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Stochastic modeling and calibration of chloride content profile in concrete based on limited available data

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Abstract

Chloride ion ingress in concrete is the main reason of concrete corrosion. In real world both uncertainty and stochasticity are main attributes of almost all measurements including testing and modeling of chloride content profile in concrete. Regarding these facts new models should be able to represent at least some of the uncertainties in the predictions. In this paper after inspiration from classical physics related to diffusion and random walk concepts a stochastic partial differential equation (SPDE) of diffusion is introduced to show a more realistic modeling/calibration scheme for construction of stochastic chloride content profile in concrete. Diffusion SPDE provides a consistent quantitative way of relating uncertainty in inputs to uncertainty in outputs. Although it is possible to run sensitivity analysis to get some statistical results from deterministic models but the nature of diffusion is inherently stochastic. Brownian motion process (Wiener process) is used in SPDE to simulate the random nature of the diffusion in heterogeneous media or random fields like concrete. The proposed method can be used to calibrate/model the chloride ion profile in concrete by only some limited data for a given depth. Then the stochastic chloride ion diffusion can be simulated by langevin equation. Results of the method are compared with data from some references and all show good agreements.

Keywords: Concrete corrosion, Markov process, Stochastic partial differential equation (SPDE), Langevin equation.

1. Introduction

Today saving the existing facilities and infrastructures is the main task of many organizations responsible for maintenance and repair issues. We should be aware of aging and performance of infrastructures under the environmental impacts.

Durability management, environmental impact assessment, and performance based design of structures are important and of main concern nowadays. Regarding concrete structures development of modeling and simulation methods for different types of concrete deteriorations is a crucial need for concrete durability evaluation.

Concrete deteriorates in different kinds of exposures. There are many concrete structures suffering from corrosion and other types of deterioration. Concrete corrosion is a widespread and epidemic problem in the world [1-3].

Considering economical conditions and limitations of budgeting concrete durability extension and service life prediction are necessary from maintenance and repair management points of view.

The main reasons for concrete corrosion are chloride ingress and/or carbon dioxide gas diffusion in concrete. Modeling and simulation of chloride ion ingress and carbon dioxide gas diffusion in porous media of concrete are needed for better decision making for maintenance and repair activities.

Diffusion is the process by which matter is transported from one part of a system to another as a result of random molecular motions. Transport of ions or molecules has been a subject of great concern in material sciences. Diffusive agents are subject to random and complex movement [4]. Considering spatial variability of governing parameters of reinforcement corrosion can lead to substantial decrease in predicted service life of RC structures [5]. Understanding their movement or transport is of fundamental and practical importance to all materials especially heterogeneous material like concrete. Concrete is an alkaline material and includes randomness from various phases such as aggregate dispersed in hardened cement paste. Alkalinity lets researchers to apply diffusion theory to deleterious material ingress in concrete [6]. This phenomenon is inherently stochastic. It means that the next step of diffusive agent movement is not dependent to the history of its previous movements or trajectory. Another characteristic of concrete material which leads researcher to

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consider randomness or stochastic concepts is that the concrete media is a random field media [7]. The next step of movement may be the position of an aggregate or hardened cement paste. Therefore this concept has direct impact on the diffusive agent's trajectory [8].

There are some simulation methods considering the modeled heterogeneous media but these methods are too complicated to be used in practical evaluations. To simplify the preliminary studies it is possible to think about concrete as a homogen material but the diffusion of deleterious materials in it is stochastic. This assumption leads us to model diffusion problems by stochastic methods [9].

There are different approaches for diffusion modeling: deterministic and stochastic. Deterministic methods are widely used to simulate diffusion of diffusive agents in concrete. Recently, stochastic methods have been under attention to estimate the depth and rate of diffusive agents. Deterministic models were attractive some years ago but there have been remarkable interests in stochastic or probabilistic methods nowadays [3]. The stochastic methods are divided to two different categories. The most popular method is using a deterministic model with probabilistic parameters as inputs. The logical deduction of this method is that the output is also probabilistic [9, 10]. The main reason that this method has been used widely is its simplicity and straightforward framework. From practical engineering point of view this method is almost accurate but to enhance our understanding and knowledge about the real behavior of concrete material in diffusion problems we need more realistic methods. Accurate simulation of diffusion in concrete is essential for durability evaluation of existing and durability design of new structures. Thus stochastic methods are basically becoming attractive as the second method of solving the problem.

