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Explainable Machine Learning for Predicting Concrete Compressive Strength from Mixture Composition and Curing Age

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ABSTRACT

The prediction of the concrete compressive strength based on composition of concrete mixtures and curing age can be used to support the preliminary assessment of concrete materials, but it is important to carefully evaluate the accuracy of the model and its explanations. In this study the five regression models were compared with UCI Concrete Compressive Strength dataset. So, 1005 observations were left after the removal of 25 duplicate observations. The composition groups were set aside in such a way that they do not overlap between train, val and test sets. Gradient Boosting was chosen for explanatory analysis because it had the lowest grouped cross validation error. The test performance gave $R^2 = 0.878$, RMS error = 6.207 MPa, and MAE = 4.249 MPa. This value of 5.797 MPa was obtained for the Extra Trees model, showing that differences existed between the models in the different evaluation stages. Permutation importance determined curing age, cement, and water to be the top three predictors. The partial dependence revealed a linear increase in predictions as age increased and a downwards trend in prediction as water content increased. The results indicate preliminary strength estimates and the need for independent estimation and experimental verification of proposed mixture adjustments.

Keywords: Concrete compressive strength, Explainable machine learning, Mixture composition, Curing age, Ensemble regression

1. Introduction

The compression strength of concrete is a fundamental indicator of the quality of the material, and also crucial in structural design. Reliable estimation can be applied to the selection of the mixtures, scheduling work and determining the appropriateness of concrete for various uses in construction. In addition to the conventional strength evaluation which relies on laboratory measurements, predictive models provide an alternative approach to performance estimation based on the available mixture information (Liu & Sun, 2023). But strength is due to interaction of constituent proportions and testing age. Research with explainable features of deep learning demonstrates the importance of encoding such relationships in the material-specific predictors instead of just the simple empirical expressions (Zeng et al., 2022).

Mixture composition is easy to predict; it is based on the fact that the composition of cement, water, aggregates, admixtures and supplementary cementitious materials interact to determine the performance of concrete. The investigations conducted on the blended concrete have shown that curing age, cement concentration, and water content are important contributors to predict the behaviour of blended concrete, thus highlighting the need to study both the composition and the time (Kashifi et al., 2024). In pozzolanic mixtures, the interactions related to binder proportions and the strength development as a function of age are further highlighted by interpretable ensemble frameworks (Jueyendah & Ağcakoca, 2026a). In addition, research on self-compacting concrete (SCC) also relates the composition, rheological properties, and strength of SCCs to explainable modelling, suggesting that the effect of the constituents should be understood in the context of their formulation (Wahab et al., 2024).

Concrete developed using alternative raw materials has stimulated interest in these relationships. By using explainable prediction for RASC, it is possible to investigate the influential mixture parameters in a material system with non-linear interactions between the constituent materials (Almutairi, 2025). Waste-glass concrete research also connects the strength estimation to the evaluation of alternative materials, reinforcing the importance of clear modelling of material substitution (Shams et al., 2026). This approach of mixture optimization can be further developed by tree-based research on the recycled aggregate fibre-reinforced self-compacting concrete (Jueyendah & Ağcakoca, 2026b). The applications encourage interpretable assessment, but do not provide evidence of environmental benefit or long term durability in terms of strength predictions.

The variety of materials that have been examined also illustrates the need for well defined limits on predictive findings. Within a manufacturing process that has other formulation requirements, explainable modelling of fly-ash-blended three-dimensional printed concrete is presented to explain mechanical performance (Iqbal et al., 2026). Ternary industrial-waste geopolymer grouting materials are studied by testing various combinations of precursors and interactions between materials (Wang et al., 2025). In addition to the curing age, ultra-high performance concrete is hybrid modelled with other material properties (fibres/silica fume) (Jueyendah & Hollý, 2026c). Therefore, the rankings or accuracy of models that have been created for a specific material system cannot be taken for granted when applied to other material systems.

There are several methods of learning the nonlinear composition–strength relationships by machine learning. Examples of comparing tree ensembles with neural networks provide a showcase of how predictive modelling could be used to explore individual input contributions through feature attribution (Fu et al., 2025). Optimization with explainable classification is also explored in EARC concrete research, demonstrating that interpretability can aid decisions beyond continuous strength estimation (Ulucan et al., 2023). However, two different requirements are predictive accuracy and explanatory usefulness. It is important to evaluate a model in groups that are also representative of specific ages and compositions, and to make comparisons in an easily understood and overt way to simpler models, in order to detect low average errors, but also to identify problems in important subgroups of ages or compositions.

