



Review on Analytical prediction of carbonation depth in Machine Learning methods

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Abstract

This study explores the review of machine learning techniques for predicting the carbonation depth of concrete. The carbonation depth is a critical parameter in determining the durability of concrete structures, and accurate prediction is essential for effective maintenance and repair. In this research, various machine learning algorithms, including artificial neural networks, decision trees, and support vector machines, were trained on a dataset of concrete samples with known carbonation depths. The models were evaluated for their accuracy and generalization performance using cross-validation techniques. The results show that machine learning models can effectively predict carbonation depth with high accuracy, and the best-performing model was able to achieve. This approach offers a promising alternative to traditional experimental methods for predicting carbonation depth and can significantly improve the efficiency and cost-effectiveness of concrete maintenance and repair.

Keywords: Carbonation, Carbonation depth prediction using analytical methods.

1 Introduction

1.1 Background

Concrete is the most prominently used construction material that moulds into any desired shape. Though the commencement of the steel as a building material and the addition of mineral admixtures into concrete business has brought about many changes in construction techniques, the use of cement as a basic binder material has not dwindled, mainly because of its excellent water resisting property.

Concrete is a composite material that consists essentially of a binding medium within which are embedded particles or fragments of aggregate (ASTM C125) [1]. The binding material being cement, hardened concrete too is impervious to water provided the concrete has less porosity. The embedded particles that are commonly used are coarse and fine aggregates. The voids of coarse aggregates are filled by fine aggregates.

The fire remains one of the serious potential risks to most of the buildings and structures and for reducing this cause few methods are also done[23]. Addition of the admixtures to concrete the strength and durability of the concrete increases with various mix proportions are been done[24,25]. Replacement of the cement in the concrete also changes the strength parameters[26,27].

Cement is a finely grounded material that by itself does not possess any binding property, but on reaction with water (hydration) develops strength. Portland cement is most widely used hydraulic cement, produced by pulverizing clinkers consisting essentially of hydraulic calcium silicates, and a small amount of one or more forms of calcium sulphate as an inter-ground addition (ASTM C150)[2]. The construction business in India consumes 400 million tons of concrete per year and will soon reach a billion-ton mark in less than 10 years



(Gowda et al. (2011)). . Addition of the alccofine in the concrete gain strength was been observed in the concrete[28].

Concrete despite its high strength and ability to resist the transport of water is susceptible to chemical attacks and deterioration. The ability of concrete to withstand the chemical attacks, weathering action, abrasion, or any sort of deterioration during its service life under a given set of conditions is called durability. The strength and durability of concrete depend on the properties of its ingredients, proportions of design mix, exposure conditions, and curing type and duration. The durability of concrete is influenced by both physical reasons and chemical reasons. The physical reasons for concrete deterioration can be broadly classified into surface wear and cracks. The surface wear is due to abrasion, erosion, and cavitation while the cracking is due to change in volume, structural loading, and exposure conditions (Mehta & Gerwick, 1982) [3]. Sesimic behaviour of the concrete can be observed in the concrete and also if need addition of the several material can be done to increase its strength and durability[29].

The chemical causes for deterioration of concrete generally, but not necessarily involve, chemical reactions between the aggressive agents in the environment and the ingredients of the cement paste. One of the reactions that influence the durability of concrete structures predominantly is corrosion of steel reinforcement in the concrete, which is mainly caused either because of chloride attack or the carbonation of concrete. Also, the porosity and interconnected permeable pores in concrete have a strong influence on its mechanical strength and durability (Kumar & Bhattacharjee (2003)) [4]. Experimental analysis was performed on the concrete to observe its strength and durability[30].

Carbonation of concrete is the reaction of calcium (Ca^{2+}) ions present in cement and carbonate (CO_3^{2-}) ions from the dissolved carbon dioxide (CO_2) to precipitate calcium carbonate (CaCO_3). Concrete possesses certain porosity when design mix proportion standards are not met. Also, upon prolonged exposure to the atmospheric fluids, the surface of concrete gets deteriorated and sometimes through its interconnected capillary pores, the deterioration progresses. Addition of the geopolymers with the admixture it was observed the rapid strength and durability in the concrete[31].

