

Original Research Paper

# Uncertainty Impact of the Effective Diffusion Coefficient on the Concrete Chemical Degradation

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**Abstract:** Reinforced concrete is the construction material widely used in civil engineering. However, knowledge of its long-term performance and the uncertain impact of the environment on his behaviour make it difficult to accurate assessment of the durability of structures with time. When a structure is put into service, it is likely to damage, which origin can be physical, mechanical or chemical. Chemical factors are frequently the most important, since the concrete can be degraded by reaction (dissolution, swelling) of the concrete constituents. In this paper, a probabilistic formulation is applied to carbonation phenomenon and statistics regarding carbonation time required for the carbonation depth reaches the reinforcement concrete are investigated by performing a parametric analysis which integrates the influence of variation of porosity and effective diffusion coefficient of carbonic gas.

**Keywords:** Chemical Factors, Carbonation Kinetics, Carbonation Time, Coefficient of Variation, Carbonic Gas CO<sub>2</sub>

## Introduction

Carbon dioxide and chlorides are the most important buildings aggressive agents which may be exposed. They are responsible for one of the main mechanisms of degradation of existing structures.

These phenomena are respectively identified by the corrosion due to penetration of chlorides or corrosion by carbonation

The speed of concrete carbonation depends mainly on the dioxide carbon penetration inside the cement matrix. Indeed, the diffusion of carbon dioxide through the porous structure of concrete is determined by the Water to cement ratio and porosity. Badaoui *et al.* (2012; Castellote *et al.*, 2001) and are identified in italic type, within parentheses.

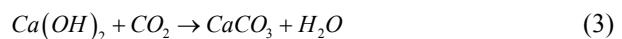
## Concrete Carbonation Theory

Carbonation originates from the low amount of carbon dioxide in the air; it reflects the action of CO<sub>2</sub> diffusion within the pores of the concrete and reactions with hydrates. When the portlandite is consumed, the pH drops to a value below 9, thus initiating the corrosion of steels (Ang and Tang, 2005).

Carbonation has a beneficial aspect of cementitious materials; crystals of calcite CaCO<sub>3</sub> that form from the

hydrates can increase the resistance of concrete to the diffusion of aggressive agents.

The Ca(OH)<sub>2</sub> reacts with carbon dioxide to form calcite, according to the following reactions (Castellote *et al.*, 2001) Equation 1-3:



Portlandite carbonation is overall accompanied by water release of structure

## Statistical Investigation of Concrete Carbonation

In this article, the statistics corresponding the time required for the carbonation depth reach the steel are studied, by performing a parametric study that incorporates the influence of the uncertainty of the effective diffusion coefficient of carbon dioxide and the porosity of the paste of the carbonated concrete on time carbonation, taking a log-normal distribution.

To evolve towards the probabilistic approach, we used the Duracrete deterministic model calculating the carbonation time  $T_1$  according to following equation (Duracrete. 2000) Equation 4:

$$T_1 = \left[ \frac{a d^2}{2 k_e k_c D_{eff} C_s t_0^{2\omega}} \right]^{\frac{1}{1-2\omega}} \quad (4)$$

$a$  is the quantity of material carbonated given by Equation 5:

$$a = \frac{\beta_{ch} CH \alpha_h M_{CO_2}}{M_{cao}} \quad (5)$$

Where:

- $M_{CO_2}$  and  $M_{cao}$  = The molar masses of carbonic gas and calcite
- $\alpha_h$  = The degree of hydration of cement
- $CH$  = The quantity of the Portland and  $\beta_{ch}$  translates the relation of the portland likely to react
- $d$  = The coating  $d = 30$  mm,  $\omega$  is the mesoclimatic factor  $\omega = 0.1$  Equation 6:

$$k_e = \left( \frac{1 - RH_{abs}^5}{1 - RH_{lab}^5} \right)^{2.5} \quad (6)$$

$$RH_{abs} = 75\%, RH_{lab} = 65\%, k_e = 0.69.$$

$k_c$  is a parameter taking account of the conditions of curing compound concrete, given by Equation 7:

$$k_c = \left( \frac{t_c}{7} \right)^{-0.56} \quad (7)$$

Where:

- $t_c$  = The duration of cure,  $t_c = 1$  day and  $k_c = 3$
- $D_{eff}$  = The effective coefficient of diffusion of  $CO_2$  Equation 8:

$$D_{eff} = 1.6410^{-6} \varepsilon_c^{1.8} (1 - RH)^{2.2} \quad (8)$$

$\varepsilon_c$  is the porosity of the paste of the carbonated concrete

$C_s$  is the  $CO_2$  pressure on the surface of the concrete,  $C_s = 6.1 \text{ kg/m}^3$

T the expiry considers (year),  $t_0$  is the reference period "28 days"

## Study Materials

The characteristics of studied concrete and cement chemical composition are shown in Table 1 and 2.