More and more software accessibility, uncertainty assessment, and engineering knowledge are needed for practical implementation. In this work, we show how computational methods for ensemble prediction and explanation can be made accessible for engineering workflows in a desktop application, ConcreteML (Abbas & Barbulescu, 2026). Explainable automated machine learning for carbon-dioxide-cured concrete is a combination of strength prediction and uncertainty quantification, where reliability reporting is crucial along with point prediction (Wang et al., 2026). Empirical relationships between knowledge and growth are incorporated into knowledge-informed neural networks for better accuracy and reliability (Zhang et al., 2026). These developments serve to promote evaluation based on both numerical performance and engineering meaning of predictions.

Validation is especially critical if there are multiple observations with identical mixture compositions. It has been

shown in independent external evaluations that the performance of predictive systems can suffer due to the change of material properties and the distribution of the datasets (Kassa et al., 2026). The above mentioned grouping by composition is therefore used in the present study to facilitate a focussed test of prediction for new formulations, by keeping measurements of the same mixture together in the data partitioning. Seven constituent quantities and curing age are selected for the analysis to compare regression models, explore prediction errors and provide an examination of model behaviour using permutation importance and partial dependence. Its contribution results in a repeatable evaluation of generalisation over composition and interpretable prediction in the available data set. The objectives of this study are as follows:

1. To characterize associations between concrete mixture composition, curing age, and measured compressive strength.
2. To compare regression models using grouped validation that evaluates predictions for previously unseen concrete mixtures.
3. To interpret influential predictors and assess prediction uncertainty and errors across curing-age and mixture categories.

2. Materials and Methods

2.1. Study Design, Data Source, and Data Quality Assessment

The Concrete Compressive Strength dataset was obtained from the public domain and originally attributed to I-Cheng Yeh (Williams, 2020); it was analysed using a quantitative study. The file that was uploaded had 1030 observations, 7 mixture constituents, curing age and compressive strength. The amounts of ingredients were presented in kg/m³, and the age in days; the strength was presented in mega Pascals (MPa). Check of missingness, numerical finiteness, duplicate records and basic plausibility were performed. It was found that 25 of the same rows had to be removed due to repeated weighting, such that there were 1,005 observations. Common constituent quantities were used to identify a common mixture.

2.2. Exploratory Analysis and Predictor Representation

Means, sample standard deviations, minima and maxima were calculated to provide descriptive statistics. Pearson and Spearman correlations were used to investigate associations between each predictor and compressive strength, and these were compared to see whether there were linear or monotonic relationships. The original eight predictors were used for model development. Presence of supplementary cementitious material was indicated by a positive sum of the quantities of blast furnace slag and fly ash. For the subsequent assessment of error, the age was stratified into four age intervals. Ingredients associations were explained in relation to the mixture distribution observed, rather than in terms of independent causes for individual ingredients.

2.3. Model Development and Validation Strategy

Randomly split the compositions into 80/20 training/testing sets using mixture identifiers with random seed 42. The following models were tested: Ridge regression, Random Forest, Extra Trees, Gradient Boosting and support vector regression. Hyperparameters were optimized by a 5-fold grouped cross validation procedure in the training data. Standardization was added to the Ridge and support vector pipelines. The model that had the lowest mean cross validation root mean squared error was chosen prior to test evaluation. Same mixture composition were discarded between the training, validation and testing partitions.

2.4. Predictive Performance and Robustness Assessment

The evaluation approach for the performance was based on use of mean absolute error, root mean squared error and coefficient of determination. Final predictions were measured on the never-seen-before grouped testing set. Observed minus predicted strength was calculated and the mean and range of the residuals was investigated. Comparisons were made between selected-model errors by curing age ranges and the categories of supplementary cementitious materials. The confidence intervals were estimated through a 1,000 bootstrap samples which resample test mixture groups with replacement. These intervals measured the uncertainty of the test sample, which was given the fitted model, and not the uncertainty over repeated training runs.

