) temperature and (b)  $C_{env}$

### 3.2 Modeling of surface chloride concentration

The model described in this subsection is used to represent the surface chloride concentration induced by de-icing salts. Due to lack of data about the variation of  $C_{env}$  during the exposure time and that various studies indicate that  $C_{env}$  has a log-normal distribution [12, 13], the stochastic process representing  $C_{env}$  is generated with independent log-normal numbers (log-normal noise). The mean of  $C_{env}$  is shown in Figure 2b and the COV used to generate the process is defined based on previous probabilistic studies [12, 13]. Stochastic representations of the surface chloride concentration are also presented in Figure 2b. This model considers that during the hot seasons  $C_{env}$  is zero, whereas during the cold seasons it becomes time-variant.  $C_{env}^{max}$  is the maximum chloride concentration that corresponds with the minimum temperature (see Figure 2b). It is worthy to clarify that the value of  $C_{env}^{max}$  has been defined by considering that the quantity of chloride ions deposited during one year be the same that the average annual concentration reported in the literature,  $C_{env}^{ave}$ . This example considers a maximum surface chloride concentration,  $C_{env}^{max}$ , equal to  $16 \text{ kg/m}^3$  which entails that  $C_{env}^{ave} = 4 \text{ kg/m}^3$  [12, 13].

### 3.3 Probability of corrosion initiation

The *time to corrosion initiation*,  $t_{ini}$ , occurs when the concentration of chlorides at the cover thickness  $c_t$  is equal to or higher than a threshold value  $C_{th}$ . For such event the limit state function becomes:

$$g(\underline{x}, t) = C_{th}(\underline{x}) - C_{tc}(\underline{x}, t, c_t) \quad (7)$$

where  $\underline{x}$  is the vector of the random variables to be taken into account and  $C_{tc}(\underline{x}, t, c_t)$  is the total concentration of chlorides at depth  $c_t$  and time  $t$  obtained from the solution of the system of PDEs presented in section 2. By evaluating the limit state function (Eq. 7), the probability of corrosion initiation is:

$$p_{corr}(t) = P[g(\underline{x}, t) \leq 0 | t] \quad (8)$$

Given the complexity of the solution procedure of the system of PDEs, simulation methods seem to be more appropriate to deal with the problem. Therefore, to reduce the computational cost, this study combines Monte Carlo simulations with Latin Hypercube Sampling.

## 4 Numerical application

This example studies the influence of the impact of the weather model, the chloride ingress induced by convection and the one- and two-dimensional flow of chlorides into concrete on the probability of corrosion initiation. Figure 3a shows the studied RC wall and column. It can be noted that for the one-dimensional exposure the chlorides come from one direction; whilst for the two-dimensional exposure there is a source of chlorides in each side. This application accounts for a continental weather which concerns the structures placed at moderate latitudes far from the ocean and the chlorides come from de-icing salts. The effect of weather is illustrated by assuming that the structure is placed in a continental environment characterized by:  $T_{min} = -10^\circ\text{C}$ ,  $T_{max} = 20^\circ\text{C}$ ,  $h_{min} = 0.6$  and  $T_{max} = 0.8$ . The probabilistic models used in this study are shown in Table 2. The mean and COV of the threshold chloride concentration  $C_{th}$  are defined based on the values reported in [13]. For this particular case,  $C_{th}$  is the critical chloride content leading to deterioration or damage of the concrete structure and is determined for partially saturated conditions. According to [13] the cover thickness,  $c_t$ , follows a truncated normal distribution with the values presented in Table 2. The means of  $D_{h,ref}$  and  $D_{c,ref}$  correspond to the values reported in [3] for water/cement ratio,  $w/c = 0.5$ . The distribution types and COV of  $D_{h,ref}$  and  $D_{c,ref}$  are assigned according to [13, 5]. Based on the experimental ranges presented by several authors (See [2]), it is supposed that  $\lambda$  and  $c_q$  follow beta distributions where the parameters vary between the experimental limits reported in the literature and their COVs are assumed. Val and Trapper [5] suggest that the age reduction factor,  $m$ , also follow a beta distribution. Finally setting as mean the typical density of concrete ( $2400 \text{ kg/m}^3$ ), it is supposed that  $\rho_c$  is normally distributed with a COV of 0.2. Other basic assumptions of the example are:

- the concrete is made with  $400 \text{ kg/m}^3$  of Ordinary Portland Cement with 8% of  $\text{C}_3\text{A}$  and water/cement ratio  $w/c = 0.5$ ;
- the constants for Langmuir isotherm are  $\alpha_L = 0.1185$  and  $\beta_L = 0.09$
- the structure is partially saturated; and
- the random variables are independent.

Table 2: Probabilistic models of the random variables.

Variable	Mean	COV	Distribution
$C_{th}$	0.5 wt% cement	0.20	normal
$c_t$	40 mm	0.25	normal (truncated at 10 mm)
$D_{h,ref}$	$3 \times 10^{-10} \text{ m}^2/\text{s}$	0.20	log-normal
$D_{c,ref}$	$3 \times 10^{-11} \text{ m}^2/\text{s}$	0.20	log-normal
$\lambda$	$2.5 \text{ W}/(\text{m}^\circ\text{C})$	0.20	beta over [1.4;3.6]
$c_q$	$1000 \text{ J}/(\text{kg}^\circ\text{C})$	0.10	beta over [840;1170]
$\rho_c$	$2400 \text{ kg/m}^3$	0.20	normal

The impact of the type of weather –i.e., mean trend and stochastic, on the time to corrosion initiation is shown in Figure 3b. The time-variant case accounts for the sinusoidal variation of temperature and humidity shown in Figure 2a; and the stochastic case considers the model presented in subsection 3.1. It can be noted that the probability of corrosion initiation increases if the randomness is included. For this particular case, at 30 years after construction, the probability of corrosion initiation can increase, from 0.48 for the mean trend to 0.78 for the stochastic model. These results highlight the importance of accounting for the uncertainty of the environment.