A stochastic differential equation is a differential equation whose coefficients are random numbers or random functions of the independent variable (or variables); therefore, it is an appropriate tool for describing systems with external noise. Stochastic partial differential equations form a computational platform by consistent quantitative way of relating uncertainty in input to uncertainty in output. Many physical, chemical or even financial problems cannot be described realistically without modeling some input data statistically. Uncertainty in input is then quantified, and it is natural to see how this uncertainty propagates through the model [11].

Numerical solution of stochastic equations is orders of magnitude more time consuming than the solution of the corresponding deterministic differential equations [12]. Contrary to this somewhat problematic disadvantage the information can be extracted from a stochastic analysis is much more comprehensive and valuable than deterministic analysis findings. For more accurate uncertainty estimates involving probabilities, for example for decision reliability calculations, the complete distribution must be computed.

In the field of diffusion problems, material properties show some sources of uncertainty those are often represented as stochastic variables or fields [12].

All properties of concrete in meso-structure level show some randomness in nature. Thus stochastic differential equations can be used for material diffusion with random media especially for concrete. One important and famous example of a stochastic differential equation which can be used for diffusion problems is the Langevin equation [13]. This equation is used in this paper to model/calibrate the chloride ion profile in concrete.

2 Diffusion partial differential equation

In many research works Fick's 2nd law is used to model the diffusion in concrete [14]. Most of the researchers use the following partial differential equation which shows the diffusion process:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} (D \frac{\partial C}{\partial x}) \tag{1}$$

where.

C = chloride ion concentration,

x = depth,

t = time, and

D = diffusion coefficient.

By applying boundary and initial conditions for semi-infinite concrete and assuming constant D the solution of Eq. 1 is:

$$C(x,t) = C_s \left[1 - erf\left(\frac{x}{\sqrt{4Dt}}\right) \right]$$
 (2)

where,

 C_s = Chloride ion concentration at surface (C(0,t)).

Typical solutions of Eq. 2 are depicted for various times in Fig 1. Solution for a specified time shows that the chloride concentration is deterministic but real measurements show that it is not true. For a given time this concentration is obviously statistical. It can be shown by some statistical distribution mainly normal distribution for any given time. Therefore stochastic representation of chloride concentration becomes necessary. This fact, at a glance, is considered in this paper in modeling approach. It is recommendable to write the diffusion partial differential equation basically in stochastic form.

The scope of this paper is to model the chloride diffusion in concrete considering the above mentioned fact. We can consider the problem as finding the chloride concentration in concrete which moves or diffuses in concrete stochastically.

In concrete corrosion study when the chloride threshold concentration reaches to the reinforcing steel bars corrosion begins. Instantly after the corrosion initiation it will be the turn of corrosion propagation which leads to more rust and extension of this detrimental effect on reinforced concrete.

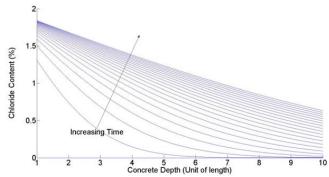


Fig. 1. Typical solution of the Eq. 2 at different times

3. Stochastic theory concepts

In this paper we are going to use stochastic partial differential equation of diffusion process. To do so it is required to define the stochastic variables. A "random number" or "stochastic variable" is an object X defined by:

- A set of possible values, called "range", "set of states", "sample space" or "phase space";
- A probability distribution over this set.

A stochastic process is simply a function of two variables one of which is the time t and the other a stochastic X as defined above [12].

From stochastic theories point of view diffusive agent movement should be modeled under uncertainty. Here we need some introductory explanations regarding the problem under investigation.