2.5. Model Explainability and Engineering Interpretation

Permutation importance and partial dependence analysis were used to attain model explanations. The contribution of each test predictor to the prediction was quantified by the increase of root mean squared error following random shuffling of predictors 30 times. The mean increase and standard deviation of repetitions were used to summarize importance. Brute force evaluation was applied to calculate the predictions of partial dependence in order to average across the training observations while varying the selected predictors. These explanations characterized the selected model's behaviour. Due to the correlation of mixture constituents, there was a cautious interpretation of shuffled and substituted combinations which were not considered as experimentally validated formulations.

3. Results

3.1. Dataset Quality and Descriptive Characteristics

The first data file had no missing values and there were 1030 records. The removal of 25 identical rows resulted in 1,005 observations corresponding to 427 different mixture compositions (see Figure 1). The split in groups was used to leave 800 observations from 341 mixtures for training and 205 observations from 86 mixtures for testing. There is significant variation in constituent quantities and strength as shown in Table 1. The mean compressive strength was 35.25 MPa, the standard deviation 16.28 MPa and the range 2.33–82.60 MPa. Curing age varied from 1 day up to 365 days, which provided an opportunity to assess the performance at various testing ages.

Table 1. Descriptive statistics of concrete composition and strength

Variable	Mean	SD	Minimum	Maximum
Cement (kg/m ³)	278.63	104.34	102.00	540.00
Blast furnace slag (kg/m ³)	72.04	86.17	0.00	359.40
Fly ash (kg/m ³)	55.54	64.21	0.00	200.10
Water (kg/m ³)	182.08	21.34	121.80	247.00
Superplasticizer (kg/m ³)	6.03	5.92	0.00	32.20
Coarse aggregate (kg/m ³)	974.38	77.58	801.00	1,145.00
Fine aggregate (kg/m ³)	772.69	80.34	594.00	992.60
Curing age (days)	45.86	63.73	1.00	365.00
Compressive strength (MPa)	35.25	16.28	2.33	82.60

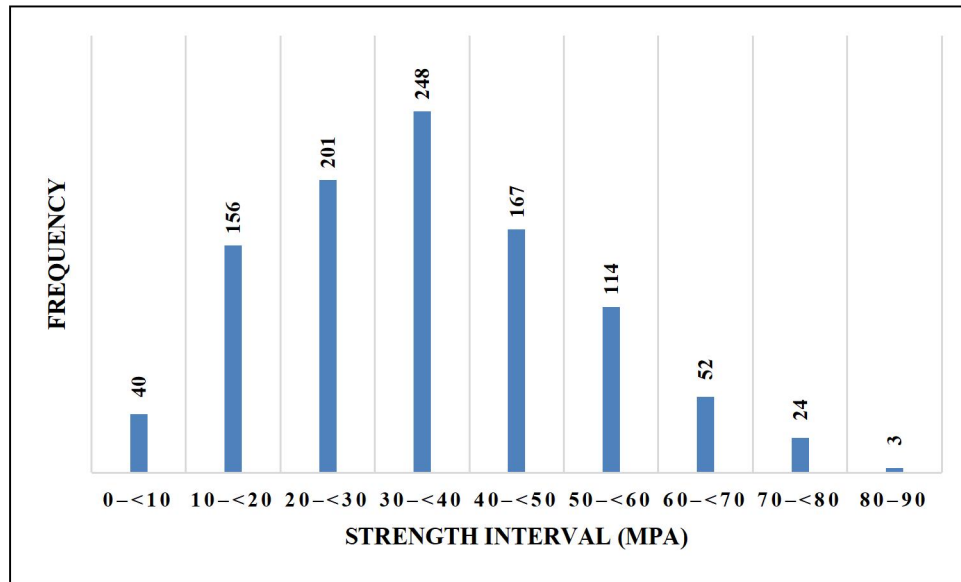


Figure 1. Distribution of measured concrete compressive strength

3.2. Composition–Age Relationships and Predictor Structure

The highest Pearson correlation was seen between cement and compressive strength (Table 2). The other two correlations, with superplasticizer and curing age, were positive, 0.344 and 0.337, respectively. For water, the negative correlation was found to be -0.270 . The strength of the monotonic association between age and strength was greater (0.605) than the Pearson coefficient (0.578). Weak marginal correlations for fly ash. These descriptive relationships accounted for the joint distribution of formulations and did not provide causal effects on any particular ingredient (Figure 2).