Carbonation of concrete is one such phenomenon where the surface of concrete gets exposed to the atmospheric carbon dioxide (0.03-0.04%) for a prolonged duration and changes the physicochemical properties of the cement hydration products. The carbon dioxide diffuses across the surface due to the difference in concentration between 3 atmosphere and concrete pore structure. A thin layer of carbonated concrete is formed initially, and the further diffusion of carbon dioxide depends on the permeability of the concrete (Mark, 2003) . And rapidly stiffness was observed check its durability and strength[32].

Carbonation is a process where dissolved carbon dioxide from the atmosphere reacts with calcium ions in cement and form calcium carbonate. The solubility of calcium carbonate is less compared to calcium hydroxide, which eventually leads to the dissolution of all calcium compounds to calcium carbonate. The end products apart from calcite are silica gels and metal hydrates. Because carbon dioxide is abundantly found in the atmosphere and the cement used in construction purposes contains calcium hydroxides, the question is not whether the process of carbonation takes place, which is evident, but how long will this process take to initiate corrosion (Lagerblad, 2005) [5]. Prior to carbonation, the reinforcement in concrete is embedded in oxygenated alkaline solution. This deposits a thin layer of insoluble oxide film preventing oxygen from reacting with steel, which inhibits corrosion.

Due to the lowering of pH value during carbonation, the passive oxide layer gets destroyed and concrete acts as an electrolyte for oxygen and moisture to penetrate. This results in corrosion of reinforcement in reinforced concrete. This situation within the concrete has created a problem for the usage of steel as reinforcing medium. There is no dearth of cases where the corrosion of reinforcement has occurred even before the carbonation has reached the reinforcement as detected by phenolphthalein indicator (Yongsheng et al. 2010) [6].



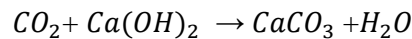
This poses a question if the phenolphthalein indicator is an accurate measure of carbonation depth. Also, though well addressed, the effect of mineral admixtures with various pore sizes on carbonation resistance is seldom studied.

1.2 Chemistry of carbonation

The process of carbonation is a surface phenomenon and hence the amount of carbonation depends on the exposure duration and the porosity of the concrete. If the surface of the concrete is porous enough, the atmospheric carbon dioxide diffuses through the pores of surface concrete and dissolves in the pore solution of concrete to form carbonate ions due to the difference in concentration between the atmosphere and concrete pore structure.

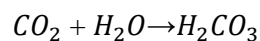
The gaseous carbon dioxide cannot react with the calcium phases of the cement. Based on the pH of the solution in which the carbon dioxide is dissolved, the carbonate ions are formed. When in contact with water at pH 7, bicarbonate ions are formed, but as the pH in the cement pore solution is high, the bicarbonates further disassociate to form carbonate ions.

Carbonation occurs when CO_2 , as natural gas in the air, penetrates the surface of concrete through the dry portions of interconnected pores in concrete microstructures, and reacts with $Ca(OH)_2$ in the moist portions of pores to form $CaCO_3$ and water (H_2O).

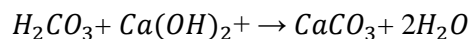


When $Ca(OH)_2$ from the paste is consumed, the hydration of calcium-silicate-hydrate (C-S-H) releases calcium oxide (CaO), which reacts with diffused CO_2 . The remaining CO_2 continues to react with C-S-H to form additional $CaCO_3$. The carbonation process requires water because CO_2 dissolves in water to form carbonic acid H_2CO_3 .

The water seeps in through small, interconnected pores, while CO_2 settles in large pores. The interconnected pores merge into large pores to supply the water required to form carbonic acid:



A chemical reaction occurs with H_2CO_3 , which is formed in the pores of the concrete, producing a desirable product of cement hydration $Ca(OH)_2$, which strengthens the concrete matrix. This reaction also produces $CaCO_3$ and water:



This process involves consumption of Ca^{2+} ions, which leads to the dissolution of predominantly available calcium hydroxide ($Ca(OH)_2$) forming new Ca^{2+} ions. Because the solubility coefficient of dissolution of $Ca(OH)_2$ is 9.95×10^{-4} mol/L and solubility coefficient of formation of $CaCO_3$ is 0.99×10^{-8} mol/L, this process continues till all the calcium ions are consumed to form $CaCO_3$ (Lager lad, 2005).

