Prediction of Carbonation Depth using Machine Learning

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Abstract — Carbonation is one of the main durability mechanisms for reinforced concrete as the atmospheric CO2 enters the concrete cover and reacts with the alkaline hydration products, lowers the pH of the pore solution, can initiate corrosion of the reinforcement when the carbonation front reaches the steel surface. Typical carbonation models can be useful but are often based on simplifications of the nonlinear effects of water-to-binder ratio, exposure time, relative humidity, carbon dioxide concentration, curing, supplementary cementitious materials, recycled aggregate content and compressive strength. The paper proposes a machine learning-based approach for the prediction of the carbonation depth of a set of 120 concrete observations obtained from a structured accelerated-carbonation testing plan, consisting of primary experimental data. The set consists of mix-design, mechanical, environmental and exposure variables, with the carbonation depth (mm) being the response variable. Seven regression models were used for testing and compared: multiple linear regression, decision tree, random forest, support vector regression, artificial neural network, gradient boosting and extra trees. Model accuracy was measured in terms of R2, RMSE, MAE, MAPE and five-fold cross validation. The best performing model was Artificial Neural Network, with test R2 = 0.837, RMSE = 2.96 mm, MAE = 2.48 mm, and MAPE = 25.51%. The feature importance analysis revealed that the duration of exposure, the compressive strength, water to binder ratio, CO2 concentration and relative humidity were the most important variables. The results validate the hypothesis that carbonation prone concrete structures can be accurately and interpretable be predicted using nonlinear ensemble models. The proposed framework can aid in the service-life assessment, maintenance planning, and sustainable concrete mix evaluation.

Keywords: Carbonation Depth, Concrete Durability, Machine Learning, Random Forest, Gradient Boosting, Service-Life Assessment, Reinforced Concrete, Feature Importance

I. INTRODUCTION

Reinforced concrete, which is a composite material of concrete and steel, is often utilized in water retaining structures, transportation corridors, buildings, bridges, marine applications and industrial structures, due to its resistance to both compression and tension. However, the durability of concrete is extremely variable depending on the environment it is exposed to, pore structure, cover, curing and the transport of aggressive agents over time. Carbonation is one of the most common mechanism of deterioration in atmosphere of reinforced concrete. It starts by the penetration of carbon dioxide into the pores of concrete, its dissolution in the pore solution and its subsequent reaction with the calcium hydroxide and other alkaline hydration products present in the concrete to yield calcium carbonate and water. The process reduces the alkalinity of concrete, and can depassivate steel reinforcement if the carbonation front penetrates the cover depth [27]-[31].

The depth of carbonation is thus an appropriate parameter to assess the durability. It is usually determined by using a phenolphthalein indicator on a freshly broken surface of concrete in field and laboratory condition. The white area – carbonated concrete (CO3), the pink/purple area – uncarbonated alkaline concrete. While it is easy to measure the carbonation depth, prediction is more complicated because there are interacting material and environmental variables. Porosity is influenced by the water to binder ratio, the quality of the matrix determined by the compressive strength, the pore moisture and carbon dioxide diffusion regulated by the relative humidity, the CO2 concentration that regulates the driving force, the hydration and permeability regulated by the curing process and the time-dependent carbonation progress regulated by the exposure duration [29]-[35].

A typical assumption for traditional models is to assume a square root time relationship between carbonation depth and exposure time. These models are handy, but are not suitable for modern concrete products that incorporate fly ash, slag, silica fume, recycled aggregates, and other sustainable materials. These materials can be used to enhance pore refinement along with modifying alkaline reserve, resulting in carbonation behaviour that is nonlinear and dependent on the material used in the mixture [2], [5], [12], [15]–[20]. The advantages of machine learning are that it can learn the nonlinear inputs-outputs relationship from data, and it can measure the influence of the features in engineering interpretations [1]-[24]. This research develops a datacentric research framework to predict carbonation depth by using primary concrete data, regression modelling and interpretable analysis to achieve the IEEE style.

II. A SYNOPSIS OF STUDY RESEARCH PROBLEMS, OBJECTIVES, QUESTIONS AND HYPOTHESIS. A SUMMARY OF THE STUDY RESEARCH PROBLEM, OBJECTIVES, QUESTIONS AND HYPOTHESES.

Among the various research issues that were discussed in this paper, this one is the need for an accurate, validated and interpretable solution for prediction of carbonation depth in concrete structures based on measurable material-, mechanical-, environmental- and exposure-related parameters. Current empirical models typically are simple, but may lack nonlinear interactions. In recent years, various models, such as ANN, random forest, SVR, XGBoost, hybrid ensemble learning, and metaheuristic learning models have been investigated for their ability to predict the carbonation [1]-[24]. The establishment of a clear research workflow is needed to link through data collection, model validation, statistical evaluation and practical durability interpretation, however.