Table 2. Predictor correlations with measured concrete compressive strength

Predictor	Pearson r	Spearman ρ
Cement	0.488	0.461
Blast furnace slag	0.103	0.140
Fly ash	-0.081	-0.056
Water	-0.270	-0.284
Superplasticizer	0.344	0.322
Coarse aggregate	-0.145	-0.163
Fine aggregate	-0.186	-0.193
Curing age	0.337	0.605

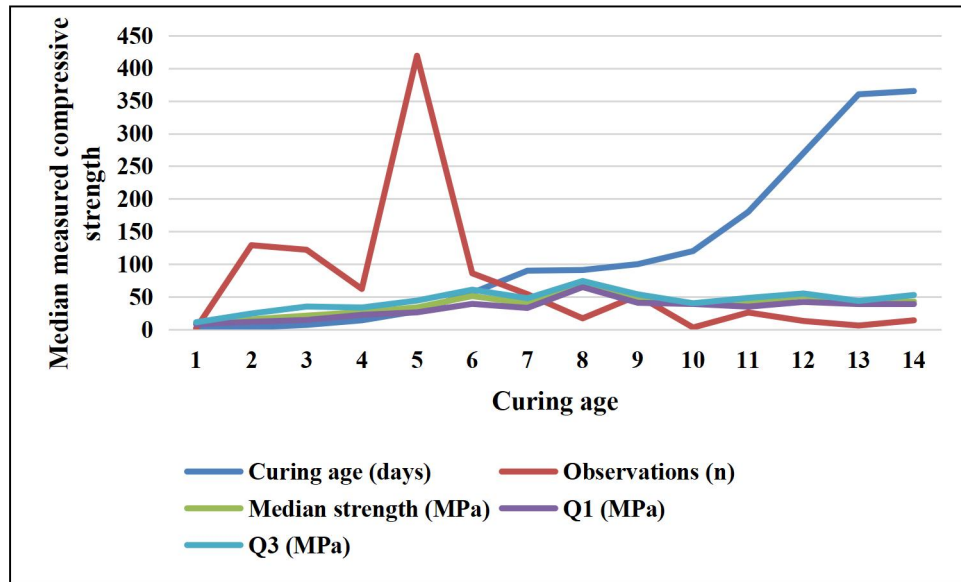


Figure 2. Median concrete strength across recorded curing ages

3.3. Comparative Model Performance

The performance of the five regression models is given in Table 3. The models with the lowest mean grouped cross validation RMSE were chosen for further investigation, with Gradient Boosting having the lowest score of 5.358 MPa. Its test MAE, RMSE, and R^2 were 4.249 MPa, 6.207 MPa, and 0.878, respectively. The results were better for Extra Trees, as they recorded an MAE of 3.705 MPa, RMSE of 5.797 MPa, and R^2 of 0.894 in the test. The test RMSE was the highest for ridge regression (10.726 MPa). As can be seen from the various validation and test ranks, the best ranking model varied with the partition being evaluated (Figure 3).

Table 3. Cross-validation and test performance of regression models

Model	CV RMSE (MPa)	Test MAE (MPa)	Test RMSE (MPa)	Test R^2
Ridge regression	10.362	8.485	10.726	0.637
Random Forest	6.159	4.175	6.007	0.886
Extra Trees	5.448	3.705	5.797	0.894
Gradient Boosting	5.358	4.249	6.207	0.878
Support vector regression	6.571	4.367	6.533	0.865

