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New Model for Natural Carbonation Prediction in Reinforced Concrete – Concept and Validation on Chemical Admixtures

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ABSTRACT

A new model for prediction of natural carbonation in reinforced concrete structures has recently been developed and presented in (Ekolu, 2018). For brevity, the model is referred to as ESS model. It employs concrete strength as the primary property depicting core carbonation behaviour of any given concrete while other factors induce secondary influence. Chemical admixtures in concrete significantly influence concrete behaviour. Using experimental data from the literature (Dan-Herrera et al., 2015), the model behaviour is verified under use of various types of chemical admixtures of concrete including internal curing, shrinkage reducing, viscosity modifying, and high range water reducing admixtures. Class F fly ash was also used in the concrete mixtures as a supplementary cementitious material. Verification results show the model predictions to be meaningful and consistent with robustness.

Keywords: Carbonation, prediction model, mathematical functions, chemical admixtures, concrete structures

1.0 INTRODUCTION

Recently, a new model for prediction of natural carbonation, abbreviated as *ESS model*, was presented in (Ekolu, 2018). The paper described the model development. The model expresses carbonation relationships versus concrete composition and versus environmental factors, using mathematical functions of algebra. Further to the description therein given, it is of interest to encapsulate the approach applied in the model development and analyse the model concept underlying its structure. This paper undertakes this scope based on considerations and understanding drawn from experimental studies reported in various literatures over the past decades.

Quite important to note is the issue of various factors that influence strength and by extension could affect model behaviour. A veracious model should be capable of accurately capturing the influence of these factors and accounting for their effects without severely altering the model's prediction behaviour. The associated earlier studies (Ekolu, 2016; 2018) did identify, evaluate and prioritize the various factors based on understanding of their influence on concrete carbonation, as reported in various literatures. However, the subject of chemical admixtures has not been given due consideration despite their indispensable use in modern concrete. In the present paper, focus is given to chemical admixtures, to evaluate whether their use in concrete could alter the model's behaviour. This verification study is based on independent data taken from the literature (Dan-Herrera *et al.*, 2015).

2.0 CONCEPT

The plausibility of a mathematical model is based on its ability to employ universal and fundamental relations to adequately represent the phenomenon, in this case, the carbonation mechanism. However, the heterogeneity of any given concrete mixture, compounded by the diverse ingredients and associated characteristics of any concrete produced from various processing methods, makes the efforts to capture its behaviour with universal material coefficients quite a complex process, which is dynamically related to environmental factors and time-dependent behaviour. In constituting a model for carbonation prediction, it is suggested that the process must incorporate the key parameters subsequently discussed.

2.1 Fundamental Mathematical Functions

Mathematical expression of phenomena requires appropriate time-dependent fundamental functions that correctly represent the unfolding of the mechanism within the material system. All the most important factors influencing carbonation behaviour primarily or secondarily must also be expressed in mathematical functions. Typically, one core property of the material has governing influence on the material response to the phenomenon while other factors secondarily influence or shift this core behaviour. The mathematical function expressing the relationship between this core property and the phenomenon, becomes the core component of the model upon which the secondary functions expressing the secondary influence by other factors, are incorporated. It should be recognized that these secondary functions only modify the core behaviour defined by the primary function.

A vast amount of research literature has shown that this core component of the model i.e. carbonation ingress or diffusion into concrete is a square-root function of time and takes the form, $d = k_c t^{½}$; where, d is the carbonation depth over time (t) while, k_c is a constant. The expression, however, is a simplification of complex behavior whose observed or measured power values reportedly fluctuate between 0.3-0.6 (Quillin, 2001). The effects of the secondary components i.e. concrete composition, environment etc. are compounded and built into a constant value, k_c which is a unique carbonation rate for a given concrete mixture under specific environmental conditions. The most complex aspect of the equation is predicting this unique value of k_c, which typically varies with each concrete mixture, material types and grades, environmental exposure conditions. Theoretically, a plausible model would attempt to accurately predict this unique rate value consistently and within the limitations and defined rules of the model applicability, which have to be established during its formulation.

2.2 Material Components

Like all porous materials, ingress of gases such as CO_2 into concrete, is inevitable. Unlike other types of ceramic materials, the presence of calcium hydroxide (lime) and moisture within the pore network of concrete enables the chemical reaction of carbonation to occur, resulting in deposition of calcite within the pores. This event immediately sparks changes in concrete that unequivocally influence concrete properties. Accordingly, by monitoring the changes in material properties of concrete under the influence of carbonation, the mechanism can be quantified. In formulating a model, therefore, the material property or parameter chosen should be sufficiently sensitive to correspondingly reflect the dynamics of progressive carbonation ingress, which involves time-dependent changes.