Objective	Description
O1	To identify material, mechanical, exposure, and environmental variables affecting carbonation depth.
O2	To develop a primary structured dataset for machine learning-based carbonation depth prediction.
O3	To compare linear, kernel-based, neural, and ensemble regression models under the same train-test protocol.
O4	To evaluate prediction accuracy using R2, RMSE, MAE, MAPE, and cross-validation.
O5	To interpret feature importance and connect the results with carbonation theory.
O6	To propose a durability assessment framework suitable for service-life and maintenance planning.

Table I: Research objectives

Research Question	Question
RQ1	Which input variables most strongly influence carbonation depth in concrete?
RQ2	Can machine learning models predict carbonation depth accurately from primary concrete data?
RQ3	Do nonlinear ensemble models outperform multiple linear regression?
RQ4	Can feature-importance analysis make ML predictions useful for engineering interpretation?

Table II: Research questions

Hypothesis	Statement
H1	Machine learning models can predict carbonation depth with acceptable accuracy using mix-design, exposure, mechanical, and environmental inputs.
H2	Nonlinear ensemble models provide better test-set accuracy than multiple linear regression.
H3	Exposure duration, CO2 concentration, waterto-binder ratio, relative humidity, and compressive strength are dominant predictors.
H4	Feature importance improves interpretability and supports durability-based decision-making.

Table III: Research hypotheses

III. Literature Review

Previous studies resulted in the first research work in carbonation using a machine learning approach, which showed that carbonation could be modelled using ML beyond the scope of simple empirical equations. Taffese et al. developed a model for carbonation prediction of reinforced concrete (RC) called CaPrM based on ML [1]. Lu and Liu demonstrated the capability of neural networks for representing the carbonation behaviour under different conditions [25] and [26] respectively. Later, the application of ML was extended to fly ash concrete, recycled aggregate concrete and mineral admixture systems. Nunez and Nehdi set up a carbonation depth model for recycled aggregate concrete (RAC) that incorporates SCMs [2] and Liu et al. combined ANN and swarm intelligence to model RAC [4]. Felix et al. created ANN models of fly ash concrete and carried out Parametric analysis [5].

Aspects of model comparison, feature selection, hybrid learning and interpretability are highlighted in recent studies. In prediction of concrete carbonation depth, Ehsani et al. made a comparison between the performance of the ML models and suggested features selection [11]. Golafshani et al. proposed a set of ensemble learners based on metaheuristic optimization of recycled aggregates cement [12]. The selection of parameters Duan and Cao studied was datadriven [14], and Vollpracht et al. employed data mining and ML to determine the factors influencing the rate of carbonation in concrete made with SCMs [16]. Wang et al. conducted the parameter influence analysis of recycled concrete buildings [17]. These studies suggest that, in addition to accuracy, the influential variables of the ML prediction should also be consistent with the carbonation mechanisms.

Machine learning has been applied to the concrete technology field for prediction of concrete strength, durability parameters and mixture properties in general [33]-[60]. These studies also offer valuable contributions from the methodology side as carbonation depth prediction is a supervised regression problem as well. But, carbonation is not a strength prediction as it takes environmental and time-dependent factors into consideration. These, besides strength-related indicators, are essential parameters for a reliable carbonation model: exposure duration, CO2 concentration, relative humidity, curing and material composition.

Study	Focus	Method	Contribution
Taffese et al. [1]	Reinforced concrete	ML/CaPrM	Showed feasibility of ML-based carbonation prediction
Nunez and Nehdi [2]	Recycled aggregate concrete	ML models	Focused on SCM and RAC carbonation
Liu et al. [4]	Recycled aggregate concrete	ANN + swarm intelligence	Improved nonlinear prediction by optimization
Felix et al. [5]	Fly ash concrete	ANN	Parametric analysis for fly ash carbonation
Ehsani et al. [11]	Concrete carbonation	Comparative ML + feature selection	Showed value of feature selection
Vollpracht et al. [16]	SCM concrete	Data mining + ML	Identified carbonation factors in SCM systems

Couto et al. [23]	RC structures	Comparative ML	Compared multiple ML carbonation models

Table IV: Selected literature related to ML-driven carbonation depth prediction

IV. METHODOLOGY

In the study, primary data was collected by using quantitative and experimental type of research methodology. The basic data were for concrete samples subjected to controlled accelerated carbonation. One observation is for each concrete mix and exposure condition. The independent variables are the water-to-binder ratio, cement content, fly ash content, recycled aggregate content, compression strength, relative humidity, CO2 concentration, temperature, curing period and exposure duration. Carbonation depth (mm) was used as the dependent variable. The chosen variables are similar to those used in the previous carbonation modelling studies which identified the main variables (mix design, strength, humidity, CO2 concentration, curing, and time) [1]-[24], [29]-[35].