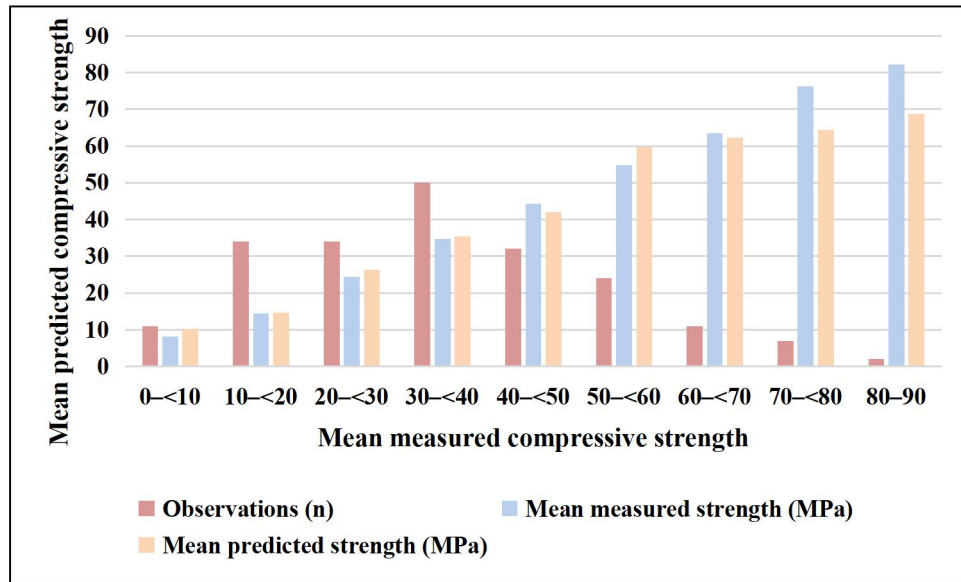


Figure 3. Comparison of mean measured and predicted concrete compressive strength across strength intervals

3.4. Prediction Errors and Robustness Across Subgroups

As can be seen in Table 4, errors in the Gradient Boosting method were found to be different among categories of curing-age and mixture. RMSE was 4.661 MPa at 1–7 days and 7.050 MPa at 29–90 days. For mixtures with supplementary cementitious materials, RMSE was 5.924 MPa, which is lower than 7.121 MPa for those without supplementary cementitious materials. The average residual bias was -0.297 MPa, which meant that on average, the model over-predicts. Bootstrap 95% confidence intervals were 3.434–5.217 MPa for MAE, 5.103–7.381 MPa for RMSE, and 0.830–0.915 for R^2 . The remaining smaller populations at older ages restricted the accuracy of the age-specific comparisons (Figure 4).

Table 4. Prediction errors across age and mixture categories

Test subgroup	n	MAE (MPa)	RMSE (MPa)	R^2
Overall	205	4.249	6.207	0.878
Curing age: 1–7 days	58	3.417	4.661	0.889
Curing age: 8–28 days	95	4.303	6.612	0.834
Curing age: 29–90 days	29	5.193	7.050	0.723
Curing age: 91–365 days	23	4.936	6.732	0.681
SCM absent	45	4.729	7.121	0.847
SCM present	160	4.114	5.924	0.888

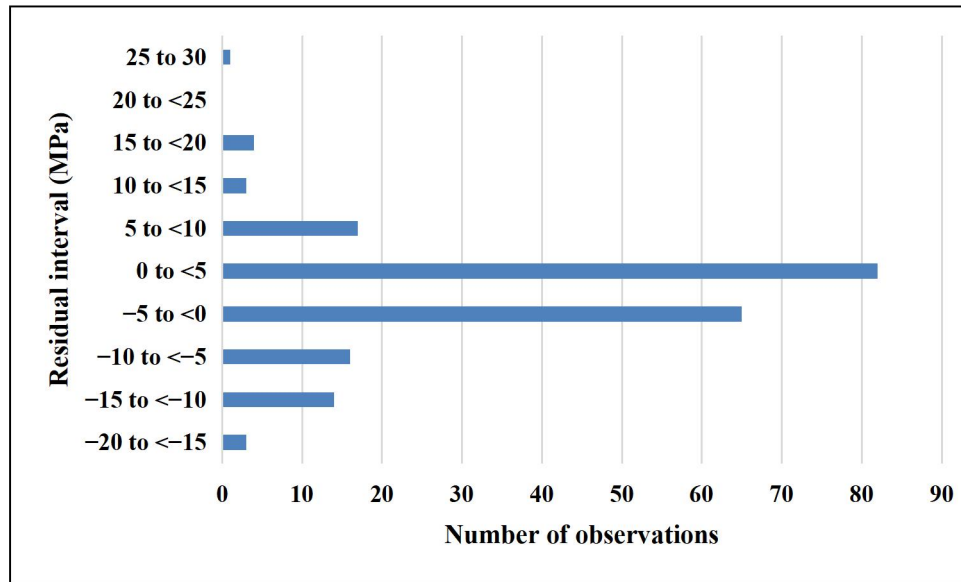


Figure 4. Distribution of test-set prediction residuals

3.5. Explainable Contributions of Composition and Age

From Table 5, it is observed that curing age and cement are the top two most important predictors in the selected Gradient Boosting model. Permuting age increased RMSE by 9.683 MPa, whereas permuting cement increased RMSE by 8.637 MPa. Water and slag came next, following with a rise of 3.914 and 2.537 MPa respectively. Average predict strength for partial dependence was 37.385MPa at 28 days and 46.166MPa at 90 days. The more water, the less was predicted. These results identify predictive dependencies within the fitted model but didn't show causal effects (Figure 5).

