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Statistical modelling of carbonation coefficient in concrete

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Abstract. Current models for the carbonation coefficient in concrete cannot comprehensively consider the impact of water-to-binder ratio, replacement of mineral admixtures, and the coupling effect of each other. To overcome this limitation, an improved model for carbonation coefficient was developed based on 96 sets of concrete carbonation test data under standard carbonization environment. Compared with the reference models, the proposed model has a higher precision.

1. Introduction

Carbon dioxide in atmospheric environment is continuously transmitted to concrete through diffusion and dissolved in concrete pore solution. It reacts with alkaline substances in concrete, resulting in the decrease in alkalinity around steel bars, thus destroying the passive film on the surface of steel bars. The reinforcement's corrosion of concrete structures compromise the structural safety of the constructions.

From references [2-5], we can found that water-to-cement ratio is closely related to the carbonation coefficient in concrete. Former researches [6-8] presented the relationship between the replacement of fly ash and carbonation coefficient. Zhou et al. [9] found that replacement of GGBFS is closely related to the carbonation coefficient in concrete. Xu [10] studied the relationship between concrete mix design parameters and carbonation coefficient in concrete containing fly ash and GGBFS. The results showed the coupling effect between replacement of fly ash and replacement of GGBFS is obvious. However, current models of carbonation coefficient in concrete could not accurately estimate the CO_2 diffusion in concrete. A more effective model for carbonation coefficient in concrete containing mineral admixtures was developed. Meanwhile, the influences of concrete mix design parameters were investigated based on the concrete carbonation tested data under standard carbonization environment. Finally, the validity of the proposed model was demonstrated in comparison with current models and tested data.

2. Statistical modelling

2.1. Database

The rate of carbonation depends mainly on CO_2 concentration, the temperature of the environment, the relative humidity, reaction rate coefficient, $Ca(OH)_2$ concentration, and CO_2 diffusion coefficient. A large of studies have been carried out to investigate the influence of concrete carbonation. The correlation between carbonation coefficient and carbonation depth can be expressed as[11]:

$$k_0 = \frac{X}{\sqrt{t}} \tag{1}$$

where k_0 is carbonation coefficient (mm/day$^{0.5}$); X is the carbonation depth (mm); t is the exposure time (day).

A sample of 96 sets of concrete carbonation test data under standard carbonization environment was obtained from the literature [4-9,12-13, 15-20]. The water-to-binder ratios ranging from 0.30 to 0.72, replacement of fly ash ranging 0.10 to 0.40, replacement of GGBFS ranging from 0.10 to 0.80. All specimens were stored in a standard curing room until the age of 28 days.

2.2. Statistical model and selection of variables

By taking into account the coupling effect of materials and environment, the carbonation coefficient in concrete can be expressed as:

$$k=F\left(X_1, X_2, X_3,\cdots, X_n\right) \tag{2}$$

where X_1, X_2 …, X_n are material parameters (water-to-binder ratio, replacement of fly ash, replacement of GGBFS) and environment parameters (the temperature of the environment, the relative humidity, CO_2 concentration) respectively.
Based on the method of polynomial expansion, Eq. (2) can be transformed into:

$$k=\mathrm{a}_0 + \sum_{i=1}^{n} a_i X_i + \sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij} X_i X_j + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} c_{ijk} X_i X_j X_k \cdots \tag{3}$$

Selecting the first and second degree of the polynomial above, one gets

$$k_0=\mathrm{a}_0 + \sum_{i=1}^{3} a_i X_i + \sum_{i=1}^{3}\sum_{j=1}^{3} b_{ij} X_i X_j \tag{4}$$

Based on the stepwise regression method[14], the carbonation coefficient can be defined:

$$k_0 = \begin{cases} k_{11}X_1 + k_{12} & \text{OPC} \\ k_{21}X_1X_2 + k_{22}X_1 + k_{23}X_2 + k_{24} & \text{FA} \\ k_{31}X_1X_3 + k_{32}X_1 + k_{33}X_3 + k_{34} & \text{GGBFS} \\ k_{41}X_1X_2 + k_{42}X_1X_3 + k_{43}X_3 + k_{44} & \text{FA\&GGBFS} \end{cases} \tag{5}$$

where X_1 is water-to-binder ratio; X_2 is replacement of fly ash; X_3 is replacement of GGBFS; k_{11}, k_{12}… are fitting coefficients. To determine the fitting coefficient, 96 sets of concrete carbonation test data regarding the carbonation coefficient in concrete were collected from the literature [4-9,12-13, 15-20]. Based on the non-linear least squares method, the fitting coefficient were determined:

$$k_0 = \begin{cases} 18.39X_1 - 4.48 & \text{OPC} \\ -4.57X_1X_2 + 10.94X_1 + 6.72X_2 - 4.82 & \text{FA} \\ 3.72X_1X_3 + 11.89X_1 + 2.58X_3 - 6.08 & \text{GGBFS} \\ 11.30X_1X_2 - 7.60X_1X_3 + 3.37X_3 - 0.61 & \text{FA\&GGBFS} \end{cases} \tag{6}$$

3. Comparison and validation

To validate the accuracy and application of the proposed model, a reference model for carbonation coefficient in concrete was compared. Zhang and Jiang [21] provided a model for the carbonation:

$$X=839\cdot\left(1-RH\right)^{1.1}\cdot\sqrt{\frac{R_{\mathrm{W/C}}-0.34}{C}}\cdot c_{\mathrm{CO_2}}\cdot\sqrt{t} \tag{7}$$

where X is the carbonation depth (mm); t is the exposure time (day); $R_{W/C}$ is water-to-cement ratio, C is the amount of cement; *RH* is the relative humidity; c_{CO_2} is the CO_2 concentration in atmosphere.