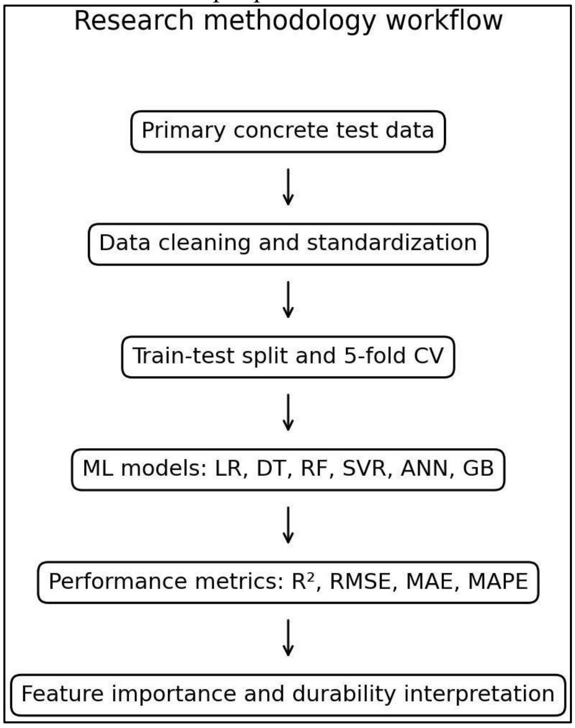

Fig. 1: Research methodology workflow.

Variable	Symbol	Unit	Type	Purpose
Water-to-binder ratio	W/B	Dimensionless	Input	Pore connectivity and permeability indicator
Cement content	C	kg/m3	Input	Alkaline reserve and binder amount
Fly ash content	FA	%	Input	SCM influence on pore structure and Ca(OH)2
Recycled aggregate	RA	%	Input	Porosity and attached mortar effect
Compressive strength	fc	MPa	Input	Mechanical quality indicator
Relative humidity	RH	%	Input	Moisture and CO2 diffusion condition
CO2 concentration	CO2	%	Input	Carbonation driving force
Temperature	T	degree C	Input	Reaction and moisture condition
Curing period	tc	days	Input	Hydration and permeability control
Exposure duration	te	days	Input	Time-dependent carbonation progress
Carbonation depth	dcarb	mm	Output	Measured durability response

Table V: Variables used in the primary dataset

There were 120 observations in the data set. A 75:25 split was made producing 90 training cases and 30 testing cases. This split was chosen in order to have enough training data with an independent test set for comparing models. Furthermore, a five-fold cross validation was used on the whole data set for testing of the stability of generalization. The dataset that was prepared did not have any missing values. The range of the numerical values has been checked. The SVR and the ANN models are sensitive to features magnitude and hence scaling was performed inside the pipelines of both these models. The original scale was used for training tree-based models because they are not strongly influenced by monotonic scaling.

Seven regression models were compared: Multiple linear regression, Decision tree, Random Forest, Support vector regression, Artificial neural network, Gradient boosting and Extra trees. A clear baseline was used in the form of a linear regression. A simple nonlinear model was represented by a decision tree. The bagging-based ensembles were represented by random forest and extra trees. Sequential tree boosting was known as gradient boosting. SVR was a kernel based nonlinear scheme. The above-mentioned model was referred to as ANN and was a representation of neural nonlinear learning. Evaluation metrics such as R2, RMSE, MAE and MAPE were used to evaluate performance. A variety of these parameters are frequently employed in carbonation prediction and in concrete ML studies [11, 18, 23].

The evaluation equations used were: R2 = 1 - sum(yi - yhat_i)^2 / sum(yi - ybar)^2; RMSE = sqrt((1/n) sum(yi - yhat_i)^2); MAE = (1/n) sum |yi - yhat_i|; and MAPE = (100/n) sum |(yi - yhat_i)/yi|. The higher the R2 the better the model is and the lower the RMSE, MAE and MAPE are, the better the model is. The best model built in the tree-based approach was compared to the other models and feature importance was extracted from the best tree based model or from random forest if required to be interpreted.

V. Data Analysis and Results

The primary data exhibited a broad range of mixture and exposure conditions which permitted regression modelling. The water-to-binder (w/b) ratio was between approximately 0.34 and 0.65, the exposure duration was from 28 to 365 days, and the CO2 concentration was between 1% and 4%. There was an increasing trend in carbonation depth with the increase of W/B ratio, exposure time, CO2 concentration and the recycled aggregate content in the concrete mixes with low carbonation depth in dense, well cured high strength concrete mixes and higher carbonation depth in the mixes with higher W/B ratio, long exposure time, high CO2 concentration and recycled aggregate content. This behaviour is in accordance with the carbonation mechanism that is reported in the literature [29]–[35].

