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https://doi.org/10.1061/41170(400)53

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**NRCC-53924**

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April 2011

A version of this document is published in / Une version de ce document se trouve dans:
International Conference on Vulnerability and Risk Analysis and Management (ICVRAM) & the Fifth International Symposium on Uncertainty Modeling and Analysis (ISUMA 2011), University of Maryland, Hyattsville, MD, USA, April 11-13, 2011, pp. 432-441

# A Polynomial Chaos Approach for Uncertainty Analysis of Chloride-Induced Corrosion in Concrete Structures

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## ABSTRACT

Chloride-induced corrosion has been identified as one of the main causes of deterioration of concrete structures, such as highway bridges, etc. The development of a performance-based approach is critical to ensure adequate safety, serviceability and durability of concrete structures, built in chloride-laden environments, as well as to help identify appropriate maintenance strategies to extend their service life. This paper presents a polynomial chaos response surface approach for the probabilistic modeling of chloride-induced corrosion of carbon steel reinforcement in concrete structures that takes into account the uncertainties in the parameters that govern the physical models of chloride ingress into concrete and corrosion of carbon steel, including concrete diffusivity, concrete cover depth, surface chloride concentration and threshold chloride level for onset of corrosion. A case study of highway bridge deck was used to illustrate the applicability, accuracy and computational efficiency when compared to crude Monte Carlo simulation.

## INTRODUCTION

In porous solids, such as concrete structures, chlorides can penetrate into concrete via different physical mechanisms, such as diffusion, capillary absorption, etc. which lead to the corrosion of the steel reinforcement. The corrosion of the steel reinforcement leads to concrete fracture through cracking, delamination and spalling of the concrete cover, reduction of concrete and reinforcement cross sections, loss of bond between the reinforcement and concrete, and reduction in strength and ductility. As a result, the safety, serviceability and service life of concrete structures are reduced. In the last decades, the Fickian diffusion process was used to model the chloride diffusion and the initiation time to corrosion using the concept of chloride threshold as an indicator of corrosion resistance of reinforcing steel to chloride attack. In practice, the design of durable concrete structures is mainly based on specifying a minimum concrete cover depth (depending on the environmental exposure), a maximum water-to-cement ratio (to achieve low chloride diffusivity), and as well the use of more corrosion resistant reinforcing steels. However, a considerable level of uncertainty may be associated with one or more of the above identified parameters. This is due to: (i) heterogeneity and aging of concrete with temporal and spatial variability of its chloride diffusivity; (ii) variability of concrete cover depth, which depends on quality control, workmanship and size of structure; (iii) variability of surface chloride concentration, which depends on the severity of the environmental exposure; and (iv) uncertainty in chloride threshold level that depends on the type of reinforcing steel, type of cementing materials, test methods, etc. It is clear that the combination of these uncertainties leads to a considerable uncertainty in the model output (e.g. the time to corrosion initiation). This uncertainty in the model output could have serious consequences in terms of reduced service life,

inadequate planning of maintenance and increased life cycle costs. The objective of this paper is twofold: (i) present physical models of chloride transport and corrosion of carbon steel reinforcement in concrete structures; and (ii) present a polynomial chaos approach for the probabilistic modeling of chloride-induced corrosion that takes into account the uncertainties in the parameters that govern the physical models. The proposed approach enables a modeling that represents the whole response of the system in a meta-model format, instead of the estimation of the mean, variance or the tail of the response.

## CHLORIDE TRANSPORT PROBLEM

### Chloride diffusion process

The main transport mechanisms of chlorides into concrete are diffusion and adsorption. However, adsorption occurs in concrete surface layers that are subjected to wetting and drying cycles, and it only affects the exposed concrete surface down to 10-20 mm (Weyers et al. 1993; Tuutti 1982). Chloride diffusion is a transfer of mass by random motion of free chloride ions in the pore solution, resulting in a net flow from regions of higher to regions of lower concentration (Crank 1975). The rate of chloride ingress is proportional to the concentration gradient and the diffusion coefficient of the concrete (Fick's first law of diffusion). Since in the field, chloride ingress occurs under transient conditions, Fick's second law of diffusion can be used to predict the time variation of chloride concentration for one-dimensional flow. It can be expressed as follows: (Crank 1975):

$$\frac{\partial C_{x,t}}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C_{x,t}}{\partial x}\right)$$

where $C_{x,t}$ is the concentration of chlorides at depth x and time t; D is the diffusion coefficient. Under the assumptions of a constant diffusion coefficient, constant surface chloride content Cs as the boundary condition, and the initial condition specified as C=0 for x>0, t=0, Crank's solution yields (Crank 1975):

$$C_{x,t} = C_s\left(1 - \mathrm{erf}\frac{x}{2\sqrt{Dt}}\right)$$

where erf(.) is the error function. In the modeling of chloride ingress as Fickian process, several simplifying assumptions are made (Zhang and Lounis 2006).