From understanding of concrete behavior, the three parameters or properties of significant importance in hardened concrete are:- mix parameters, permeability and porosity, strength. The two important mix parameters that strongly affect performance of concrete are water/cement ratio (w/c) and cement content. Indeed, research shows that carbonation responds almost linearly to changes in w/c, directly increasing with increase in w/c. Data shows carbonation to be strongly sensitive to the w/c parameter, as found by several researchers (Parrot, 1987). Changes in the w/c, however, are based on adjustments in cement content i.e. decreasing the w/c to diminish the carbonation rate, correspondingly requires increasing the cement content of the mix. It is not surprising that there is a strong relationship between the cement content of concrete and carbonation depth. Indeed, several model expressions have been proposed that are based on w/c (Parrot, 1987). However, the practicality of employing mix parameters in modelling the service life of existing structures poses insurmountable problems. The w/c used in mix design is not necessarily the effective value in hardened concrete. Besides, it is often the case that for most aged structures, there are no original design and construction documents available, having been lost either during change of ownerships or during some unfortunate past event(s). If a prediction model is to be applied to such a structure, the required information would have to be extracted through measurements on the existing structure. Unfortunately, determination of w/c in hardened concrete is complex and may require sophisticated equipment. Moreover, the typical achievable accuracy is at the level of ± 0.1 using analytical techniques (BS 1881: Part 124, 1988). Such low accuracy is not of much use given that w/c significantly impacts concrete properties at the level of two orders of its magnitude. The reportedly best achievable accuracy for w/c determination is ± 0.05 (Neville, 2003) using optical microscopy (ASTM C 457-12, 2012; Ekolu 2008). This too is a tenuous and expensive procedure requiring specialized expertise. These difficulties in determining the correct value of w/c ratio from hardened concrete, also similarly apply to cement content determination. Regardless of the potential ability of these mix parameters to predict carbonation ingress in concrete, the foreseeable difficulties of obtaining reliable data of mix parameters from concrete structures, diminishes their practical value. Mix parameters are therefore not preferred for use in modelling. This leaves two performance properties which are also known to be defining characteristics for durability i.e. permeability and strength.

Permeability has been recognized as perhaps the most important governing property of concrete which controls its durability performance. Measurement of gas permeability is therefore naturally the closest emulation of CO_2 diffusion into concrete. However, there are relatively few proposed models where permeability or diffusion has been employed as the performance property for carbonation prediction (Parrot, 1987). The main reason for this curtailed use of permeability is two-fold: Firstly, permeability measurement is costly and requires expensive equipment. Secondly, there are no universally accepted and standardized permeability test methods, despite intense research in this area over the past 50 years. The main reason for lack of fully fledged standardized permeability test methods is squarely a problem of poor reproducibility of data. It has been shown that the coefficient of variation for permeability measurement is high and varies widely, in the range of 30-50% (Hooton, 1988). Data given in Stanish et al. (2004) found the oxygen permeability coefficients of variation to be 23.7-53.9%, which is consistent with Hooton’s (1988) findings. These reasons place the potential use of permeability as a performance property for carbonation prediction to a significant disadvantage. However, some few permeability-based test methods and prediction models appear to be gaining general acceptability, mainly as experimental tools, such as the permeability-based model by Parrott (1994), Torrent et al. (2014) and more practically, the diffusion model, fib-Model Code (2010). The nuances associated with the permeability property, give preference to strength as the better performance property for carbonation prediction. Compressive strength is as sensitive to carbonation effects as permeability is, and its data are advantageously available, at all ages of the structures lifetime ranging from the design stage to quality control during construction. If, however, there is no past strength data available, it is a simple matter to extract cores from an existing structure for strength testing, as is commonly done during repair and maintenance. Of all concrete tests, compressive strength data are the most abundant and most readily available.

Compressive strength property also has an overriding advantage over permeability for its relatively low coefficient of variation, being 20 to 30% (Shimizu, 2000; Ekolu, 2010) compared to 30 to 50% (Hooton, 1988; Stanish et al., 2004) for permeability. It can be concluded generally that strength may be considered the preferred performance property for use in carbonation prediction.