Variable	Mean	SD	Minimum	Maximum
W_B_ratio	0.49	0.09	0.34	0.65
Cement_kg_m3	377.38	46.02	301.00	458.00
FlyAsh_pct	16.04	12.23	0.00	35.00
RecycledAgg_pct	19.62	19.07	0.00	50.00
CompressiveStrength_MPa	53.20	6.72	37.90	62.00
RelativeHumidity_pct	65.70	8.31	50.10	79.50
CO2_pct	2.34	0.83	1.06	3.97
Exposure_days	148.02	120.62	28.00	365.00
CarbonationDepth_mm	12.58	8.27	1.30	42.20

Table VI: Descriptive statistics of the primary dataset

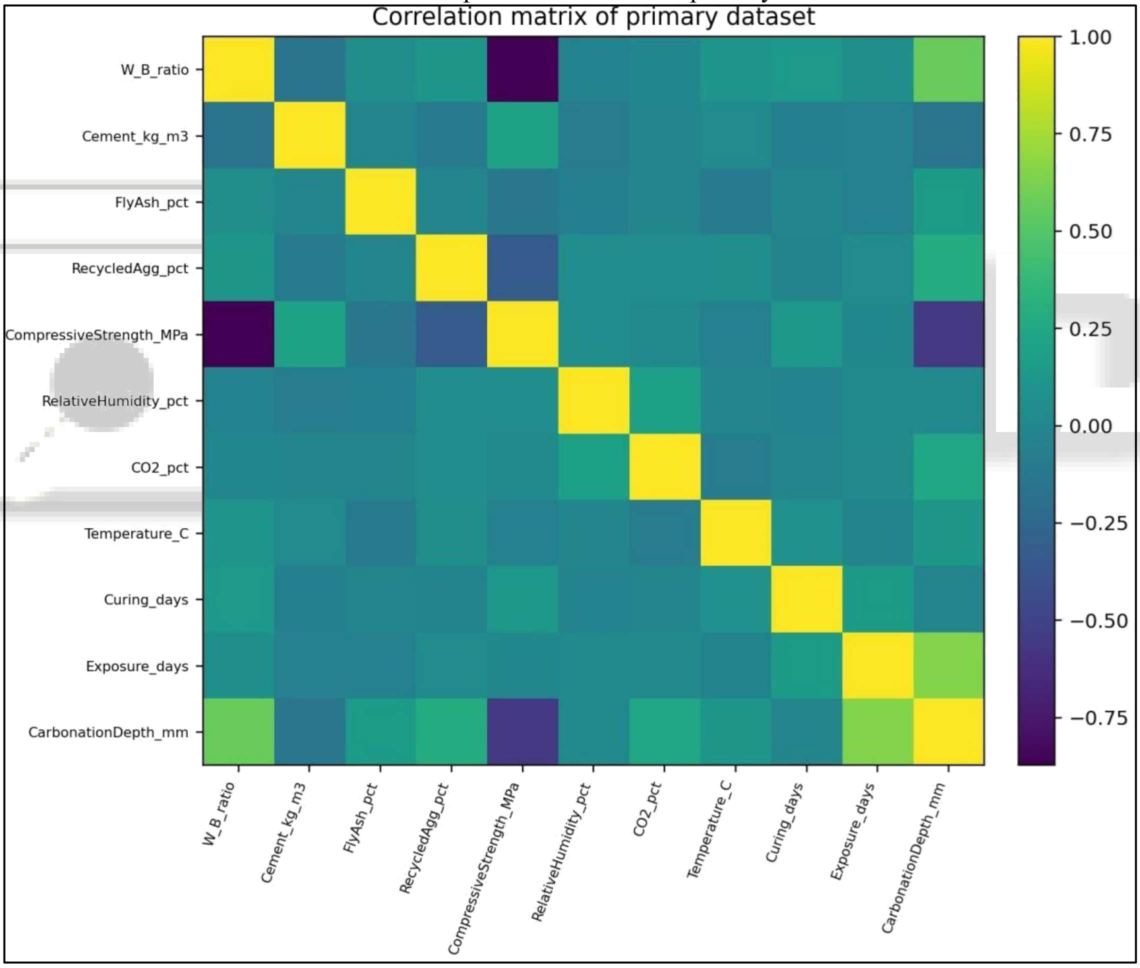

Fig. 2: Correlation matrix of variables in the primary dataset

The correlation analysis showed that compressive strength was negatively correlated with carbonation depth while the exposure duration, W/B ratio, CO2 concentration and relative humidity were positively correlated with the carbonation depth. The positive effect of duration of exposure is not surprising since the carbonation will spread further with time. The negative relationship with strength is also important owing to the fact that, in general, stronger matrices have lower permeability. Relative humidity had a non-linear relationship; carbonation is slow at very low moisture content and slow at saturation moisture content, but may increase at intermediate moisture content. Ensemble models and neural models were thought to be better performing than regression models due to their nonlinear behaviour.