2. Overview of Machine learning methods proposed

2.1 Woubishet ZewduTaffese, EskoSistonen and Jari Puttonen 2015 (DECISION TREES)

Three concrete carbonation depth prediction models based on decision tree method are presented. To



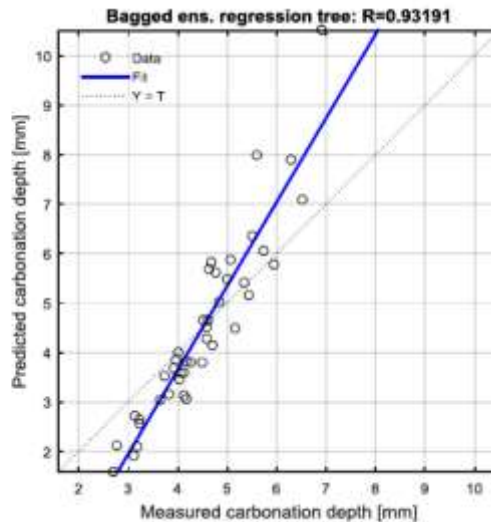
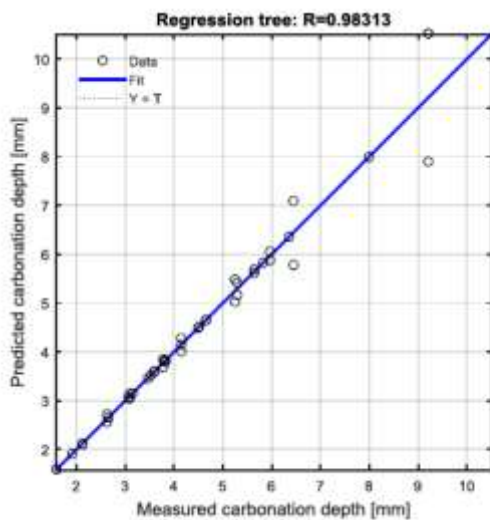
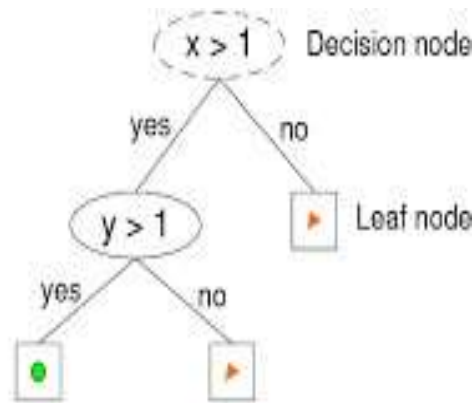
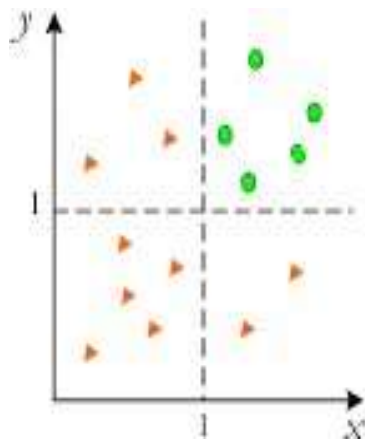
develop the models, three different decision trees were adopted. They are regression tree, bagged ensemble regression tree and reduced bagged ensemble regression tree. The model's prediction capacity was examined based on mean square errors and mean absolute error.

2.1.1 Regression tree

The structure of the regression tree is the same as that of the tree presented in Figure 1. The only difference is the leaves which contain real numbers instead of class labels. The regression tree is trained over the training dataset. The performance of the developed tree is measured by mean square error (MSE) and mean absolute error (MAE) on both training and testing dataset. MSE, the mean square error between predicted output (\hat{Y}_i) and target (Y_i), is the most common measure of accuracy, Eq. . The MAE of Eq. is the more intuitive measure and is less sensitive to outliers.

$$MSE = \frac{1}{N} \sum_{i=1}^N (Y_i - \hat{Y}_i)^2$$
$$MAE = \frac{1}{N} \sum_{i=1}^N |Y_i - \hat{Y}_i|$$

where \hat{Y}_i is the predicted output value, Y_i is the measured target value, and N is the number of observations. The resulting MSE values for training and test dataset were 0.0416 and 4.3108, respectively. Significant difference in MAE of training and testing dataset is also observed. All these show that the developed regression tree generalized the test data poorly because it overfitted the training data as seen in the regression plot.