### Corrosion initiation

The corrosion initiation stage corresponds to the process of chloride ions (chlorides) ingress into concrete, while the steel remains passivated. The corrosion initiates when the concentration of chloride ions in contact with the steel reaches a threshold level $C_{th}$ (Tuutti 1982) that destroys the passivation of the steel. Therefore, the duration of the initial stage, which is often used as a quantitative indicator of service life or durability of concrete structures, depends on the rate of chloride penetration in concrete. Ideally, the corrosion initiates at time $\widetilde{\boldsymbol{T}}_{\boldsymbol{i}}$ at which the concentration of chlorides at the steel level becomes equal or greater than the chloride threshold ($C_{th}$):

$$C_{d,\widetilde{T}_i} \geq C_{th}$$

Where d represents the concrete cover depth of the steel. From this equation, the approximated initiation time to corrosion can be deduced as follows:

$$\widetilde{T}_i = \frac{d^2}{4D\left[erf^{-1}\left(1 - \frac{C_{th}}{C_s}\right)\right]^2}$$

In this deterministic model, the four governing parameters are assumed as independent that are critical for corrosion protection: (i) structural parameter: concrete cover depth d; (ii) material parameters: chloride diffusion coefficient D, which is an indicator of the rate of chloride penetration into concrete, and chloride threshold value $C_{th}$, which is an indicator of the corrosion resistance of reinforcing steel; and (iii) environmental parameter: surface chloride concentration $C_s$, which is a measure of the corrosivity or load or exposure risk of concrete structures. Given the inherent complexity and heterogeneity of concrete as a corrosion medium, there exists a large uncertainty in the above mentioned parameters and in the proposed model. In the following section, a probabilistic approach based on the polynomial chaos expansion will be used to model the uncertainties in the above four parameters.

## PROBABILISTIC MODELING OF CORROSION USING POLYNOMIAL CHAOS EXPANSION

### Uncertainty modeling

As mentioned above, the model and its associated parameters can exhibit a considerable level of variability (e.g. concrete cover depth, diffusion coefficient, etc.), which may have coefficients of variation of 20% or higher while the concrete cover for high quality control can present a narrow scatter with lower coefficients of variation (Stewart and Rosowsky 1998; Lounis and Mirza 2001). The values of these parameters used in deterministic models are mainly based on the mean values or some conservative characteristic values of the variables. The deterministic models can predict only two states, i.e. corrosion or non- corrosion. It is clear that the use of deterministic models, which assume concrete as a homogeneous medium, cannot predict the extent of corrosion for a reference period of time (it is either 0% or 100% corrosion). Although such models present a powerful tool for selection of proper parameters at the design stage for new structures, they have serious shortcomings regarding the selection of appropriate maintenance strategies for structures in service. A probabilistic modeling of the performance of concrete structures has much to offer with regard to simplicity as compared to attempts to formulate purely deterministic models (Frangopol *et al.* 1997; Mori and Ellingwood 1993).

### Prediction of Corrosion Probability

In order to calculate the probability of corrosion of reinforcing steel embedded in concrete structures several methods can be used, depending on the complexity of the model (e.g. linear or non-linear …) and the accuracy desired. The probability of corrosion corresponds to the integral of the probability density function $f_X(x)$ on the corrosion domain (See equation below).

$$P_f = \int_{g(\mathrm{Cs,\,d,\,D,\,Cth}) < 0} f_Y(C_s, d, D, C_{th})dx$$

$$\text{With } \mathrm{g(C_s, C_{th}, D, d)} = \mathrm{C_{th}} - \mathrm{C_s}\left(1 - \mathrm{erf}\frac{\mathrm{d}}{2\sqrt{\mathrm{Dt}}}\right)$$

Where g is the limit state or performance function, which is a highly nonlinear function.

To calculate this integral (i.e. probability of corrosion $P_f$), several methods can be proposed. The most obvious and simple to implement is the Monte Carlo Simulation (MCS). This method attempts to characterize the whole domain of failure so it needs an important number of simulations (i.e. slow convergence rate). Advanced methods use a more efficient way to select simulations, which are based on two main concepts: (i) the approximation of the nonlinear state function; and (ii) efficient method of simulations (e.g. experimental designs).