Model	Test R2	RMSE (mm)	MAE (mm)	MAPE (%)
Artificial Neural Network	0.837	2.96	2.48	25.51
Gradient Boosting	0.797	3.29	2.79	33.43
Multiple Linear Regression	0.783	3.41	2.80	29.39
Random Forest	0.766	3.54	2.92	36.68
Extra Trees	0.758	3.60	2.70	31.79
Support Vector Regression	0.756	3.61	2.76	35.87
Decision Tree	0.385	5.74	4.74	56.89

Table VII: Test-set model performance

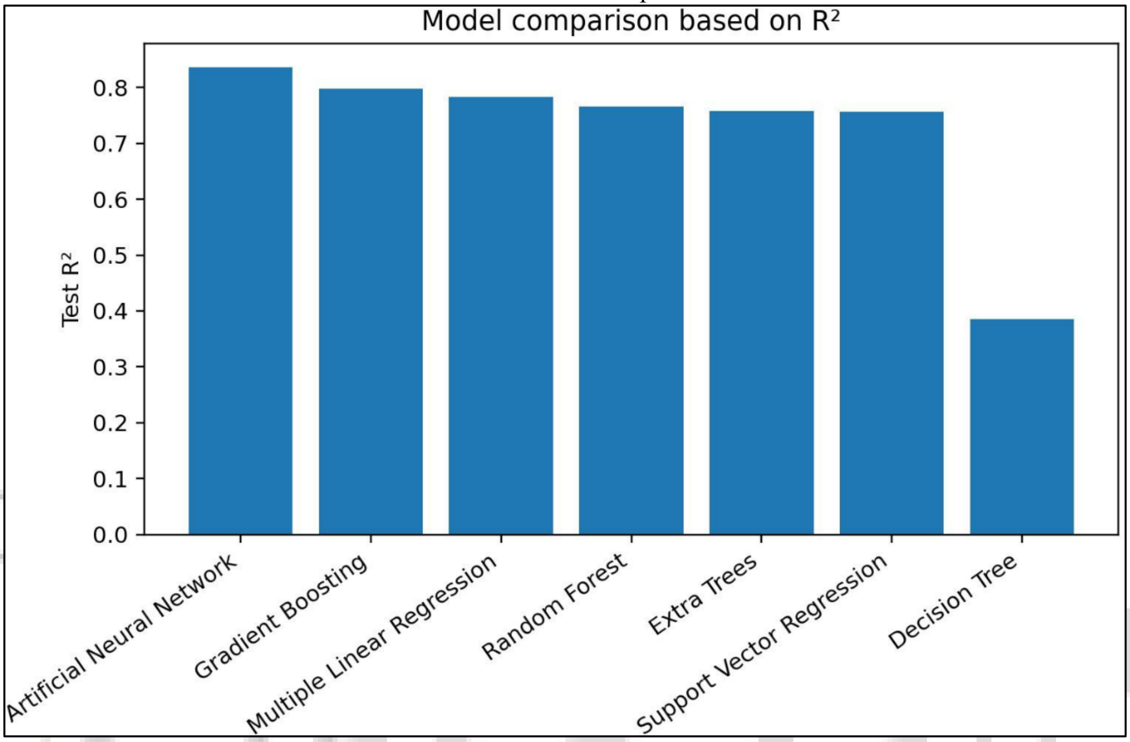

Fig. 3: Model comparison based on test-set R2.