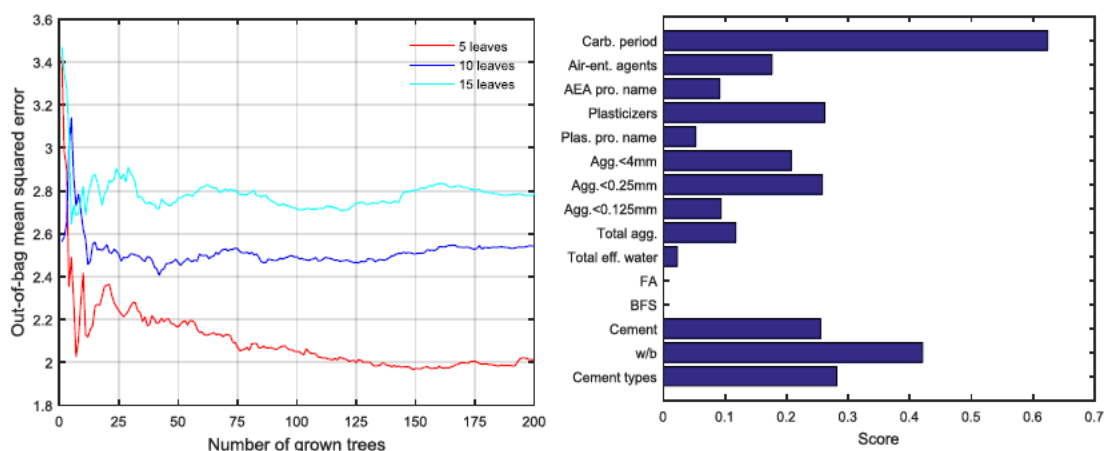


Regression plot of predicted vs measured carbonation depth on training dataset for regression tree (left) and bagged ensemble regression tree (right).

2.1.2 Bagged ensemble regression tree

Bagging is one of the most effective methods that can be used to improve the predictive performance of a tree model by reducing the variance associated with prediction. This technique draws multiple bootstrap samples from the training dataset and generates multiple predictor trees, and then, the results are combined by averaging to obtain the overall prediction [21, 22].

After determining good predictors and an ensemble size from the out-of-bag error, a new bagged ensemble regression tree was constructed to enhance its performance further. In this case, the optimal number of leaf and trees was chosen as 5 and 150, respectively. Two parameters, BFS and FA, were reduced out of the total 15 features since they are unimportant to predict the carbonation depth in this dataset. The MSE of training and testing dataset of this model was 0.9536 and 2.2990. Figure illustrate the predicted and the measured carbonation depth with the predicted error.



Out-of-bag mean square error vs number of grown trees (left). 3b: Relative importance of the input variables of the bagged ensemble regression tree (right).

2.1.3 Reduced bagged ensemble regression tree

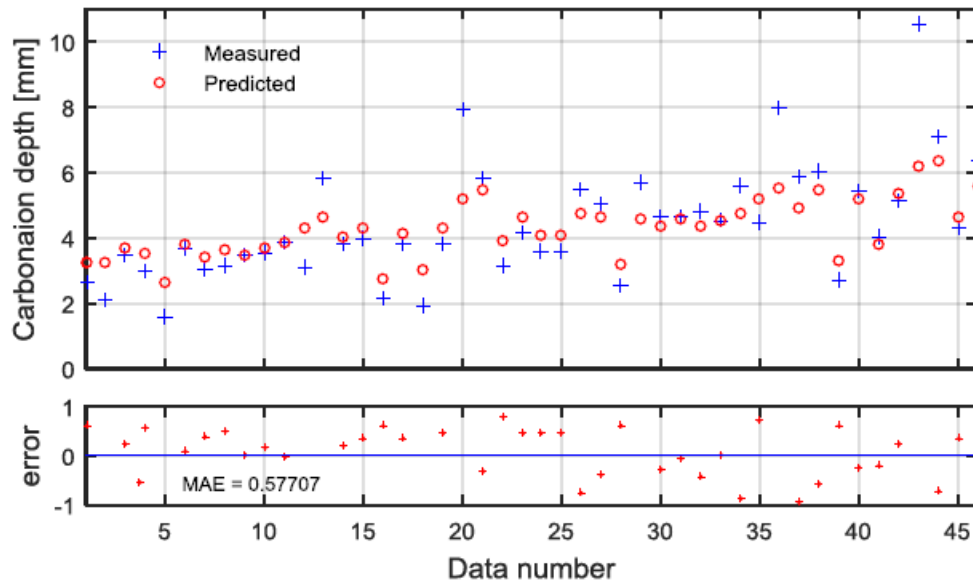
In order to minimize the prediction error of the bagged ensemble, we compute predictions for trees with different leaf sizes on its out-of-bag observations, Figure .