Other methods attempt to represent the whole response of the system, such as a polynomial chaos expansion that allows constructing a probabilistic response surface. The response of a concrete structure subjected to chloride attack is a random output that can be explicitly represented in a suitable space using the polynomial chaos (PC) basis (Soize & Ghanem 2004). The response is thus cast as a series of multivariate polynomials. In this setup, characterizing the random response is equivalent to computing the coefficients in the representation, i.e. the coordinates of the response in the PC basis. This can be efficiently achieved by using non intrusive approaches, namely the projection strategy and the regression strategy. These schemes allow one to compute the coefficients of the PC expansion by means of a set of deterministic model evaluations, i.e. without modifying the underlying computer code. Inexpensive moment, sensitivity and reliability analyses (Sudret 2008) are then easily carried out using a suitable post-processing of the PC expansion coefficients.

**Polynomial chaos representation**

Consider a structural system described by a numerical model that can be analytical or more generally algorithmic (*e.g.* a finite element model). Suppose that this model has $M$ uncertain input parameters that are represented by *independent* random variables $\{X_1,...,X_M\}$ gathered into a random vector $\boldsymbol{X}$ of prescribed joint probability density function $f_{\boldsymbol{X}}(\boldsymbol{x})$. Hence the model response denoted by $Y = \mathcal{M}(\boldsymbol{X})$ is also random. For the sake of simplicity, $Y$ is assumed to be scalar throughout the paper (in case of a vector response $\boldsymbol{Y}$, the following derivations hold true for each component). Provided that the random variable $Y$ has a finite variance, it can be expressed as follows (Soize & Ghanem 2004):

$$Y = \mathcal{M}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^M} a_{\boldsymbol{\alpha}}\, \psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \qquad (1)$$

This expansion is referred to as the *generalized polynomial chaos* (PC) *representation* of $Y$. The $a_{\boldsymbol{\alpha}}$'s are unknown deterministic coefficients and the $\psi_{\boldsymbol{\alpha}}$'s are multivariate polynomials, which are orthonormal with respect to the joint PDF $f_{\boldsymbol{X}}$ of the input random vector $\boldsymbol{X}$, *i.e.* $\mathrm{E}\left[\psi_{\boldsymbol{\alpha}}(\boldsymbol{X})\, \psi_{\boldsymbol{\beta}}(\boldsymbol{X})\right] = 1$ if $\alpha = \beta$ and 0 otherwise.

**Basis of polynomial chaos expansion**

As emphasized above, it is supposed that the input random vector $\boldsymbol{X}$ has independent components $X_i$, $i=1..M$. Thus, its joint probability density function (PDF) may be written as:

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i=1}^{M} f_{X_i}(x_i)$$

where $f_{X_i}(x_i)$ = the marginal PDF of $X_i$.

Let $\left\{\pi_j^{(i)},\ j \in \mathbb{N}\right\}$ be a family of orthonormal polynomials with respect to $f_{X_i}$. Most common distributions can be associated to a specific type of polynomials, *e.g.* normalized Hermite (resp. Legendre) polynomials for standard normal variables (resp. uniform variables over [-1,1]). The multivariate basis $\{\psi_{\boldsymbol{\alpha}}, \boldsymbol{\alpha} \in \mathbb{N}^M\}$ of the representation in Eq. 1 is built by from the $M$ resulting families of univariate polynomials as follows:

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \prod_{i=1}^{M} \pi_{\alpha_j}^{(i)}(X_i)$$

For computational purposes, the series in Eq. 1 are truncated in order to retain only a finite number of terms. One commonly retains those polynomials whose total degree $|\boldsymbol{\alpha}| = \sum_i \alpha_i$ does not exceed a given $p$:

$$Y = \mathcal{M}(\boldsymbol{X}) \approx \sum_{|\boldsymbol{\alpha}| \leq p} a_{\boldsymbol{\alpha}}\, \psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \qquad (2)$$

Characterizing the random response $Y$ is thus equivalent to computing the finite set of unknown coefficients $\{a_{\boldsymbol{\alpha}}, |\boldsymbol{\alpha}| \leq p\}$. This may be achieved using non intrusive techniques respectively known as *projection* and *regression* methods, as shown in the sequel.

**Estimation of coefficients of polynomial chaos expansion**

The estimation of the coefficients can be done by many strategies, including:

- classic simulation strategy like Monte Carlo Simulation, Latin Hyper Cube
- projection strategies.