As shown in Figure 1, the results of the proposed model distribute near the equality line, which indicates that the proposed model agree well with test data.

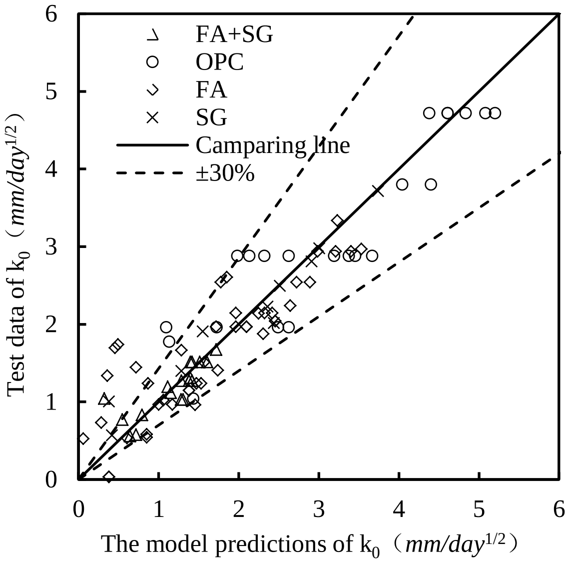

Figure 1. The prediction of the proposed model.

As shown in Figure 2, tested data regarding the concrete coefficient in concrete were collected to compare the accuracy and application between the proposed model and reference model. It is clear that the dispersal of the reference model is much larger than the proposed model. This is because the reference model does not take into account the replacement of fly ash, the replacement of GGBFS, and the coupling effect of each other. Finally, the accuracy and applicability of the multi-factor coupled model of concrete carbonation analysis were validated by 96 sets of concrete carbonation test data under standard carbonization environment.

Furthermore, the predicted values of the proposed model are much closer to the equality than the reference model, thus demonstrating the high accuracy of the proposed model. The residual mean square error which describes the deviation of one model from the tested data is defined as:

$$\delta_e = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(k_0^i - \hat{k}_0^i\right)^2} \tag{8}$$

Which k_0 and $\hat{k}_0^i$ are the *i*th set of the carbonation coefficient in concrete; *n* is the total number of concrete specimens. The residual mean error of the reference model and proposed model were obtained. As listed in Tab.1, the residual mean error of the proposed mode is quite smaller than the reference model, which demonstrates that the accuracy of the proposed model is much higher than the reference model.

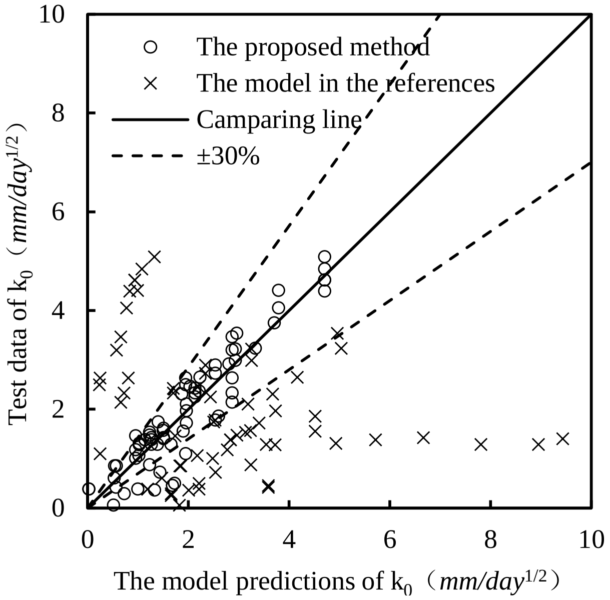

Figure 2. Comparison of the reference model and the proposed model.

Table 1. Comparison between the precision of reference model and the precision of proposed model.

Numble	The residual mean square error (δ_e)		(R^2)	
	Reference [21] model	Proposed model	Reference [21] model	Proposed model
OPC	1.322	0.223	0.825	0.909
Mineral admixtures	7.192	0.372	0.379	0.888

4. Conclusion

This work suggests one model to predict carbonation coefficient in concrete, which takes into account the influence of water-to-binder ratio, replacement of fly ash and replacement of GGBFS. The following conclusions can be drawn:

1. The carbonation coefficient in concrete is influenced by both water-to-binder ratio and replacement of mineral admixtures.
2. Compared with the reference models, the proposed model has a higher precision.

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