Table 5. Permutation importance of composition and age predictors

Predictor	Rank	Mean Δ RMSE (MPa)	SD of Δ RMSE (MPa)
Curing age	1	9.683	0.681
Cement	2	8.637	0.516
Water	3	3.914	0.483
Blast furnace slag	4	2.537	0.335
Fine aggregate	5	1.234	0.117
Superplasticizer	6	0.752	0.203
Coarse aggregate	7	0.357	0.136
Fly ash	8	0.203	0.102

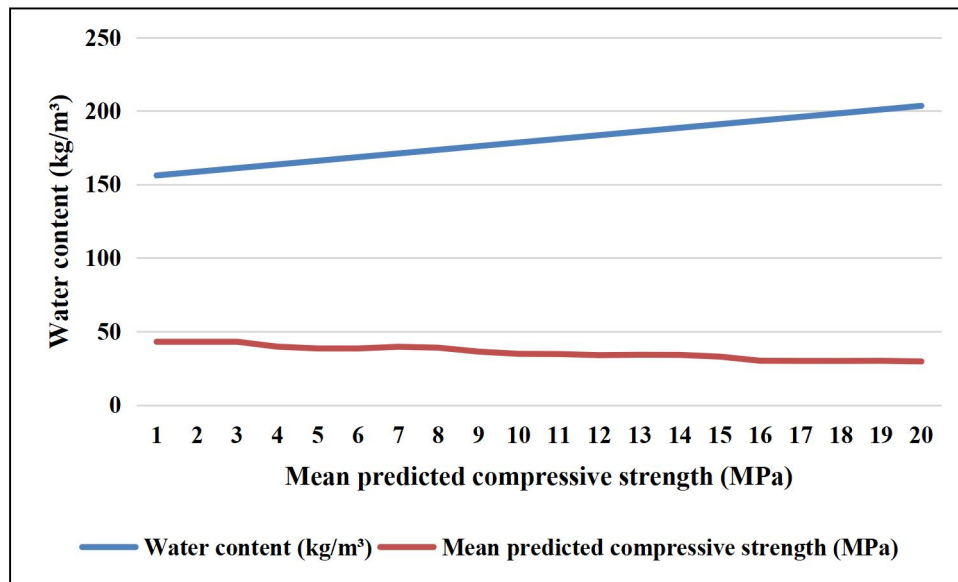


Figure 5. Partial dependence of predicted strength on water content

4. Discussion

Non-linear ensembles describe the relationships between the variables of mixture composition, curing age, and compressive strength better than linear regression. Using Gradient Boosting, test RMSE was lowered from 10.726 MPa (Ridge) to 6.207 MPa ($R^2 = 0.878$). Generally consistent with previous studies that reported an XGBoost R^2 of 0.91 and RMSE of 4.37 MPa on the same underlying concrete data (Elhishi et al., 2023). The values are unable to demonstrate model superiority, however, due to differences in pre-processing and validation. The mix variables used in the mixture and the age are also common to research using the UCI benchmark for predicting concrete strength (Nikoopayan Tak et al., 2025).

However, there was a critical difference in the validation versus test performance that emerged with model selection. The grouped CV RMSE for Gradient Boosting was the lowest, while the test RMSE for Extra Trees was the lowest (5.797 MPa). The results do not exclude ensemble modelling, but do not imply that there is any one superior algorithm. In comparison, high-strength concrete models achieved reported R^2 values over 0.96 for a number of optimized models of XGBoost optimisation (Sapkota et al., 2025). Those results show optimization within their data set, but they don't prove that they can do the same here. However, if the tuning adjustment is to be repeated in groups, one would have to confirm that the tuning adjustment is consistent and that the performance is improved by the change.

The present evaluation is relevant to predicting strengths of previously unseen mixtures, by keeping each mixture composition inside a partition. Similarly, a similar focus on validation is observed in the coconut-fiber concrete study, which employed the use of the nested grouped cross-validation and locked test set with the optimized XGBoost model yielding the test $R^2 = 0.953$ (Alawi Al-Naghi et al., 2026). The purpose of the present study is similar to that of preserving group separation, but without using nested cross-validation. Numerical comparisons are further restricted by variations in fibre content and recycled aggregates, as well as coverage of samples and optimization. The differences in these indicate that validation design and material coverage should be taken into account in addition to reported accuracy when analyzing predictive reliability.