Table 1. Portland cement chemical composition CEM I 52.5R

Parameter	Value
Cement	365 Kg/m <sup>3</sup>
Aggregates	1850 Kg/m <sup>3</sup>
Water	182 Kg/m <sup>3</sup>
Thermal cure (free cooling)	6H à 60°C
Cure time	1 day
Water to cement ratio	0.5

Table 2. Concrete composition studied

SiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	Fe <sub>2</sub> O <sub>3</sub>	CaO
22%	5.02%	2.94%	64.36%
K <sub>2</sub> O	Na <sub>2</sub> O	SO <sub>3</sub>	MgO
0.47%	0.26%	1.94%	2.07%

For the composition of concrete proposed, the effective coefficient of diffusion can be estimated at  $D_{eff} = 3.92 \cdot 10^{-12} \text{ m}^2/\text{s}$ , with a value of porosity  $\varepsilon_c = 0.45$ ,  $\alpha_h = 80\%$ ,  $\beta_{ch} = 85\%$  and  $a = 65.2 \text{ kg/m}^3$  (Badaoui *et al.*, 2012).

It is considered that this concrete is located inside of a building where the humidity of the ambient air is medium or high. It is therefore subject to the exposure class XC3, the numerical values for the composition parameters are identical to those of the class XF1 (Norm NA 16002, 2004; Norm NA 442, 2006).

## Numerical Implementation of the Simulations

One has to solve a conventional random problem for a large number of input parameters by using Monte Carlo simulations (Rubinstein and Kroese, 1981).

About 10000 independent samples of the parameters  $D_{eff}$  and  $\varepsilon_c$  with a log-normal distribution are generated and the deterministic numerical procedure is applied to each individual simulation, providing 10000 values of the time carbonation parameters. Finally, statistics of the depth and time factors (mean, standard deviation and confidence interval) are calculated.

The parameters of the lognormal distribution of  $D_{eff}$  and  $s$  are expressed as follows Equation 9-12:

$$\sigma_{\ln D_{eff}}^2 = \ln \left( 1 + \frac{\sigma_{D_{eff}}^2}{\mu_{D_{eff}}^2} \right) \quad (9)$$

$$\mu_{\ln D_{eff}} = \ln(\mu_{D_{eff}}) - \frac{1}{2} \sigma_{\ln D_{eff}}^2 \quad (10)$$

$$\sigma_{\ln \varepsilon_c}^2 = \ln \left( 1 + \frac{\sigma_{\varepsilon_c}^2}{\mu_{\varepsilon_c}^2} \right) \quad (11)$$

$$\mu_{\ln \varepsilon_c} = \ln(\mu_{\varepsilon_c}) - \frac{1}{2} \sigma_{\ln \varepsilon_c}^2 \quad (12)$$

where,  $(\mu_{D_{eff}}, \sigma^2_{D_{eff}})$  and  $(\mu_{\epsilon_c}, \sigma^2_{\epsilon_c})$  are statistics (mean and variance) of  $D_{eff}$  and  $\epsilon_c$  respectively.

The mean value of the effective coefficient of diffusion is  $D_{eff} = 3.92 \cdot 10^{-12} \text{ m}^2/\text{s}$  and the coefficient of variation  $Cv_{D_{eff}}$  varies between 0 and 0.1.

For the porosity  $\epsilon_c$ , the mean value is  $\mu_{\epsilon_c} = 0.45$  and its coefficient of variation  $Cv_{\epsilon_c}$  also varies between 0 and 0.1.