It is essential that the time-dependence of a given concrete property which is used to represent carbonation progression into concrete, is incorporated into the model equation as a mathematical equation. Again, strength is the core or most critical parameter in this regard, of which the 28-day strength may be adopted as the baseline value to be used for prediction of carbonation at different ages. However, the use of different ingredients in concrete, specifically supplementary cementing materials (SCMs) such as fly ash (FA), silica fume (SF), slag (SG) etc., introduces variations to the strength growth curve. It is well established that these SCMs tend to promote carbonation even when used within conventional proportions of typically 5-10% SF, 20-30% FA, and 30-50% SG. The dual effects of SCMs on both strength and carbonation progression have to be accounted for by introducing the adjustment coefficients or factors, depending on the mathematical expression of model formulation.
Air content is another mix factor that is known to influence strength. However, the effect of entrained air is mostly limited to compressive strength, in which case an appropriate adjustment coefficient, would be sufficient. Also, air entrainment is not commonly practiced in tropical countries.

The common aggregates used in concrete are considered to be inert and may not be involved in chemical interactions. Aggregates of special categories, especially recycled and lightweight types are known to show significant influence on carbonation, with lightweight concretes giving lower carbonation than normal concretes, while recycled aggregates tend to increase carbonation (Lo et al., 2008; Ryu, 2002). Accordingly, models would need to incorporate correction factors to account for aggregate types in lightweight and recycled aggregate concretes. The influence of processing factors including compaction and normal or heat curing can be built into the strength property and need not be considered separately for carbonation prediction (Ekolu, 2004; 2016).

2.3 Environmental Factors

The natural CO_2 concentration is typically 300-400 ppm, however, it often fluctuates seasonally over the year, as well as locally within the exposure site as influenced by industrial activities, traffic, wind factors and ventilation. Besides, the worldwide atmospheric CO_2 concentration has been rising since AD 1700's and this trend is projected to continue over the next 100 years (Quillin, 2001; Parrot, 1987). While it may presently be sufficient to assume that natural CO_2 concentration is constant at 350-400 ppm, it should be acknowledged that this assumption may fail in the nearby future.

Relative humidity (RH) is of absolute importance to carbonation. Carbonation intensity is confined to a range of 50-70% RH. At low RH, there isn't sufficient presence of moisture to support carbonation reactions, while at RH >80%, CO_2 diffusion into the nearly saturated concrete would be inhibited (Quillin, 2001; Parrot, 1987). 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 (Eludoyin et al., 2013). Indoor and outdoor exposure conditions are known to differently influence concrete carbonation, with indoor conditions generally exhibiting relatively higher carbonation progression.

Similarly, concrete that is sheltered from rain e.g. the concrete section at the soffit of a horizontal structural element, will expectedly experience greater carbonation than those concrete sections that are unsheltered. Direct exposure of structural concrete to rain, causes blockage of the surface pore network which in turn prevents carbonation progression during wet cycles, unlike sheltered concrete which remains partially saturated throughout the various seasons of the year. Carbonation can be expected to thrive at the exposure classes of XC3 (moderately wet, typically 70%RH) and XC4 (alternating wet and dry, typically 85-90%RH) (BS EN 206, 2000; Kulkarni, 2009). These exposures classes are also the predominant conditions in tropical climates.

3.0 MODEL

The model is given in Eqs. (1) to (7). The expressions represent various relationships which together estimate the carbonation behavior of concrete. These relationships constitute the three major components of the model, comprising: (1) the material performance property, being concrete strength, (2) the concrete compositional characteristics represented by the cementitious material type, and (3) environmental factors i.e. RH, [CO_2], sheltering from rain. It should be recalled that use of the model is applicable within its limitations that are given in (Ekolu, 2018).

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

Environmental factors for relative humidity and shelter:

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

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

Environmental factors for varied CO_2 concentrations:

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

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

Table 1. Correction factors for varied CO_2 concentrations and strength grades

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
		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

$$a = 0.35,\ b = 0.6 - t^{0.5}/50 \quad (5a)$$

(ii) Long-term ages, t ≥ 6 years

$$a = 0.15t,\ b = 0.5 - t^{0.5}/50 \quad (5b)$$

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

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

$$a = 0.35,\ b = 1.15 - t^{0.6}/50 \quad (6a)$$

(ii) Long-term ages, t ≥ 15 years

$$a = 0.15t,\ b = 0.95 \quad t^{0.6}/50 \quad (6b)$$

Cement factors for carbonation conductance: (7)

Table 2. Materials and conductance factor

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 cementing materials

Notes: Cube strength (f_c) is related to core or cylinder strength (f_{cyl}) through the conversion, $f_c = 1.25\ f_{cyl}$. Strength values used in the equations must be ≥ 20 MPa. Moist-cured 28-day strength (f_{c28}) is related to insitu strength (f_{cbn}) using the expression, $f_{cbn} = f_{c28}+13$.