Here below, an overview of the main projection strategies is given:

*(i) Integration strategy*

Due to the orthonormality of the PC basis, the PC coefficients can be computed by pre-multiplying Eq. 2 by $\psi_{\boldsymbol{\alpha}}$ and by taking their expectations. Therefore, the exact expression of each coefficient $a_{\boldsymbol{\alpha}}$ can be written as follows:

$$\boldsymbol{a_\alpha} = \boldsymbol{E}[\boldsymbol{\psi_\alpha}(\boldsymbol{X})\, \boldsymbol{\mathcal{M}}(\boldsymbol{X})] \equiv \int_{\boldsymbol{D_X}} \boldsymbol{\psi_\alpha}(\boldsymbol{x})\, \boldsymbol{\mathcal{M}}(\boldsymbol{x})\, \boldsymbol{f_X}(\boldsymbol{x})\, \boldsymbol{dx}$$

where $D_{\boldsymbol{X}}$ denotes the support of the random vector $\boldsymbol{X}$. The multidimensional integral in the above equation may be computed either by simulation techniques, such as Monte Carlo simulation, Latin Hypercube (McKay et al. 1979) or quadrature (Sudret 2008).

*(ii) Regression strategy*

Another alternative is the *regression* strategy, which consists in adjusting the truncated PC expansion to the model under consideration. It is possible to recast Equation 2 using a vector notation as follows:

$$Y = \mathcal{M}(\boldsymbol{X}) \approx \mathcal{M}_p(\boldsymbol{X}) = \boldsymbol{a}^{\mathrm{T}} \boldsymbol{\psi}(\boldsymbol{X})$$

where $\boldsymbol{a}$ (resp. $\boldsymbol{\psi}$) gathers the coefficients $\{a_{\boldsymbol{\alpha}}, |\boldsymbol{\alpha}| \leq p\}$ (resp. the basis polynomials $\{\psi_{\boldsymbol{\alpha}}, |\boldsymbol{\alpha}| \leq p\}$). Sudret (2008) shows that the PC coefficients in Equation 2 are the solution of the optimisation problem below:

$$a^{*} = \underset{a \in IR^{P}}{\operatorname{argmin}} \int_{D_X} (M(x) - a^{T}\psi(x))^{2} f_X(x)\, dx$$

where $P$ denotes the number of multi-indices in the set $\{a_{\boldsymbol{\alpha}}, |\boldsymbol{\alpha}| \leq p\}$, which is given by:

$$P = \binom{M+p}{p}$$

This problem can be solved by an integral discretization and by choosing a suitable *experimental design* (using the PDF of X). Hence, let us consider an experimental design $\mathbf{X} = \{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}\}^{\mathrm{T}}$ such that $\mathbf{X}$ represents a set of $N$ realizations of the input random vector, and $\mathbf{Y} = \{y^{(1)}, \ldots, y^{(N)}\}^{\mathrm{T}}$ be the corresponding model evaluations $\{y^{(i)} = \mathcal{M}(\boldsymbol{x}^{(i)}),\ i = 1, \ldots, N\}$. In this case the estimated coefficients are those that minimize the following squared residual:

$$\widehat{\boldsymbol{a}} = \underset{\boldsymbol{a} \in \mathbb{R}^{P}}{\operatorname{argmin}} \left[ \sum_{i=1}^{N} \left( \mathcal{M}(\boldsymbol{x}^{(i)}) - \boldsymbol{a}^{\mathrm{T}} \boldsymbol{\psi}(\boldsymbol{x}^{(i)}) \right)^{2} \right]$$

The solution reads as:

$$\widehat{\boldsymbol{a}} = (\boldsymbol{\Psi}^{\mathrm{T}}\boldsymbol{\Psi})^{-1}\boldsymbol{\Psi}^{\mathrm{T}}\mathbf{Y}$$

where the *data matrix* $\boldsymbol{\Psi}$ is defined by:

$$\boldsymbol{\Psi} = \begin{pmatrix} \psi_{\boldsymbol{\alpha}_1}(\boldsymbol{x}^{(1)}) & \cdots & \psi_{\boldsymbol{\alpha}_P}(\boldsymbol{x}^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_{\boldsymbol{\alpha}_1}(\boldsymbol{x}^{(N)}) & \cdots & \psi_{\boldsymbol{\alpha}_P}(\boldsymbol{x}^{(N)}) \end{pmatrix}$$

upon introducing the ordering $\{|\boldsymbol{\alpha}| \leq p\} \equiv \{\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_P\}$ of the multi-indices. Note that in order to make this problem well-posed, the experimental design $\mathbf{X}$ must be selected in such a way that the *information matrix* $\boldsymbol{\Psi}^{\mathrm{T}}\boldsymbol{\Psi}$ is well-conditioned. This implies that the size $N$ of the design (*i.e.* the number of model evaluations) has to be large enough, and necessarily greater than $P$.