In order to determine the time carbonation, the Chi-Square goodness of fit test is used to evaluate the fit of the assumed carbonation parameters probability distribution and the shape of the corresponding histograms suggests a log-normal distribution, which is adopted in this study is shown in Fig. 1

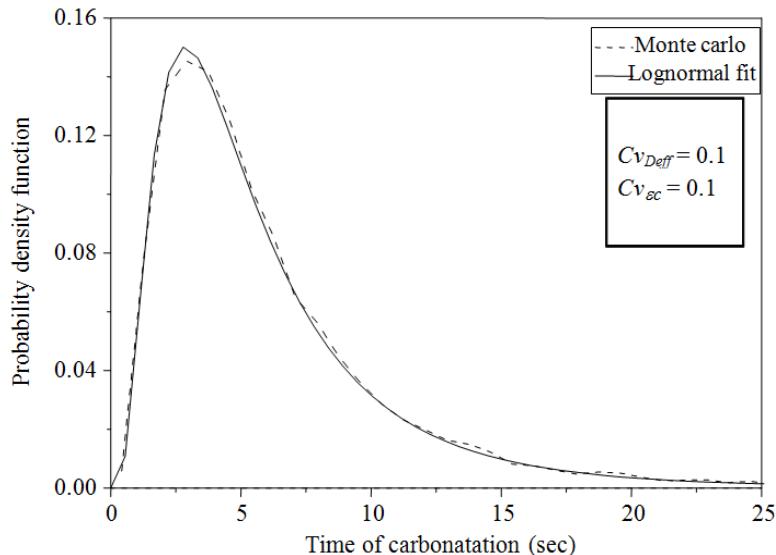


Fig. 1. Probability density function of the carbonation time versus  $D_{eff}$  and  $\epsilon_c$

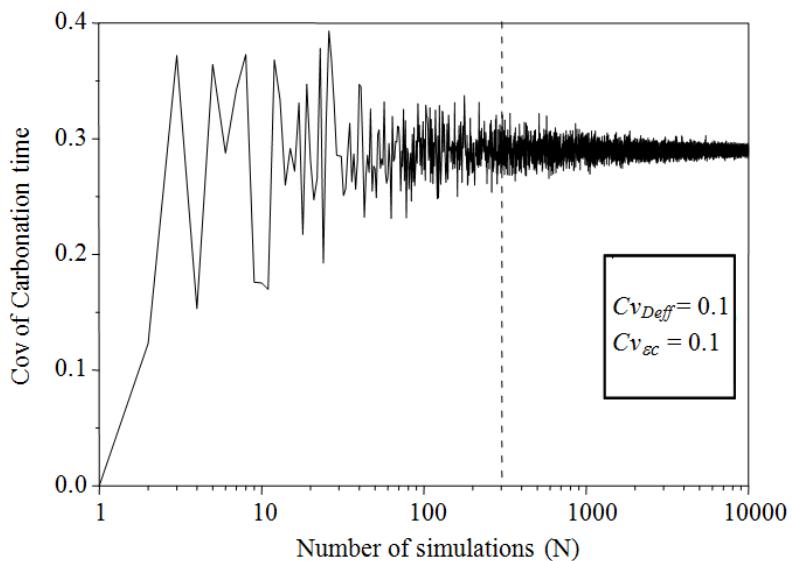


Fig. 2. Carbonation time coefficient of variation versus  $D_{eff}$  and  $\epsilon_c$