It can be observed that the out-of-bag error decreases well with the number of grown trees for leaf size of five. The relative importance of the input variables of the bagged ensemble regression tree is illustrated in Figure . It can be clearly seen that the carbonation period and w/b are the foremost influential predictors for this dataset.

Next to these variables, amount and types of cement, plasticizer and the distribution of aggregate play considerable role in predicting the carbonation depth for this dataset. This is a useful finding because plasticizer and aggregate distribution were overlooked in several existing analytical models.

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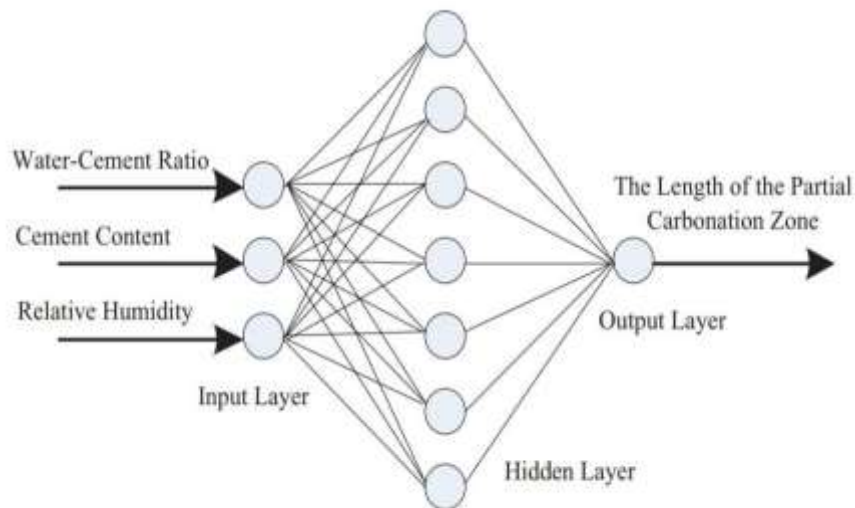
Measured and predicted carbonation depth using bagged ensemble regression tree with the prediction error

Models	MSE		MAE	
	Train	Test	Train	Test
Regression tree	0.0416	4.3108	0.0740	1.3437
Bagged ensemble regression tree	0.9701	2.7223	0.4927	0.6283
Reduced bagged ensemble regression tree	0.9536	2.2990	0.4755	0.5261

Performance comparison of carbonation depth prediction models.

2.2 Daming Luo, DitaoNiu, and Zhenping Dong, 2014 (Neutral network based algorithm)

1. Since the particle swarm algorithm is an optimization process under the guidance of individual learning and social information-sharing principles, and the BP algorithm completes its optimization process in accordance with the specified anti-gradient descent trajectory, the routes of the two processes do not coincide.
2. The optimizing of PSO algorithm on BP neural network can greatly shorten the training time and improve the prediction accuracy. The factors affecting concrete carbonation depth are complex and with interactions among them. This article only focus on the nonlinear relationship among the cement content, water–cement ratio, relative humidity, and the length of the partial carbonation zone with $9 < \text{pH} < 11.5$.
3. Further research work can be performed to get a more comprehensive analysis of various factors and improve prediction accuracy. The accumulation of field-measured value and laboratory results is very important to the artificial neural networks for the establishing of concrete carbonation depth prediction model.
4. Due to the fact that the sample data is limited, the type of concrete, the strength of concrete, the thickness of concrete cover, and other factors are not considered in this article. It is necessary for additional work to be undertaken for a further in-depth study.