The largest increases in prediction error were induced for the ages, the cement and the water, which highlights the importance of these variables for the fitted model. Also, the Spearman correlation was stronger than Pearson correlation for the age, suggesting a non-linear relationship. The significance of age-dependent behaviour is aligned with the study of interpretable strength research that is specifically focused on the curing-age segmentation (Lv et al., 2025). In a similar study on recycled-aggregate self-compacting concrete, Miao et al. (2025) used SHAP to determine that age and cement were major positive predictors. These variables are not identical measures of importance as predicted by the model and should not be confused with each other.

The lower significance of fly ash and aggregates must, therefore, be considered in this context and not as a lack of significance of the material. Predictive rankings rely on the variable available, the relationships between the

variables, and the mixtures in training. Similarly, ensemble learning with feature selection and SHAP was applied to study the dependency of strength prediction on cement composition in the research on calcium sulfoaluminate cement (Arachchilage et al., 2023). The various binder system makes it difficult to transfer the rankings of the features directly to the current concrete mixtures. The comparison provides an argument for invoking explanations to discover model dependence and to not lose material specific interpretation, especially in extrapolating beyond the compositions included in a benchmark database.

Partial dependence gave an overview that as water content increased, the predicted strength decreased, while curing age increased, the predicted strength increased. The patterns help make the behaviour of the model easier to examine and share the focus of explanation for the previous work on concrete strength prediction that was done at the concrete level (Pandey et al., 2026). However, averaging predictions after changing one variable can create combinations which are poorly represented or physically impractical. The resultant curves represent model responses and not real strength changes. As such they may support hypotheses and find possible predictions of problems, but proposed mixture adjustments have to be evaluated by experiments and also the workability and composition considerations should be taken into account.

Prediction accuracy also depends on interpretation along with the property being modelled. M & Janamala (2026) conducted research on permeability of high performance concrete with the focus on durability in an explainable framework by applying permutation importance, partial dependence and error assessment. The present study offers the same transparency for compressive strength but does not predict permeability or long term performance. Furthermore, the average residual bias, -0.297 MPa, was small while the individual errors were quite large. The bootstrap RMSE interval (5.103 – 7.381 MPa) represents uncertainty in the aggregate performance given the fitted model and does not give an uncertainty interval for a single concrete specimen.

Lastly, differences between subgroups illustrate why overall accuracy is not enough to make practical interpretation. The RMSE values obtained for the mixture of slag (or fly ash) were 5.924 MPa while the RMSE value obtained for the mixture without slag (or fly ash) was 7.121 MPa. These categories are not controlled substitutions as in material-specific modelling with recycled-aggregate concrete with supplementary cementitious materials (Miao et al., 2025). The error difference, therefore, can no longer be used to show a benefit in strength of causality. Unequal subgroups, along with relatively poor performance at older ages, also are worthy of additional research. Future experiments with new mixtures and independently determined curing conditions would validate the framework's applicability to other cases.

5. Conclusion

The importance of explainable machine learning in predicting concrete compressive strength based on its mixture composition and curing age. Nonlinear ensemble models performed better than Ridge regression suggesting that the data did not follow a linear relationship. Gradient Boosting had the lowest grouped error from cross validation and was consequently chosen for the explanatory analysis: test $R^2 = 0.878$ and test RMSE = 6.207 MPa. The test RMSE of Extra Trees is 5.797 MPa lower than the test RMSE of the other models, indicating that there is some difference between validation and testing. The strongest predictors were identified as curing age, cement and water through permutation importance and increasing predicted strength with age and decreasing with increasing water content was uncovered by partial dependence. These explanations are about the behaviour of the fitted model, and not about causal effects from the adjustment to mixtures. In practice, the framework might be used for preliminary estimation of strength and prioritizing mixtures for experimental testing. It is still limited in its applications due to dataset coverage, subgroup imbalances and prediction errors per individual. Repeated grouped evaluation, independent data sets with new, unseen compositions, and laboratory confirmation of proposed mixtures should be used to further validate. Further research is also needed to evaluate the quality of explanation and calibrated prediction intervals for models. These would help to make it clear how reliable the prediction is and at the same time maintain the conclusion always to the actual outcome of the concrete compressive strength.

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