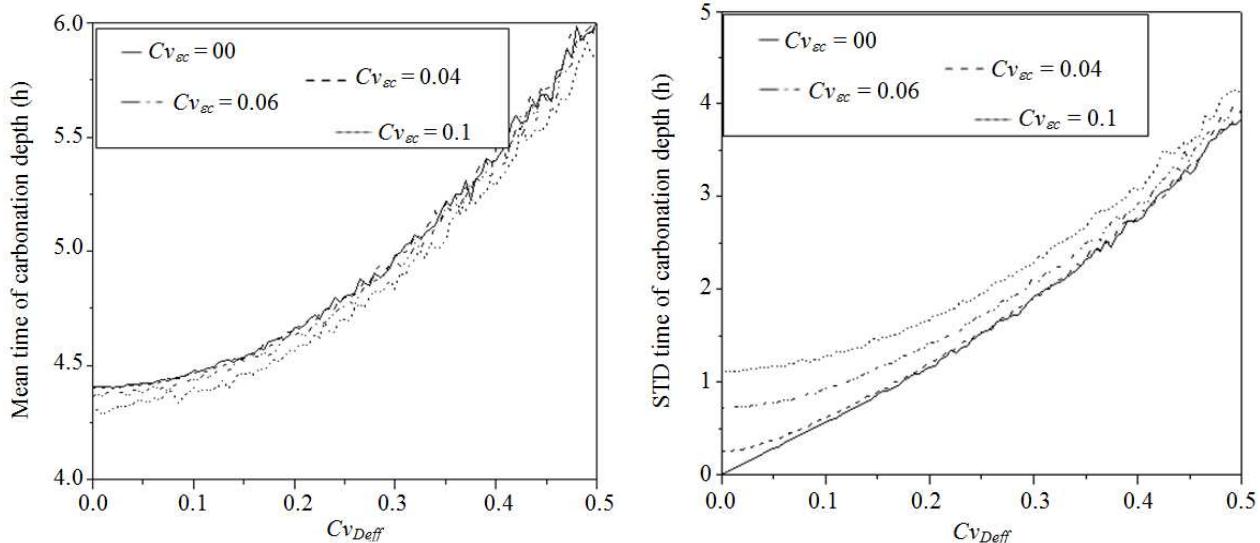


Fig. 3. Time of carbonation statistics versus  $Cv_{D_{eff}}$  coefficient of variation

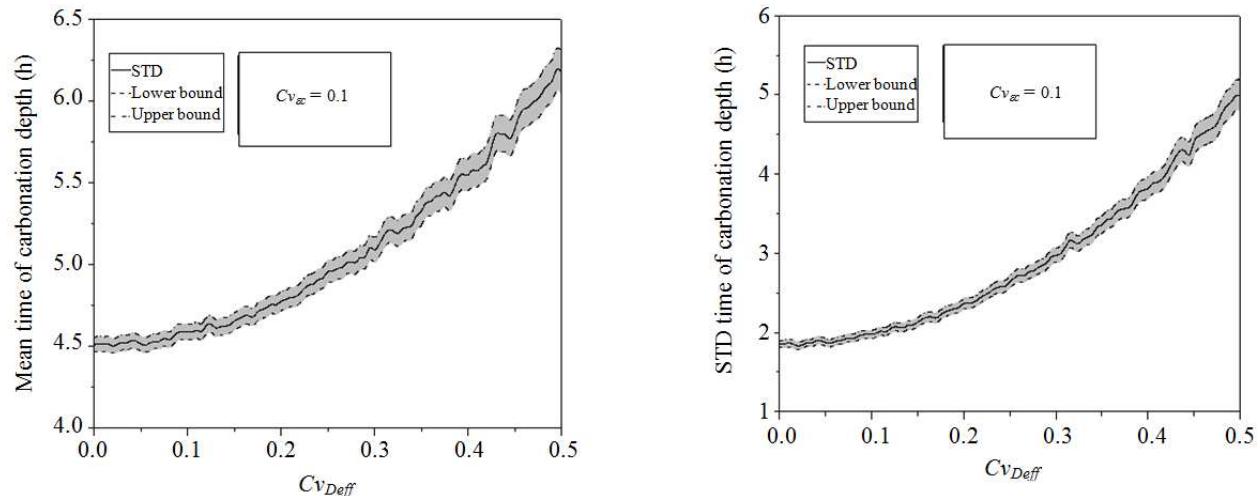


Fig. 4. Time of carbonation statistics and confidence intervals versus  $Cv_{D_{eff}}$  coefficient of variation

We remark that when  $Cv_{D_{eff}}$  and  $Cv_{ec}$  increase, the mean and the standard deviation augment significantly; indicating that the diffusion of  $\text{CO}_2$  from the outside to the heart of the concrete requires a longer time.

The confidence intervals are important indicating that the variability of the  $D_{eff}$  affects the carbonation time.

The SDT value of the carbonation time increases which indicates that the uncertainty on the  $ec$  causes a delay in the carbonation process.

Reacting the hydrate of concrete with carbon dioxide leads to the production of water.

Greater the quantity of carbon dioxide released into the pores is larger, the amount of water formed during carbonation is important, this formation will

also affect the process and increase the time of carbonation.

## Conclusion

Carbonation of the concrete has an impact on the effective diffusion coefficient; this coefficient is decreased after carbonation. The interaction between the ions of carbon dioxide and the Calcium Silicate Hydrate surface (C-S-H) negatively charged form an electric double layer on the pores surface of the and slows the  $\text{CO}_2$  diffusion.

Indeed, the time required for the carbonation depth reaches the reinforcement concrete depends on the effective diffusion coefficient of  $\text{CO}_2$ , " $D_{eff}$ ", which is

linearly related to water to cement ratio and relative humidity.

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## Ethics

This article is original and contains unpublished material. The corresponding author confirms that all of the other authors have read and approved the manuscript and no ethical issues involved.

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