2.3 Hyungmin Lee a, Han-Seung Lee , Prannoy Suraneni

1. Carbonation of concrete, which can accelerate corrosion, is one of the major deterioration mechanisms in reinforced concrete structures. Experimental data has been used to develop carbonation prediction models, however, the service life predicted from various models can differ significantly. A potential solution is the application of an artificial neural network algorithm.
2. Machine learning can be divided into three categories: supervised learning, unsupervised learning, and reinforcement learning.
3. Deep learning is used, which is a supervised learning technique that uses various training data to inform the results. In general, supervised learning is used for regression analysis and classification, and unsupervised learning is used to find patterns in data.
4. The input layer passes the given input data to nodes in the next hidden layer. Each node multiplies the value of the input data by the weight of the corresponding node through an activation function and transmits the result to the next layer.

2.3.1 Machine learning

A short introduction to machine learning and its various approaches is presented in this subsection and the next; readers who are familiar with such concepts may skip these sub-sections. Machine learning can be divided into three categories: supervised learning, unsupervised learning, and reinforcement learning [7,8]. In this study, deep learning is used, which is a supervised learning technique that uses various training data to inform the results. In general, supervised learning is used for regression analysis and classification, and unsupervised learning is used to find patterns in data. Reinforcement learning is used to train robots that improve their behavior according to their relationships with the environment. Typical algorithms that have been studied include K-Nearest Neighbours [9], Decision Tree, Support Vector Machine (SVM) [10],



Naive Bayes and Neural Networks [11–13]. In general, the performance of machine learning increases as the number of input variables increases. Deep learning is defined as a machine learning algorithm that generalizes a high-level predictive model through a combination of several nonlinear analysis techniques. It utilizes deep neural networks (DNNs) [14], which are algorithms that mimic the way the human brain perceives patterns. DNNs consist of input layer, hidden layer, and output layer. The input layer passes the given input data to nodes in the next hidden layer. Each node multiplies the value of the input data by the weight of the corresponding node through an activation function and transmits the result to the next layer. After analyzing the errors on the test and validation data at the nodes in the output layer, reverse learning is performed to minimize them. This single process is defined as one Epoch. The main technical difference between deep learning and machine learning is the self-identification of variables and the adjustment of weights. Fig. shows a schematic diagram of the deep neural network.

2.3.2 Gradient descent method:

Gradient descent method is the most general method to minimize the error function of the input and output values. A gradient that represents the differential value of the error function with respect to the weight vector x is calculated, and the algorithm proceeds to converge to the minimum value. The parameter E is the cost function for the learning weight vector. If the input value of the output layer j is x_j through the neuron of the hidden layer the predicted output value \hat{y}_j is expressed by Eqs, where σ represents the activation function.

$$E = \frac{1}{2} \times \sum_{j=1}^m (y_j - \hat{y}_j)^2$$
$$\hat{y}_j = \sigma \times \left(\sum_i w_{ij} \times x_i \right)$$

$$w(t + 1) = w(t) + \Delta w(t)$$

The expression of the gradient descent method is shown in Eq. The aim of the gradient descent method is to obtain $\Delta w(t)$ in Eq. (6), which is an algorithm that is corrected to $\Delta w(t)$ at any starting point on the plane and is directed to the minimum point. The weighting vector $\Delta w(t)$ requires components of direction and magnitude. The direction is expressed by $\frac{\partial E}{\partial w}$, since it is a gradient of the error function. The magnitude refers to the distance from the current step (t) to the next step ($t+1$). The amount that the weights are updated during training is referred to as the step size or the learning rate α . The learning rate is a configurable parameter used in the training of neural networks that has a small positive value, often in the range between 0.0 and 1.0. If the learning rate is low, a number of iterations must be repeated until the algorithm converges, and if the local minimum occurs within a certain number of repetitions, then learning may be stopped by recognizing the local minimum as a global minimum. By contrast, if the learning rate is high, it is possible to quickly approach the minimum value, but there is a possibility that the global minimum value cannot be found by diverging around the minimum value. Therefore, effective learning rate adjustment is needed. In this study, the optimal learning rate is derived to minimize the error between the input and output values. Eq. can be expressed as a function of