The Markov process, also called the Markov chain, is defined as a stochastic process that the future development of the process only depends on the present value, not on the past ones [10, 12 & 15]. In other words,

$$P(x_n, t_n | x_1, t_1, \dots, x_{n-1}, t_{n-1}) = P(x_n, t_n | x_{n-1}, t_{n-1})$$
(3)

where $P(x_n, t_n | x_1, t_1, ..., x_{n-1}, t_{n-1})$ is the transition probability of a diffusive agent to be in position x_n at time t_n given all previous positions $[x_1, x_1, ..., x_{n-1}]$ at previous time $[t_1, t_1, ..., t_{n-1}]$, and $P(x_n, t_n | x_{n-1}, t_{n-1})$ represents the transition probability conditioned only on the diffusive agent.

Markov process has the property that given the present state, the past states have no influence on the future. The advantage of the Markov process lies in both its broad applications to engineering systems and its simplicity. Herein, diffusive agent movement in concrete porous media is assumed to follow the Markov chain.

A standard Brownian motion or a standard Wiener process governs the behavior of the random variable W(t) in continuous time interval $0 \le t \le T$. The standard Brownian motion satisfies the following conditions [11, 16]:

- 1. W(0)=0 with probability 1.
- 2. If 0 < s < t < T, then the random variable $\Delta W = W(t) W(s)$ is normally distributed with a zero mean and a variance (*t-s*), and satisfies $\Delta W \sim \sqrt{t-s} N(0,1)$
- 3. If 0 < s < t < u < v < T, $\Delta W_1 = W(t) W(s)$ and $\Delta W_2 = W(v) W(u)$, then ΔW_1 and ΔW_2 are independent.
- 4. Stochastic diffusion processes

Diffusion processes (specially, Brownian motion) originated in physics as mathematical models of the motions of individual molecules undergoing random collisions with other molecules in a gas or liquid. Long before the mathematical foundations of the subject were laid, Albert Einstein realized that the microscopic random motion of molecules was ultimately responsible for the macroscopic physical phenomenon of diffusion, and made the connection between the volatility parameter of the random process and the diffusion constant in the partial differential equation governing diffusion.

The connection between the differential equations of diffusion and the random process of Brownian motion has been a recurring theme in mathematical research ever since [8].

Einstein realized that the quantity involving Brownian motion that can be best observed under a microscope in an experiment is the "diffusivity":

$$D = \lim_{t \to \infty} \frac{\left| X(t) - X(0) \right|^2}{2t} \tag{4}$$

Where X(t) denotes the observed displacement of the Brownian particle along a fixed direction at time t. In practice, t is simply taken as some satisfactorily long time of observation, and there is no need for fine temporal resolution as there would be if the velocity were to be measured. Einstein employed a random walk model for his analysis and showed that the diffusivity defined in Eq. 4 is identical to the diffusion constant that describes the macroscopic evolution of the concentration density n(x,t) of a large number of Brownian particles:

$$\frac{\partial n(x,t)}{\partial t} = D \sum_{k=0}^{3} \frac{\partial^{2} n(x,t)}{\partial x^{2}}$$
 (5)

where D is diffusion coefficient [13].

If we allow for some randomness in some of the coefficients of a differential equation we often obtain a more realistic mathematical model of the situation. All kinds of dynamics with stochastic influence in nature or man-made complex systems can be modeled by SPDEs.

A stochastic differential equation (SDE) is a differential equation in which one or more of the terms are a stochastic process, thus resulting in a solution which is itself a stochastic process. In other words a stochastic differential equation is a differential equation whose coefficients are random numbers or random functions of the independent variable (or variables). Hence stochastic differential equations are the appropriate tool for describing systems with external noise [12].

In its simplest form, diffusion is the transport of a material or chemical by molecular motion. Individual particles or molecules will follow paths sometimes known as "random walks." In such processes, a chemical initially concentrated in one area will disperse. That is, there will be a net transport of that chemical from regions of high concentration to regions of low concentration [4].

The diffusion Eq. 1 has multiple historical origins each building upon a unique physical or chemical interpretation. This partial differential equation (PDE) also encompasses many ideas about probability and stochasticity and its solution will require that we delve into some challenging mathematics.

