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Experimental study to evaluate the performance of a natural carbonation prediction (NCP) model

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Abstract

This paper presents an evaluation of a recently developed natural carbonation prediction (NCP) model. In the present study, the NCP model was evaluated using data from an experimental investigation conducted using concrete mixtures of 0.5 water - cementitious (w/cm) ratios, and of various concrete strengths. CEM I 52.5N ordinary Portland cement was used in the mixtures, with or without 10% silica fume, 30% fly ash and 50% slag. Concrete cubes of 100 mm size were cast and cured in water for 7 days then exposed outdoors to undergo carbonation under the natural environment in Johannesburg, South Africa. The cube samples were stored at an urban outdoor site. After 6 years of outdoor exposure of the samples, carbonation measurements were done to generate data sets used to evaluate the model. Results show that the model's predictions were in agreement with actual carbonation measurements. Findings of this study confirm the model's accuracy, and also imply that the NCP model can potentially be used under different environments for various concrete structures.

Keywords: natural carbonation; prediction model; service life; reinforced concrete; corrosion

1. INTRODUCTION

With ongoing worldwide climate change associated with rise in carbon-dioxide (CO_2) concentration in the atmosphere along with rise in global temperature, it can be expected that long-term durability aspects of concrete structures, are being adversely affected. As such, there is a crucial need for practical carbonation prediction models, that can be employed to define specifications for use to build future climate resilient structures, as old and current standards are quickly becoming inadequate under the changing global climate conditions.

Assessment of carbonation-induced damage upon service life, whether for new or existing reinforced concrete, involves consideration of two stages: (1) initiation period during which the carbonation front under CO_2 diffusion, penetrates the cover concrete such that the loss of alkalinity causes de-passivation of reinforcing steel. (2) propagation period in which, depending upon the local moisture conditions, the de-passivated steel corrodes. The corrosion products then cause expansive stresses that crack the cover concrete. Further corrosion then progressively leads to spalling, delamination and loss of steel area thereby causing structural damage.

Service life is the total time duration comprising the sum of initiation and propagation periods. It is known that propagation period is very short being about 2 to 5 years in concrete structures that may have an initiation period of typically more than 30 to 50 years. On this basis, it can be reasonable to neglect propagation time while giving consideration specifically to initiation period as the basis for determining service life. This approach is evident in the literatures, with most researches focussing upon development of carbonation prediction models without much emphasis on propagation models.

A closer look into the various factors influencing the mechanism, highlights the complexity of carbonation modelling, more so with ongoing climate change. Since 2015, the natural CO_2 concentration in the atmosphere has exceeded 400 ppm, however, it fluctuates seasonally over the year, as well as locally within the exposure site as influenced by industrial activities, traffic, wind factors and ventilation. Also, relative humidity (RH) is of absolute importance to carbonation. Maximum carbonation intensity occurs at 50 to 70% RH. At low RH, there isn't sufficient presence of moisture to support carbonation reactions, while at RH > 80%, the saturated concrete hinders CO_2 penetration into concrete [1, 2]. RH varies widely with seasonal changes in the tropical regions, and may range from 40% RH in dry season to 80% RH during wet season [3]. Indoor and outdoor exposure conditions are known to differently influence concrete carbonation, with the former giving generally higher carbonation ingress.

Nearly all the carbonation models proposed in the literatures are experimental techniques that have not been evaluated against real – life behaviour of concrete structures, with very few exceptions such as the fib-Model Code [4] and the natural carbonation prediction (NCP) model [5]. Comparison done in Ekolu 2018 [5] showed that the NCP and fib-Model Code models exhibit a similar level of prediction accuracy. In Ekolu 2020a [6], the NCP model was employed to predict carbonation in 69 existing concrete structures located worldwide in the urban settings of Johannesburg (South Africa), Bhopal (India), Brasilia (Brazil), Blenio (Switzerland), Tallin (Estonia), Seoul (South Korea), Taipei (Taiwan) and Turin (Italy). It was found that the NCP model made realistic predictions of actual ongoing carbonation in the existing concrete structures. Independent researches have also shown that the NCP model outperforms most other models [7, 8].