## ILLUSTRATIVE EXAMPLE

The probabilistic model proposed herein is illustrated on a high performance concrete (HPC) highway bridge deck reinforced with conventional carbon steel with two different types of HPC mixes that yield similar diffusion coefficients of 0.2 $cm^2$/yr. HPC1 is made with a low w/c ratio (no supplementary mineral admixtures) and HPC 2 contains 10% of silica fume. The parameters values are based on examples taken from Lounis and Daigle (2008) and are listed in Table 1:

**Table 1. Data for Bridge Deck Case Study**

| | $C_s$ $Kg/m^3$ | Depth mm | Diffusion $cm^2$/year | $C_{th}$ $Kg/m^3$ |
|---|---|---|---|---|
| Mean value | 6 | 70 | 0.2 | 0.7 |
| Coefficient of variation | 30% | 20% | 25% | 20% |

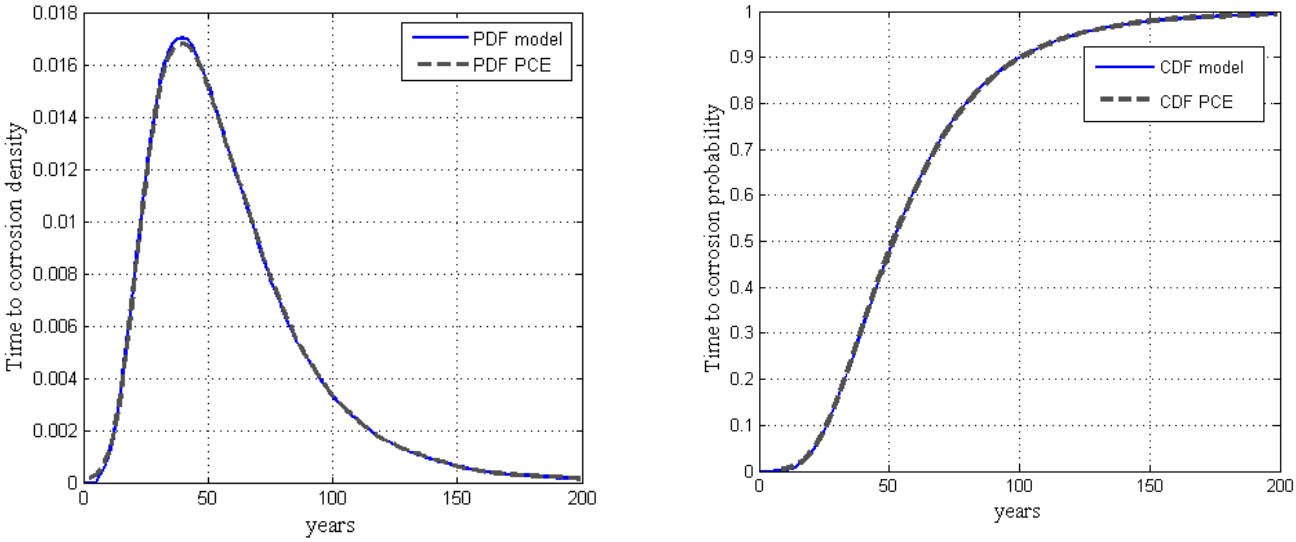


**Figure1. PDF and CDF of corrosion initiation time using PCE and MCS models**

In this example, the parameters are assumed to be independent and follow lognormal distributions. The time-varying probability of corrosion is evaluated over 200 years. Fig.1 shows the probability density function (PDF) and cumulative density function (CDF) of the corrosion initiation time obtained using the polynomial chaos expansion (PCE) with 200 simulations. Fig.1 shows also the PDF and CDF of the corrosion initiation time using Monte Carlo simulations (MCS) with 100,000 simulations. It can be seen from Fig.1, that PCE with only 200 simulations provides similar predictions to MCS with much higher number of simulations. This example illustrates the following: (i) the applicability of the polynomial chaos expansion for non-linear chloride transport and corrosion problems; (ii) Accuracy of the PCE when compared to MCS; and (iii) PCE can provide reliable results at a lower computational cost.

## CONCLUSIONS

In this paper, a probabilistic modeling of chloride transport and chloride-induced corrosion of concrete structures using the polynomial chaos expansion (PCE) is presented. It is found that the PCE approach provides accurate results and is more efficient than Monte Carlo simulation, even for the highly nonlinear performance function. The case study showed that similar results are obtained using PCE with much lower computational cost.

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