$\Delta w(t)$ using the learning rate. Eq. (4) can be substituted into Eq and then Eq can be expressed using the chain rule.

$$\begin{aligned}\Delta w(t) &= -\alpha \frac{\partial E}{\partial w} \\ \Delta w_{ij}(t) &= -\alpha \frac{\partial \frac{1}{2} \times \sum_{j=1}^m (y_j - \hat{y}_j)^2}{\partial w_{ij}} \\ &= \alpha \times \sum_{j=1}^m (y_j - \hat{y}_j) \frac{\partial \hat{y}_j}{\partial w_{ij}} \\ w(t+1) &= w(t) + \alpha \times \sum_{j=1}^m (y_j - \hat{y}_j) \times \sigma' \left(\sum_i w_{ij} \times x_i \right) \times x_i\end{aligned}$$

2.3.3 AIJ model :

In order to compare the accelerated carbonation experiment results with the existing carbonation prediction model, the results from the Architectural Institute Japanese model [15], were obtained. While this model is commonly used for buildings, work has shown that it can also be used for acceleration carbonation experiments [16,17]. Table 1 shows the parameters for the AIJ model

Eqs. and show the AIJ carbonation prediction model.

$$\begin{aligned}C &= A\sqrt{t} \\ A &= k \times \alpha_1 \times \alpha_2 \times \alpha_3 \times \beta_1 \times \beta_2 \times \beta_3\end{aligned}$$

where C is carbonation depth (mm), t is time (year), α_1 is the coefficient for concrete type, α_2 is the coefficient for cement type, α_3 is the w/c coefficient, β_1 is temperature, β_2 is humidity, β_3 is CO₂ concentration, and K is the coefficient of the Kishitani model.

2.3.4 FEM analysis

FEM analysis was carried out to predict the carbonation through the LECCA2 program, a durability prediction program from the Japan Concrete Institute. The concrete input parameters for FEM analysis are shown in Table. FEM analysis was performed on the input variables using Eqs. [18,19]. The determination of the carbonation depth in the FEM analysis was based on the assumption of carbonation when the concentration of Ca(OH)₂ was reduced to 50% of the initial value [20].

$$\begin{aligned}C_{s0} &= p \times S \\ P &= D_{CO_2} \times S\end{aligned}$$

where Cs0 is concentration of CO₂ on concrete surface (%), p is CO₂ pressure on concrete surface (Pa), Dco2 is diffusion coefficient of CO₂ (m²/s).

Input variables for applying the FEM analysis.



Parameter	Input Value
Concentration of CO ₂ (%)	5,20
Thickness of concrete specimen (cm)	20
Diffusion coefficient of CO ₂ in concrete (cm ² /day)	5.00×10^{-7}
Rate constant (k) of reaction between CO ₂ and Ca(OH) ₂ (1/day)	500,000
Ca(OH) ₂ concentration on specimen surface (mol/cm ³)	3.00×10^{-6}
Ca(OH) ₂ loss (%)	50

P is air permeability (cm³ (STP) X cm/(cm² X sec X cmHg)), S is solubility coefficient of CO₂ (mol/m³ X Pa). Obviously, some variation can be expected in these input variables as a function of w/c, which can somewhat affect the results, and such variation can be simulated in the FEM analysis, if desired. As an example, different Ca(OH)₂ concentration values can be used, depending on the w/c, though these are not expected to significantly change for w/c 0.55 and 0.65.

Conclusion

1. The bagged ensemble regression tree identified important variables that influenced the carbonation rate which was not considered in the existing analytical models. The models have potential to be part of a service life management system.
2. The model developed using the former method has superior performance with relatively better generalization capability.
3. Models developed using bagged ensemble with and without features extraction predict the carbonation depth with reasonably low error.
4. Carbonation depth values of FEM and AJJ model are similar to the expected experimental program.
5. If the addition of the fly ash is done then the carbonation depth of the concrete increases.
6. Errors in FEM analysis and AJJ model are significantly higher at CO₂ concentration 20% and w/c 0.65 not in case of machine learning.

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