In this study, experimental investigation was conducted using concrete mixtures of 0.5 water - cementitious (w/cm) ratios, and of various concrete strengths. CEM I 52.5N ordinary Portland cement was used in the mixtures, with or without 10% silica fume, 30% fly ash and 50% slag. Concrete cubes of 100 mm size were cast and cured in water for 7 days then exposed outdoors to undergo carbonation under the natural environment in Johannesburg, South Africa. Data of this study were used to evaluate a recently developed NCP model [5]. After 6 years of outdoor exposure of the samples, carbonation depth measurements were done, then the results were compared with the model's predictions.

2. EXPERIMENTAL DETAILS

2.1 Test Samples

The cement types, w/cm ratios and supplementary cementitious materials (SCM) employed, are given in Table 1. After casting, the hardened concrete samples were cured for 7 days in water at 23 °C and subsequently, four contiguous surfaces of cube samples were coated with epoxy. The remaining non-coated opposite cube sides were exposed to natural carbonation under sheltered or unsheltered outdoor conditions until the testing date. Also, the four concrete mixtures were tested for compressive strength at the age of 28 days, giving the results presented in Table 1.

Table 1: Cement types, w/cm ratios and SCMs used.

Mix	Type of SCM	Cement type	%SCM	w/cm	28-day strength (MPa)
PC5	Ordinary Portland cement	CEM I	0	0.50	38.2
FA5	Fly ash	CEM IIB-V	30	0.50	27.2
SG5	Slag	CEM IIIA	50	0.50	22.8
SF5	Silica fume	CEM IIA-D	10	0.50	30.0

2.2 NCP Model

The NCP model [5] is given in Eqns (1) to (7). The mathematical equations represent various relationships which once combined, estimate carbonation depth in concrete at any given age. The three major components of the model are: (1) concrete strength, (2) the type of cementitious material, and (3) environmental factors comprising RH, CO_2 concentration, and sheltering from rain.

$$d_{f,t} = e_h.e_s.e_c.cem(F_{c,t})^g.\sqrt{t} \quad (1)$$

where e_h, e_s, e_c are environmental correction factors for RH /temperature, shelter effect and CO_2 concentration, respectively. $F_{(c,t)}$ is the function for strength growth with time (t), which in turn is converted into carbonation progression using the scalar quantity, *cem*, coupled with exponent, *g*, both factors being dependent on the type of cement.

Environmental factors for relative humidity (RH) and shelter:

$$e_h = 16\left(\frac{\mathrm{RH}-35}{100}\right)\left(1-\frac{\mathrm{RH}}{100}\right)^{1.5} \text{ for } 50\% \leq \mathrm{RH} \leq 80\% \quad (2)$$

This factor is applicable under tropical annual ambient temperatures of 10 to 30°C.

$$e_s = \begin{cases} 1.0 \text{ for sheltered outdoor exposure} \\ f_c^{-0.2} \text{ for unsheltered outdoor exposure; } f_c \text{ is 28-day strength} \end{cases} \quad (3)$$

Environmental factors for varied CO_2 concentrations:

$$e_c = \begin{cases} \alpha f_c^r \text{ for } 20 < f_c < 60 \text{ MPa} \\ 1.0 \text{ for } f_c \geq 60 \text{ MPa} \end{cases} \quad (4)$$

where α and r, are correction factors for natural carbonation under varied CO_2 concentrations:

28 - day strength (MPa)	Correction factor		CO_2 concentration level (ppm)				
			200	300	500	1000	2000
$20 < f_c < 60$	$e_c = \alpha f_c^r$	α	1.4	1.0	2.5	4.5	14.0
		r	-1/4	0	-1/4	-2/5	-2/3
$f_c \geq 60$	$e_c = 1.0$						

Time-dependent strength growth function ($F_{c,t}$):

$F_{c,t} = \frac{t}{a+bt} . f_c$, where $f_c = f_{c28}$ or f_{cbn}

(a) Using 28-day strength (f_{c28})

(i) Short-term ages, t < 6 years (5a)

$$a = 0.35, b = 0.6 - t^{0.5}/50$$

(ii) Long-term ages, t ≥ 6 years (5b)

$$a = 0.15t, b = 0.5 - t^{0.5}/50$$

(b) Using long-term insitu strength (f_{cbn})

(i) Short-term ages, t < 15 years (6a)

$$a = 0.35, b = 1.15 - t^{0.6}/50$$

(ii) Long-term ages, t ≥ 15 years (6b)

$$a = 0.15t, b = 0.95 - t^{0.6}/50$$

Cement factors for carbonation conductance: (7a)