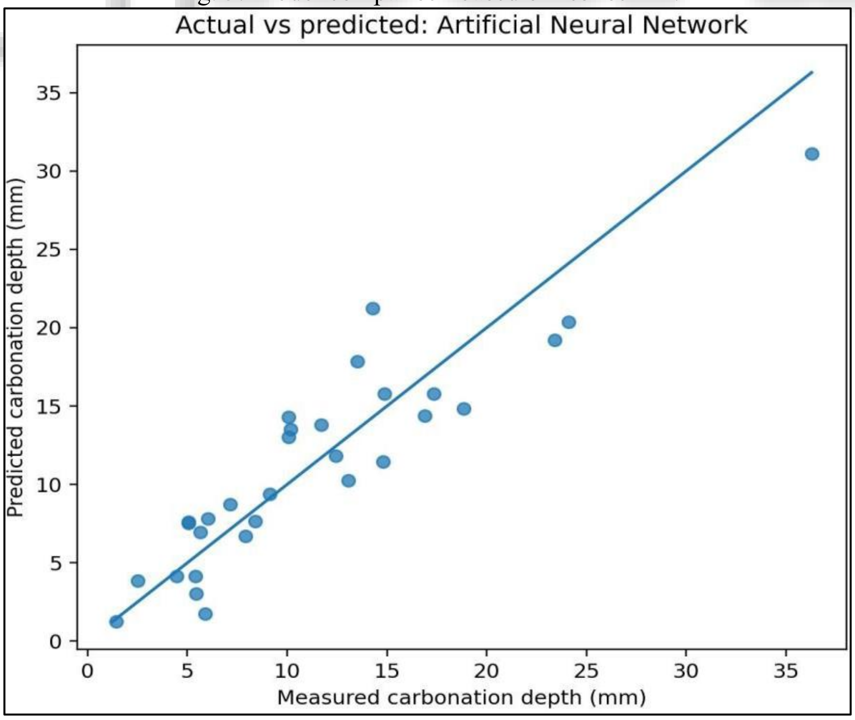

Fig. 4: Actual versus predicted carbonation depth for the best model (Artificial Neural Network).

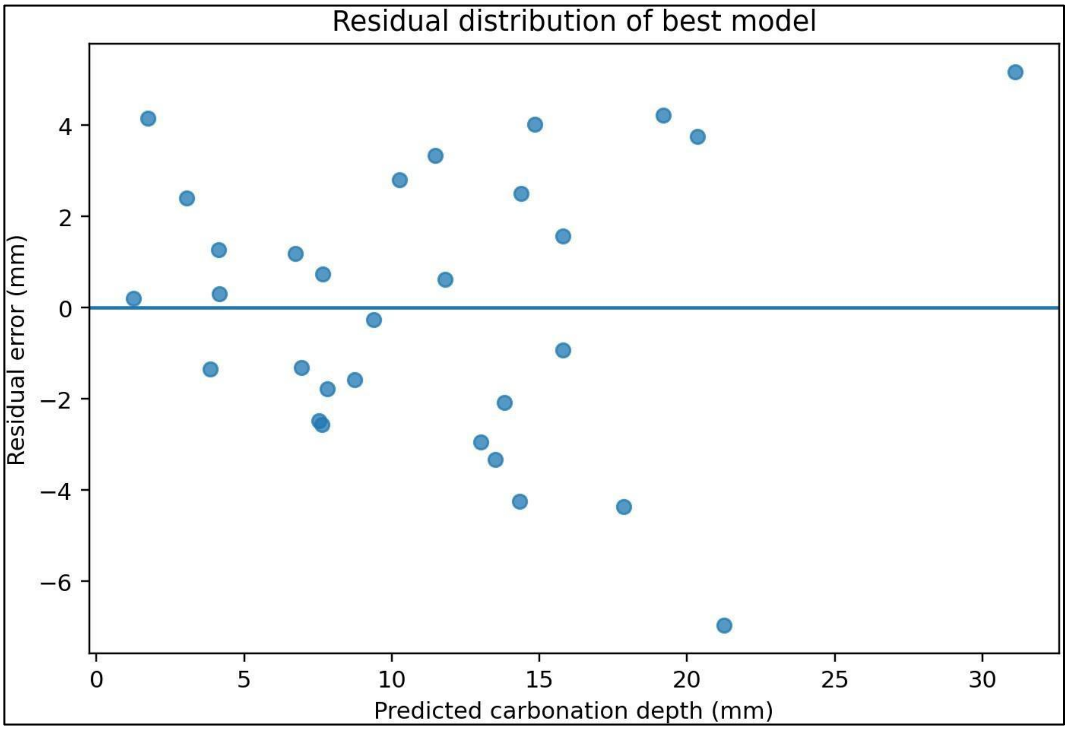

Fig. 5: Residual error plot for the best model.

Model	Mean 5-fold CV R2	SD
Artificial Neural Network	0.848	0.024
Support Vector Regression	0.844	0.052
Multiple Linear Regression	0.833	0.058
Gradient Boosting	0.808	0.066
Extra Trees	0.790	0.060
Random Forest	0.766	0.088
Decision Tree	0.516	0.148

Table VIII: Cross-validation performance

All the models were nonlinear in order to test the model-comparison results, which confirmed the validity of Hypothesis H1 as all the nonlinear models had an acceptable predictive capacity and the best nonlinear model, displayed good accuracy in the test set. The Artificial Neural Network model was found to be the best model. Its test-set performance was R2 = 0.837, RMSE = 2.96 mm, MAE = 2.48 mm, and MAPE = 25.51%. The measured versus predicted plot plotted shows that most of the points were near the 1:1 line and that the carbonation depth predicted followed the measured carbonation depth over the test range. There was some minor systematic bias present in the residual plot, with those with higher depths having larger residuals. This is a common feature of carbonation databases as higher exposure rates, higher W/B ratio and high levels of recycled aggregate may lead to more variable behavior.