4.0 COMPARISON OF MODEL PREDICTIONS VERSUS EXPERIMENTAL RESULTS

All data used under this section was extracted from (Duran-Herrera et al. 2013). These data were used as inputs into the carbonation prediction model. The literature gave experimental data of accelerated and natural carbonation measurements for a set of seven (7) concrete mixtures. The experimental study investigated carbonation resistance of concretes in which chemical admixtures of various types were used including high range water reducing admixture, internal curing admixture, shrinkage compensating admixture, and viscosity modifying admixture. Five (5) mixtures of ordinary Portland cement (OPC) concretes and two mixtures containing 20% Class F fly ash, were prepared. Only the data for natural carbonation exposure were used in the present paper, as the model is not applicable under accelerated carbonation. In the literature, compressive strength results were given for 14, 28, 90 and 180 days. For model predictions, the 28-day strengths were employed to predict carbonation depths at 28, 90 and 180 days. The predicted carbonation depths were then compared with the measured depths recorded in the data.

It was indicated in Duran-Herrera et al. (2013) that ambient temperature at site of the experiment ranged from 27-45ºC, while annual RH was between 18-60%. In the absence of any further detailed records, average annual RH of 41% was assumed and used in the model prediction calculations.

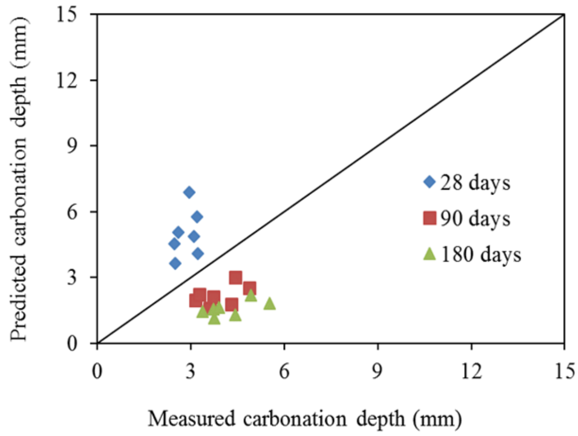

Fig. 1. Comparison of predicted carbonation depths with measured depths

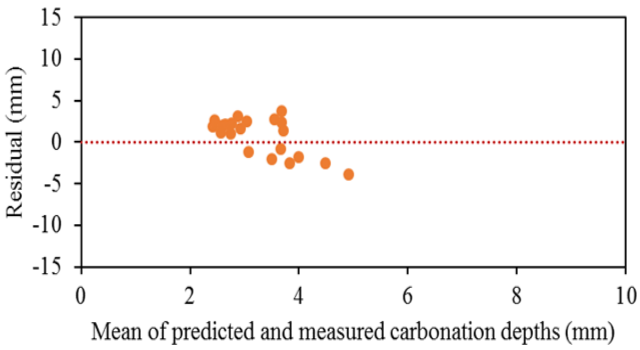

Fig. 2. Plot of residuals for model predictions

It can be seen in Fig.1 that there is a reasonably good correlation between the predicted carbonation depths and the measured depths. Calculations gave a root mean square (RMS) of error of 2.31, which is quite acceptable although the coefficient of variation (CV) of error determined to be 62.8% is fairly high, compared to the typical CV of about 40-50% (Ekolu, 2018). The high CV obtained is attributed to the wide scatter of data seen in Fig.1, which may be related to the assumptions made due to absence of detailed data of environmental factors. A RH of 41% was assumed for model predictions, whereas the actual value may have been different. Also, the CO_2 level at site of exposure reportedly varied from 200-900 mg/kg but no consistent mean values were given. Accordingly, no corrections were made for [CO_2] due to absence of detailed data records. By default, it was assumed that the average [CO_2] concentration was within the normal range of 300-400 mg/kg, in which case the correction factor was α = 1.0 (Eq. 4). The calculations are based on sheltered exposure.

A plot of residuals is shown in Fig. 2, which indicates fanning out as the carbonation depth increases. This behaviour was also reported in Ekolu (2018) and is associated with increase in variability for highly carbonating concretes, due to their relatively lower quality.

5.0 CONCLUSION

In the foregone study, a concept overview and theoretical considerations in the model development were described. Furthermore, the model was verified against natural carbonation measurements obtained from experimental work in the literature (Duran-Herrera et al. 2013), on concretes in which different types of chemical admixtures, were used. Although assumptions on the input parameters of relative humidity, sheltering, and [CO_2] had to be made, the model's veracity and robustness is demonstrated as it gave meaningful carbonation predictions, regardless of the chemical admixture types used in the concretes.

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