SCM	Cement types	Scalar, *cem*	Conductance factor, *g*
20% any	CEM I, CEM II/A	1000	-1.5
30% fly ash	CEM II/B, CEM IV/A	1000	-1.4
50% slag	CEM III/A, CEM IV/B	1000	-1.4

*SCM – supplementary cementitious material

Alternatively, g, may be determined using the equation

$$g = \frac{\%SCM}{500} - 1.5 \tag{7b}$$

Footnote: Cube strength (f_c) is related to core or cylinder strength (f_{cyl}) through the conversion, $f_c = 1.25\ f_{cyl}$. The cube strength values used in the model's equations must be ≥ 20 MPa.

2.3 Carbonation Measurement

After exposure of samples outdoors for 6 years, they were split then the fresh surfaces were sprayed with phenolphthalein indicator solution. The depth of carbonation was recorded 24 h after spraying the indicator solution, as recommended by RILEM CPC-18 [9]. For each split surface, the measurements for depth of carbonation were performed at 11 points along each opposite end of the surface, and the 22 values thus obtained were averaged.

3. RESULTS AND DISCUSSION

The 28-day strength results of the concrete cubes, are given in Table 1. The carbonation depths were measured 6 years after initial casting of the concrete cubes. The model employs RH, 28-day concrete strength, cement type, CO_2 concentration and time, as its input data (Section 2.2). The comparison of results can be seen in Figures 1 and 2.

An average annual relative humidity of 60 % was used in the model, along with an average CO_2 level of 400 ppm. These values of the environmental factors were based on air quality readings recorded at the outdoor exposure site. The age for each sample was taken as the precise duration from the date of casting to the date of testing for carbonation depth.

The measured results were compared against carbonation depth values predicted by the model. In Figure 1, the predicted values and measured values of carbonation depths show a strong agreement with points lying along the line of equality. Evidently, the model's predictions are realistic for concretes subjected to natural carbonation under both *sheltered* and *unsheltered* outdoor exposure conditions.

It is notable that values of carbonation depths greater than 10 mm exhibited significant dispersion, with predicted values tending to be relatively higher than measured results. A close look at the data shows that this tendency was associated with mixtures that had lower strength. For example the mix SG5 that had 22 MPa strength, gave the measured carbonation of 11.82 mm which was lower than the predicted 18.4 mm depth. Similarly, the mix FA5 which had concrete strength of 27.2 MPa, gave 8.5 mm carbonation depth while the predicted value was 14.1 mm. The mixtures PC5 and SF5 that had concrete strengths of 38.2 MPa and 30 MPa, gave values of measured and predicted values that were generally in agreement, falling close to the line of equality (Figure 1). The foregoing observation underscores the necessity of the condition given in the footnote of Eqn (8), requiring that cube strength must be greater than 20 MPa, as lower strength values invariably alter predictions of the model to give disproportionately high values.

Prediction accuracy of the model was evaluated using statistical error parameters comprising the root mean square of error (RMSE) and coefficient of variation of error (CVE), calculated as given in Eqns (8) and (9).

$$\mathrm{RMSE} = \sqrt{\sum_{1}^{n} \frac{(\mathrm{Residual})^2}{n}} \tag{8}$$

$$\mathrm{CVE}\ (\%) = \frac{\mathrm{RMSE}}{\overline{\mathrm{X}}_{\mathrm{mv}}} . 100 \tag{9}$$

where *residual* is the difference between the predicted and corresponding measured value, n is total number of paired data points, and $\overline{\mathrm{X}}_{\mathrm{mv}}$ is the mean of measured values.

The CVE and RMSE values obtained were 36.9% and 2.87, indicating that the model's predictions were accurate and consistent with those reported in the earlier associated studies [5, 6, 10, 11]. The prediction accuracy of the NCP model is also similar to those of code-type models which give typical CVE values of 20 to 50% [6].

The residuals seen in Figure 2 show more dispersion with increase in carbonation depth, due to lower quality concretes which tend to carbonate faster. This observed pattern is consistent with similar findings reported in the previous studies [5, 11]. It may be recalled that lower quality concretes are typically those of lower strength, which in turn exhibit correspondingly higher variability, which explains the observed fanning out heteroscedasticity seen in Figure 2.