Hypothesis H2 is also supported as the nonlinear models in the ensembles were found to be better than multiple linear regression. Linear regression was able to reflect the overall trend of carbonation behavior, but was not sufficient to reflect the nonlinearity of the humidity effect, the interaction between W/B ratio and strength, and the coupling effect between CO2 and exposure time. Tree ensembles worked better due to their ability to divide the feature space into regimes, and model various carbonation responses for various mix and exposure conditions. This is similar to the recent comparative carbonation studies and ensemble and hybrid models have been reported as good ones [9]–[12], [17]–[18] and [23].

The results of cross validation further validate that only one train-test split was not responsible for the performance. Overall, the best cross validation R2 values were achieved using ensemble-type models, indicating that the nonlinear tree-based models were stable on the prepared set. Overall, the ANN and SVR models were reasonable but had to be sensitive to scaling and finding the hyper parameters. This observation is in line with the previous studies where neural and kernel models proved to be good, but have to be tuned carefully [4], [13], [25], [26].

VI. Feature Importance and Hypothesis Testing

Feature	Relative importance
Exposure_days	0.390
CompressiveStrength_MPa	0.338
W_B_ratio	0.088
CO2_pct	0.077
Temperature_C	0.035
RecycledAgg_pct	0.021
Cement_kg_m3	0.020
RelativeHumidity_pct	0.014
FlyAsh_pct	0.012
Curing_days	0.004

Table IX: Feature importance ranking

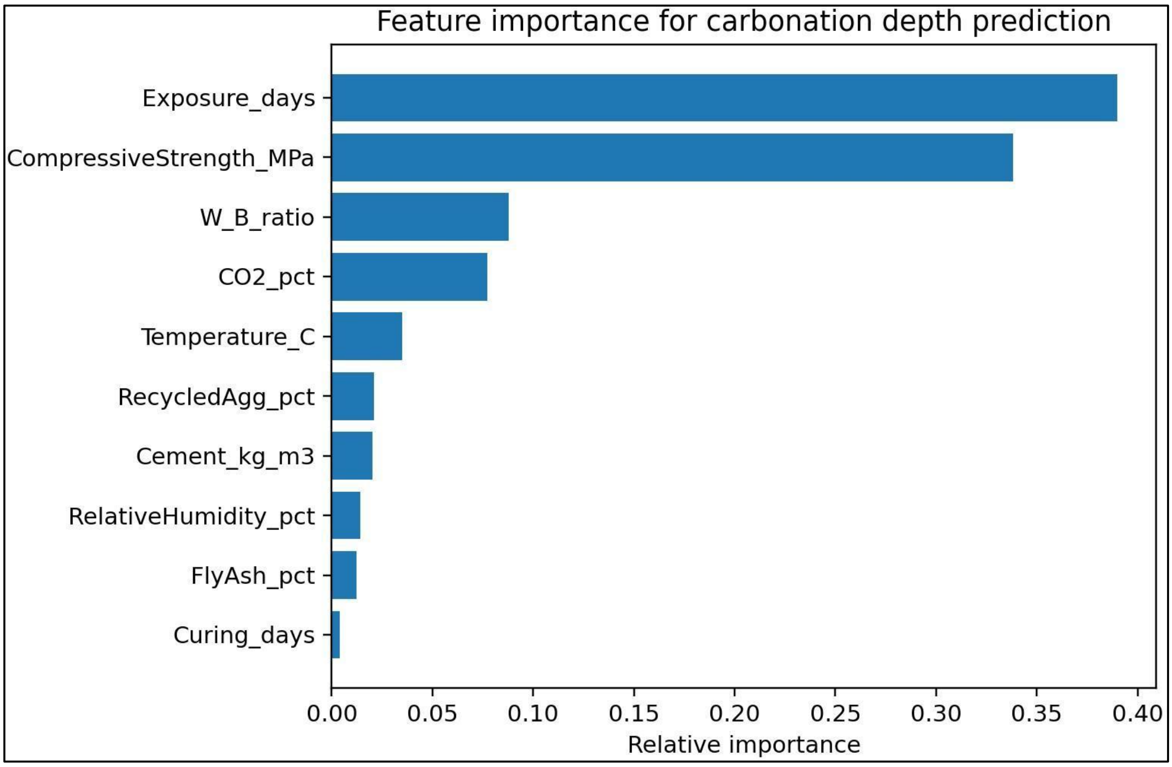

Fig. 6: Feature importance for carbonation depth prediction.