The above definition of stochastic process allows us to talk about the statistics of random chloride profile in concrete in N dimensions. By random, we mean the movement at one moment in time cannot be correlated movement at any other moment in time, or in other words, there is no deterministic/predictive power over the exact motion of chloride concentration. Already this means we must abandon Newtonian mechanics and the notion of inertia, in favor of a system that directly responds to fluctuations in the surrounding environment.

The classical diffusion Eq. 1 governs the scaling limit of a random walk where diffusive agent jumps have zero mean and finite variance. The probability density c(x, t) of the Brownian

motion scaling limit W(t) solves the diffusion equation, and represents the relative concentration of a cloud of chloride concentration in concrete.

In this paper we concentrate on stochastic partial differential equation (SPDE) of diffusion. Stochastic partial differential equation of diffusion for chloride concentration trajectory has been introduced based on the above definitions and explanations, thus making a further step to build a practical stochastic model for diffusion problems.

One example of a stochastic differential equation is the Langevin equation. A stochastic theory based on chloride concentration movement or simply diffusion model can be derived from the Langevin equation by considering some changes to the concepts of its variables. This model as opposed to deterministic methods can provide more comprehensive information such as mean, variance and other statistical characteristics of chloride concentration profile in concrete.

Langevin equation was the first example of the stochastic differential equation with a random term X. Each solution of Langevin equation represents a different random trajectory and, using only rather simple properties of X (his fluctuating force), measurable results can be derived [17].

Compared to the deterministic diffusion equation, this modeling scheme has the advantage of capturing any randomly selected scenarios of chloride concentration in concrete. The trajectory of a chloride concentration is stochastic because of the probabilistic nature of its movement in diffusion problem.

Mathematical Brownian motion is often referred to as the Wiener process [18-20]. This idealized Brownian motion has independent increments (no inertia). Physical Brownian motion, of course, has some small inertia as well as several other complicating influences from the fluid environment and from the presence of other nearby Brownian particles [21]. These extra features can be built into a dynamical description using the mathematical Brownian motion as the basic noise input with influence mediated by the other physical parameters. The mathematical Brownian motion has a similar role in modeling noise input in a wide variety of stochastic models in physics, biology, finance, and other fields. More precisely, the Levy-Khinchine theorem indicates that in any system affected by noise in a continuous way such that the noise on disjoint intervals is independent can be modeled in terms of mathematical Brownian motion [22].

Based on the above introduction a typical stochastic partial differential equation is of the following form:

$$X_{t} = \mu(X_{t}, t)dt + \sigma(X_{t}, t)dW_{t}$$
(6)

where W_t denotes a Wiener process (Standard Brownian motion).

Eq. 6 characterizes the behavior of the continuous time stochastic process X_t as the sum of an ordinary Lebesgue integral and an Itō integral. A heuristic (but very helpful) interpretation of the stochastic differential equation is that in a small time interval of length δ the stochastic process X_t changes its value by an amount that is normally distributed with expectation $\mu(X_t, t)\delta$ and variance $\sigma(X_t, t)^2\delta$ and is independent of the past behavior of the process. This is so

because the increments of a Wiener process are independent and normally distributed. The function μ is referred to as the drift coefficient, while σ is called the diffusion coefficient. The stochastic process X_t is called a diffusion process, and is usually a Markov process [9, 11].

5. Langevin equation and its solution

Particles moving in a liquid without forces acting on the particles, other than forces due to random collisions with liquid molecules, are governed by the Langevin equation [17].

Based on the experience and investigation of several test results it is obvious that the more real solution of the diffusion partial differential equation cannot be a smooth curve for concrete. It shows that there is a tendency to statistical or stochastic form for solution curve. Therefore stochastic method is an appropriate approach to model the diffusion in concrete.

To fully describe the movement of chloride concentration in concrete, a stochastic differential equation should consist of a drift, a diffusion coefficient, and a driving Wiener process. The best choice is the Langevin equation which shows outcomes of exponential decay with noise. It is the most fitted function form for the diffusion of chloride concentration in porous media of concrete.