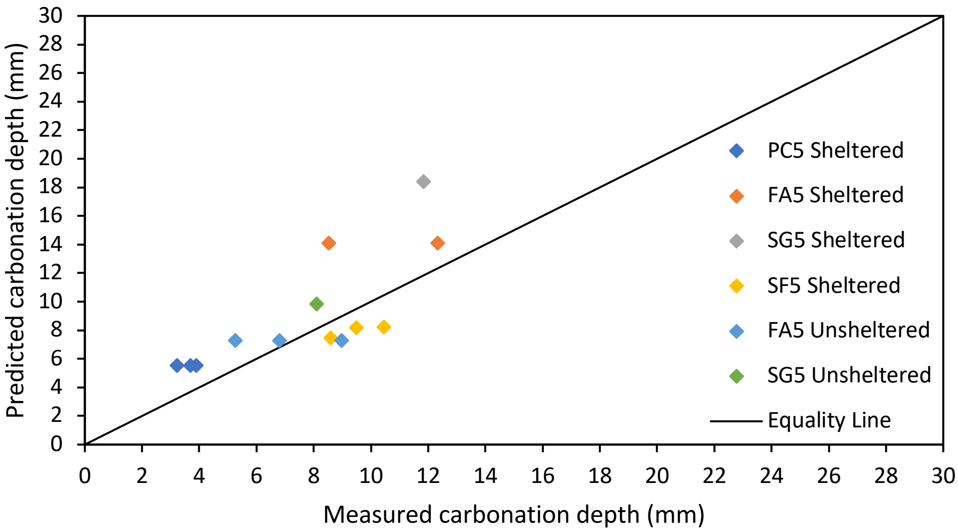

Figure 1: Plot of predicted carbonation depths against measured carbonation depths.

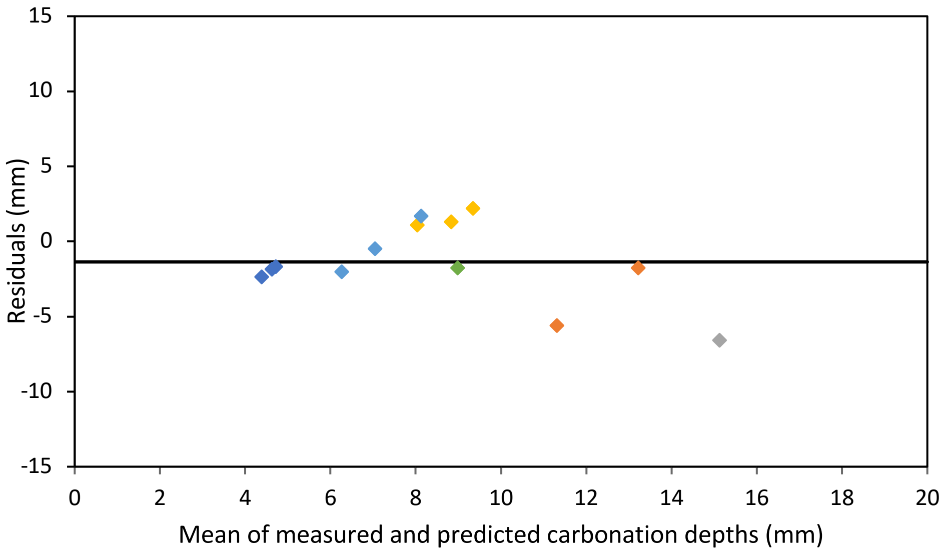

Figure 2: Plot of residuals against mean of measured and predicted carbonation depths.

4. CONCLUSIONS

In this study, an outdoor experiment of 6 years was carried out to obtain data used to evaluate the NCP model. The experiment involved exposure of concrete cubes outdoors for natural carbonation to occur under *sheltered* and *unsheltered* exposure conditions in Johannesburg, South Africa. The measured carbonation depths were compared with values predicted by the model.

Comparison of predicted carbonation depth values versus actual measured values, showed strong agreement which depicts the potential of the NCP model for use under different environmental exposure conditions.

Findings of the present study also confirm that the NCP model is applicable to various concretes including those containing supplementary cementitious materials such as fly ash, slag and silica fume, amongst others. The prediction accuracy of the NCP model was shown to be similar to those of code-type models, typically giving 20 to 50% coefficient of variation of error.

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