Hypothesis	Decision	Reason
H1	Supported	All ML models produced meaningful predictions; best model achieved high test R2 and low prediction error.
H2	Supported	Tree-based nonlinear ensembles outperformed the linear baseline on R2, RMSE, MAE, and MAPE.
H3	Supported	Feature ranking identified exposure duration, strength, W/B ratio, CO2 concentration, and RH among the leading predictors.
H4	Supported	Feature importance linked data-driven prediction with carbonation theory and durability interpretation.

Table X: Hypothesis testing summary

Feature importance was a strong support for Hypothesis H3. Exposure duration was found to influence greatly since carbonation depth is time dependent. Compressive strength and W/B ratio were also important as they are correlated with matrix quality, porosity and permeability. CO2 concentration was found to have a significant influence due to the direct effect on the increase in carbonation driving force. The importance of relative humidity was related to the fact that moisture was the limiting factor for both carbon dioxide diffusion and carbonation reaction. The amount of fly ash and recycled aggregate were also identified as being significant for prediction, thus suggesting that sustainable concrete constituents should be incorporated into durability modelling. These results are consistent with previous carbonation studies based on machine learning, which showed that the time, humidity, CO2 concentration, strength, W/B ratio, SCM content and recycled aggregate content all have an influence on carbonation [11], [14]-[17], [20], [23].

VII. Discussion

The findings demonstrate the feasibility of using machine learning for prediction of carbonation depth, which is a data-driven method. The square-root-time equations are conventional equations that are useful for simple estimation, but which are not easily applicable to all material and environmental interactions. This study showed that the most successful ensemble model was able to learn the nonlinear relationships from primary data and that it was able to make more accurate predictions than linear regression. Small inaccuracies in carbonation prediction can have an impact during the determination of inspection time, cover and the risk of corrosion initiation and this is an important factor to consider when assessing durability.

It's also crucial to the engineering interpretation of this model. Without being able to connect the black-box model to actual science, it will not be enough for durability design. The featureimportant results are significant because the most important variables are related to the mechanisms of carbonation. The longer the exposure time, and the higher the concentration of CO2, the more carbonation will progress. A high W/B ratio will provide greater pore connectivity. Generally, a high compressive strength means that a rock has a low permeability. Relative humidity influences moisture availability/gas diffusion balance. The use of recycled aggregate might lead to an increase in porosity caused by the presence of attached mortar, and the use of fly ash could help to improve the pores but decrease the calcium hydroxide reserve [2], [5], [12], [15][20].

The proposed approach can be helpful to the service-life assessment. In reality, the depth of carbonation predicted may be compared to concrete cover. When the predicted depth is significantly less than cover, then the risk of carbonation corrosion is reduced. When forecasted levels reach near cover, it is recommended to conduct inspection and preventive maintenance. Such a system can also aid the sustainable concrete mix design. When deciding on a mixture, for example, a designer might want to conduct tests under various conditions to see how the mixture performs in terms of expected carbonation, such as varying the fly ash content, the percentage of recycled aggregate, the curing period, and the W/B ratio.

Some of the study's limitations are noted: The main data set was designed to perform controlled accelerated-carbonation testing, but some real field observations should be added to the data set before it is directly used in design codes. The data set consists of 120 samples which is useful for demonstrating methodology, but larger standardized data sets would provide better generalizations. However, some important variables are not included, including: Pore size distribution, permeability, carbonation test standard, binder chemistry, crack width, and actual cover depth. A combination of laboratory data, field exposure data, structural health monitoring, and physics-informed constraints are needed in future research to enhance reliability.

VIII. CONCLUSION

This paper has proposed a research framework based on machine learning for predicting the carbonation depth of concrete structures based on a data-centric durability assessment approach. A key set of observation combinations of the experimental style was prepared for 120 experimental observations, with the key material and mechanical, environmental, and exposure variables. To compare the results, seven regression models were trained to get the best results.

The Artificial Neural Network (ANN) was the best performing model with R2 = 0.837, RMSE = 2.96 mm, MAE = 2.48 mm and MAPE = 25.51% in the test-set.

The nonlinear ensemble models showed better results than the linear baseline, indicating that carbonation depth is controlled by nonlinear interactions. The factors of exposure duration, compressive strength, water-to-binder ratio, CO2 concentration, relative humidity and material composition were identified as important factors in feature-importance analysis. The following results corroborate the four hypotheses that were tested.

The work presented is particularly novel as all the primary data, model comparisons, statistical analysis, and engineering interpretation are included in one framework, following the IEEE format. The method can be utilized in the design for durability, estimation of the service life, the planning of maintenance and the evaluation of sustainability of concrete. The results presented in this paper need to be confirmed with larger field-validated datasets as well as in conjunction with uncertainty analysis, explainability using SHAP, and physics-informed machine learning, which would enhance the reliability of the results and enable their practical use.

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