The effect of convection on the probability of corrosion initiation is depicted in Figure 4a. These curves were obtained by modeling the weather stochastically. It can be observed from Figure 4a that accounting for the chloride ingress by convection increases the probability of corrosion initiation. This increment is explained by the addition of a second mechanism of chloride ingress (see Table 1) which augments the chloride concentration at the corrosion cell reducing the time to reach the threshold concentration.

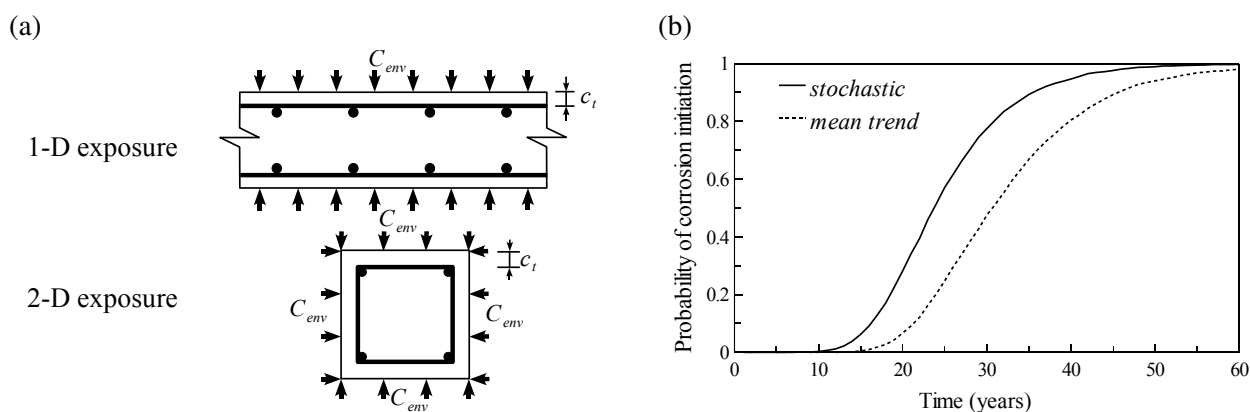


Figure 3: (a) Considered cross-sections. (b) Influence of the randomness.

Finally, the variation of the probability of corrosion initiation for 1-D and 2-D exposures is presented in Figure 4b. Both cases include the probabilistic nature of the environmental actions and the chloride ingress by convection. As expected the higher probabilities correspond to the 2-D exposure. The reduction of the corrosion initiation time is due to the exposure to chlorides on both sides of the structural element. For instance, for 30 years of exposure the probability of failure is increased by 27% when 2-D exposure is considered. These results stress the importance of including a two-dimensional analysis for correct prediction of corrosion initiation in small RC elements as columns and beams.

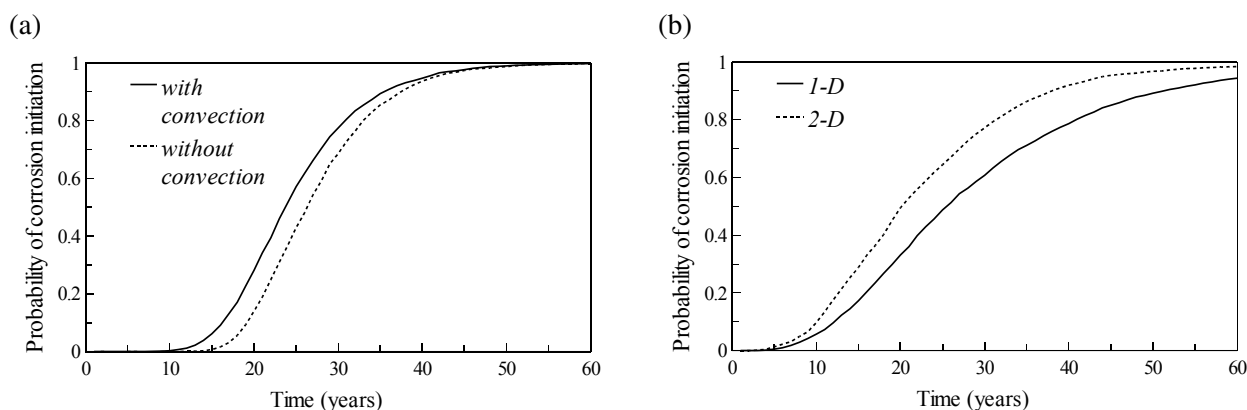


Figure 4: Effect of: (a) convection and (b) one- and two-dimensional modeling

## 5 Conclusions

This paper presented a numerical solution of the governing equations of diffusion/convection in a stochastic framework. The proposed methodology was applied to diffusion of chloride ions into concrete. The model of chloride ingress accounted for the effects of chloride binding, temperature, humidity, concrete aging, and convection. To better understanding the effects of the uncertainties, the mechanical model of chloride ingress was introduced into a probabilistic framework where the reliability analysis was carried out by using Monte Carlo simulations and Latin hypercube sampling. A numerical example illustrated about the effects of the weather model, the chloride ingress induced by convection and the one- and two-dimensional flow of chlorides into concrete on the probability of corrosion initiation. Overall behavior indicated that the probability of corrosion initiation increases when the random nature of humidity and temperature, convection convection and two dimensional flow or chlorides were considered. These results highlight the importance of including comprehensive model for both chloride penetration and randomness for a satisfactory lifetime assessment of structures subject to chloride ingress.

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