The problem of predicting stochastic chloride concentration profile in concrete is of Langevin type with trajectories between fixed concentrations at surface of concrete and relatively deep points in it. This type of problem is studied by different researchers [23].

Continuum theories of such diffusive systems describe the concentration field by the Nernst-Planck equation with fixed boundary concentrations. On the other hand, the underlying microscopic theory of diffusion describes the motion of the diffusing particles by Langevin's equations. This means that on a microscopic scale there are fluctuations in the concentrations at the boundaries. The question of the boundary behavior of the Langevin trajectories, corresponding to fixed boundary concentrations, arises both in theory and in the practice of particle simulations of diffusive motion [23].

The solution of Langevin SPDE looks like the curves in Fig. 1 for a given time but it is not smooth. Langevin equation which is used in this paper is as follows [9, 11]:

$$dX(t) = -aX(t)dt + \sigma dW(t) \tag{7}$$

where a is the drift coefficient, while σ is the diffusion coefficient. X(t) is the trajectory of chloride content in the concrete medium at time t; the realization X ranges over a probability space, and W is the Wiener process or the Brownian motion which is defined above. Now it is easy to depict the stochastic chloride concentration profile by the results of Eq. 7.

6. Discussions

The best method of the solution of the Langevin equation is a numerical solution. In this paper a simple program is written in MATLAB® to solve this SPDE. The results of the langevin equation solution are some trajectories. In the solution of the

Langevin equation two variables play the main role. Changing a affects the slope of the trajectories and changing σ results in variance of the trajectories. Based on these capabilities the above mentioned program can be used in two ways. Firstly by changing the coefficients one can find many trajectories like Fig. 2. Secondly, as shown in Fig. 3, if σ is equal to zero the mean curve for Chloride content can be found. In other words the solution can be considered both stochastic and deterministic. Obviously it is brilliant that the stochastic mode of solution is of more advantages comparing to deterministic mode.

Results of the solution shown in above figures contain useful information. Fig. 2 shows that the solution is inherently stochastic. There are many answers to the question. Each answer is a trajectory of the chloride content in concrete. In other words each trajectory can be a possible solution. This is due to this fact that we have basically written the diffusion SPDE in stochastic form. There is no need to find the deterministic answer and then conduct sensitivity analysis to find some statistics. This is an advantage for this type of modeling method in comparison to the other methods used by other researchers.

Fig. 2 also shows that we can define any confidence intervals or percentiles for the chloride content profile. It is a useful tool for probabilistic or stochastic durability design methods. Here the confidence interval shows that there is 95% confidence that the front depth being between 2.5% and 97.5% of the results at any time. In the written computer program it is

possible to change confidence intervals to any required range by changing the upper and lower limits.

Another important finding from Fig. 2 is that after a lot of runs simulation shows that the mean value curve of the front depth is almost same as the deterministic smooth curve. This important fact is needed for future works when the real test results are going to be used together with the results of simulations. This is the next step of this research work which has been already started. In order to check and verify the capabilities of the proposed modeling method results from other researchers are used [24, 6, 25, 26 & and 5]. Here some typical results of the proposed method are shown to compare with the data in different references [24, 25]. These references have real test results for different kind of concretes. All findings show good and practical results for the proposed modeling method in this paper.

Typically Fig. 4 to Fig. 6 show comparison of the obtained results in this paper with the results from reference [24]. Fig. 4 shows the results of chloride content from core samples in wharf-8 structure with sound concrete (uncracked). Here in order to show how the proposed method can be used only the results at 2.5 cm inside concrete are considered for calibration of the simulations. Assuming only at 2.5 cm depth the chloride content is known the many trajectories are calculated so that the mean shows the mean point of the simulated curve and the scatter of the trajectories at 2.5 cm is same as the real test results. In other words the real test results at this specific depth

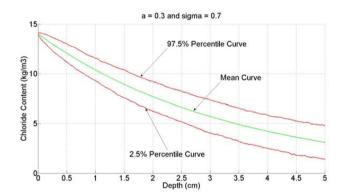


Fig. 2. Typical Trajectories of Chloride Content vs. Concrete Depth (Stochastic solution mode)

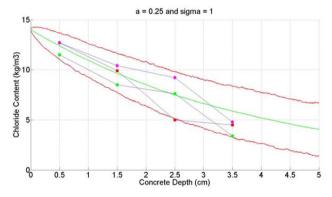


Fig. 4. Comparison of simulated stochastic chloride content profiles calibrated by test data for wharf-8 structure at only x = 2.5 cm in reference [24]

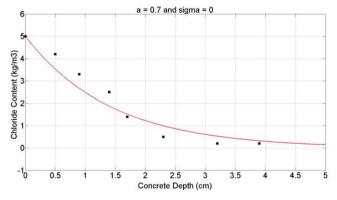


Fig. 3. Typical Mean Trajectory of Chloride Content vs. Concrete Depth (Deterministic solution mode)

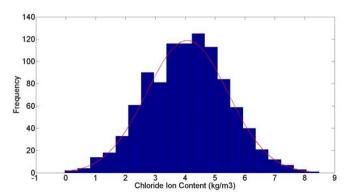


Fig. 5. Histogram and distribution of the simulated stochastic chloride content at x = 5 cm in Fig. 4

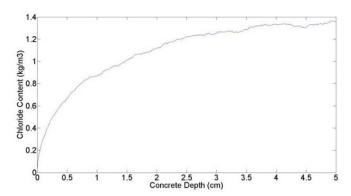


Fig. 6. Standard Deviation of the Chloride Content Profiles vs. Concrete Depth in Fig. 4

are used to calibrate the proposed method for both a and σ coefficients. It is clear that only by this limited data all the chloride content data from real test results in different depths can be shown by the proposed method in this paper. It means extrapolation is also possible.

Fig. 5 depicts that the output for any given depth (here x=5 cm) is normally distributed. Fig. 6 shows by increasing concrete depth standard deviation of the chloride content profiles at first increases rapidly and then it becomes pretty constant.

Fig. 7 to Fig. 9 show the simulated results for comparison

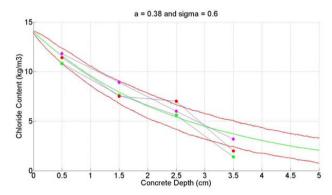


Fig. 7. Comparison of simulated stochastic chloride content profiles calibrated by test data for wharf-11 structure at only x = 1.5 cm in reference [24]

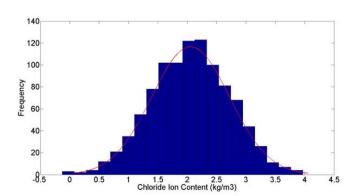


Fig. 8. Histogram and distribution of the simulated stochastic chloride content at x = 5 cm in Fig. 7

with other real test data from reference [24]. Here again findings are same as the previous example.

Two more verification examples are included in this section from another reference [25]. In this reference there are many test results for concrete chloride content in different type of concretes at two different exposures. Fig. 10 to Fig. 15 show that the proposed simulation method is capable of being used for prediction of stochastic chloride ion profile in concrete based on the available test data.

The coefficients a and σ in Langevin equation show some physical meanings. Coefficient a shows how fast or slow the slope of chloride ion profile is descending. It may be regarded as the strength of chloride ion binding effect of concrete and its probable high density. In other words concrete permeability is very small. This coefficient physically means like an opposing force or active barrier against diffusing chloride ion in concrete. Also coefficient σ shows the variance of diffusing chloride ion in concrete which in turn can be a sign of the degree of concrete homogeneity. Overall finding shows that both a and σ may be accepted as two measures for concrete quality when durability is the main concern.

It should be noted that since the proposed method is using limited available real test data simulations can be used for different kind of concretes. Therefore this hybrid method based on the theoretical simulations calibrated by real test

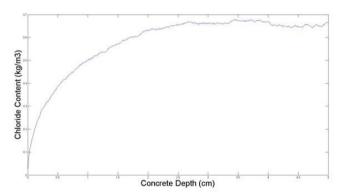


Fig. 9. Standard Deviation of the Chloride Content Profiles vs. Concrete Depth in Fig. 7

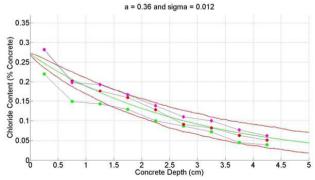


Fig. 10. Comparison of simulated stochastic chloride content profiles calibrated by test data for concrete at the Weka Bay exposure site in New Zealand after 60 months at only x = 2.25 cm in reference [25]

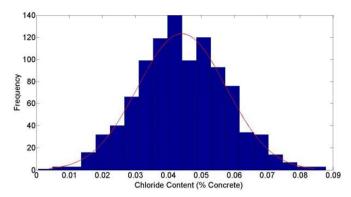


Fig. 11. Histogram and distribution of the simulated stochastic chloride content at x = 5 cm in Fig. 10

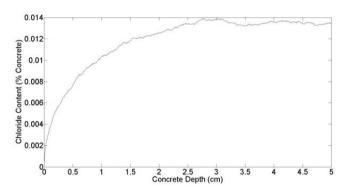


Fig. 12 - Standard Deviation of the Chloride Content Profiles vs. Concrete Depth in Fig. 10

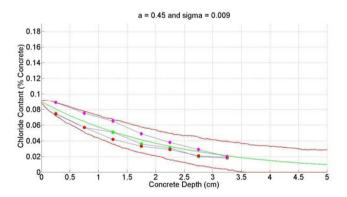


Fig. 13 - Comparison of simulated stochastic chloride content profiles calibrated by test data for concrete at the Oteranga Bay exposure site in New Zealand after 60 months at only x = 1.25 cm in reference [25]

data is more practical than merely theoretical methods or expensive-time consuming experimental works. One of the most particular attentions due to lack of budgeting in many countries is to optimize the management of the two main items in bridge management systems (BMS). These activities are repair projects and maintenance activities with their associated data [27]. The limited data associated with them is apparently valuable and can extend possible application of the Langevin equation for concrete deterioration prediction and enhances the capabilities of managerial actions.

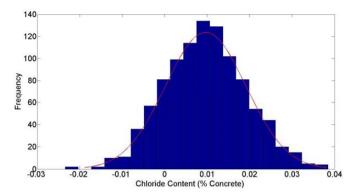


Fig. 14. Histogram and distribution of the simulated stochastic chloride content at x = 5 cm in Fig. 13

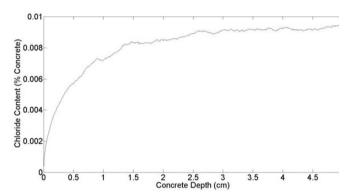


Fig. 15 - Standard Deviation of the Chloride Content Profiles vs. Concrete Depth in Fig. 13

7. Conclusions

In this paper a new approach is introduced in calibration/modeling of the diffusion based deterioration of concrete. Stochastic partial differential equation (SPDE) of diffusion, specifically Langevin equation is used to simulate stochastic chloride content profile vs. time. The major findings are:

- 1. The famous Langevin equation which is a wide used SPDE in physics and chemistry can be applied in diffusion based problems of concrete deterioration successfully.
- 2. The proposed method has the advantage of capturing an instantaneous chloride content profile in concrete including not only the mean but also the variance compared to the deterministic diffusion equation.
- 3. The ensemble mean of the proposed stochastic model based on a large number of runs agrees with the solution of deterministic diffusion equation very well.
- 4. A stochastic solution provides more detailed information as opposed to deterministic methods such as mean, variance and other statistical characteristics of chloride content profile at any depth in concrete.
- 5. Such information regarding the mean and variance of chloride content profile in concrete is valuable for concrete durability design/evaluation and service life prediction of concrete structures as well.
- 6. Drift and diffusion coefficients of Langevin equation may be considered as two measures for concrete quality when durability is the main concern.

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