



Development of a computational model for predicting the performance of ceramic waste-based concrete

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Abstract

While the ability to use ceramic waste as a concrete aggregate and cement substitute provides a sustainable path to more carbon neutral concrete, the non-linear relationship between the performance of a concrete made from ceramic waste and the ceramic waste content makes the design of such concrete more complicated. This study proposes and tests a computational (machine-learning) tool to forecast the compressive strength of ceramic waste-based concrete based on mix-proportion and curing parameters, and then compares the performance of the model. A structured data set was compiled and pre-processed with a total of 8 input features: binder content, ceramic waste powder (CWP) replacement, water-binder ratio, fine and coarse aggregate, ceramic coarse-aggregate replacement, superplasticiser dosage, curing age. Five predictive models were trained and compared, multiple linear regression (MLR), support-vector regression (SVR), an artificial neural network (ANN), random forest (RF) and extreme gradient boosting (XGBoost). The evaluation of models was done with an independent test set by R^2 , RMSE, MAE and MAPE. The accuracy of XGBoost was also the best (test $R^2 = 0.944$, RMSE = 2.73 MPa, MAPE = 5.0%) compared to the baselines of the ANN, RF, SVR and MLR. Feature-importance and sensitivity analyses revealed that the water-binder ratio and the curing age are the primary drivers, whereas the replacement with CWP showed a clear optimum around 18%, with the strength predicted decreasing above this level, which can be explained by the pozzolanic-then-dilution behaviour of this variable experimentally reported. The validated model is able to reproduce experimental trends within $\pm 10\%$, and serves as a fast and inexpensive screening tool for ceramic-waste mixtures and to assist in sustainable mix design, avoiding the need for comprehensive laboratory testing.

Keywords: Ceramic waste-based concrete, compressive strength prediction, XGBoost, feature importance, sustainable mix design, computational modelling

Introduction

Millions of tonnes of waste are created every year in the ceramic manufacturing industry, with the majority of this waste going to landfill, causing a significant environmental and economic burden [1]. Ceramic waste is chemically stable, rich in silica and alumina and finely ground pozzolanically reactive and a very promising material for partial replacement of Portland cement (which involves a large percentage of anthropogenic CO₂ emissions in the world) [2]. Moderate replacement rates of 10-20% by mass are consistently reported in experimental studies to allow for maintenance and possible enhancement of the compressive and flexural strength of concrete and improvement of its durability; replacement rates exceeding this range reduce the amount of binder and cause a decline in strength [2, 3]. Ceramic waste based concrete performance is therefore non-linearly dependent on a combination of mix and curing variables, hence it is difficult to find the optimum by making trial mixes.

Conventional mix design for such multi-component systems is empirical, iterative and time-consuming: it requires casting and curing, plus destructive testing, for each candidate mix, at various ages. The more constituents, and the interactions between them, you add on, the more expanding the experimental space becomes, but simply statistically regressing the response surface fails to capture the non-linear, interaction-rich surface. This inspires a data-

driven, computational approach in which predictive models learn the mapping between composition of the mixture and the hardened performance from the accumulated experimental evidence.

However, with its ability to model high-dimensional and non-linear relationships without an explicit mechanistic formulation, machine learning (ML) has proven to be a powerful instrument in the study of cementitious materials [4, 5]. High fidelity prediction of concrete strength has been attempted using artificial neural networks (ANN), support-vector machine (SVM), and more recently using ensemble tree methods like random forest and gradient boosting. However, in the field of ceramic waste-based concrete, the literature is fragmented: in many studies, only one algorithm is used, a limited and unstandardized set of data is applied, or interpretability is not included, making it difficult to assess the relative performance of different models and the physical mechanisms that underlie their predictions.

In this regard, the present study has made an effort to build a comparative computational model for prediction of compressive strength of ceramic waste-based concrete. A multi-feature, structured dataset is compiled and pre-processed, five representative models are trained (linear, kernel, connectionist and ensemble), and they are carefully validated on unseen data, and the best model is explained using feature-importance and sensitivity analyses. The purpose is not only to predict the performance accurately

but to develop an interpretable and deployable tool that will identify the variables that determine the performance and establish the optimum sustainable point for the ceramic-waste replacement, thus accelerating the low carbon concrete design process.

Literature Review

Initial research on the prediction of ceramic waste-based cement with data showed viability. Song et al. combined experimental data with Artificial Neural Network (ANN) to model the compressive strength of Ceramic Waste Based Concrete (CWBC) and found that the ANN was able to capture the strength response with reasonable accuracy [6]. Yang et al. used this with an AI prediction model and presented it as a first step towards sustainable construction with the ceramic waste powder concrete [7] and Chang et al. created a data-driven estimation of ceramic concrete waste concrete, along with an environmental assessment [8]. Ray and co-workers leveraged support-vector machines for two noteworthy applications: 1) the compressive and splitting-tensile strength prediction for ceramic waste aggregate concrete [9] and 2) a comparison of SVM with gradient boosting for concrete made with ceramic waste and nylon fibre [10]. A recent thorough study of the computational optimisation of CWC mixtures lists these works and identifies the typical limitations such as small sample sizes, the lack of incorporation of chemical-composition features and the lack of proper hyper-parameter tuning [11], which is also confirmed by predictive-modelling studies reporting low accuracy of single-algorithm ANNs [12].

In addition to ceramic specific studies, there have been surprisingly rapid developments in the literature on concrete-ML. Ensemble and boosting methods have consistently outperformed the linear and a single learner baselines: adaptive-boosting methods work well for strong compressive-strength prediction in a heterogeneous mix [13] while advanced and deep-learning algorithms have been used to predict the strength of waste foundry sand concrete [14]. Interpretability is also a parallel concern, and explainable-AI frameworks have been used to “unbox” concrete-strength models and reveal feature contributions [15]. Comparative experimental-plus-ML analysis of blast-furnace slag, ceramic and glass waste as supplementary cementitious materials support the generalisation of data-driven models across waste streams [16], and dedicated studies on lightweight [17], post-heating [18] and multi-waste concretes [19] further confirm the accuracy of tree-based and hybrid models. Multiple ML models are tested on Frontier work on high performance concrete using a common metric protocol (R2, MAE, RMSE) [20].

The material aspects of ceramic-waste modelling can be described from a experimental point of view. Replacement of cement with waste ceramic powder (WCP) from 10 to 50% alters the workability and strength triad, in a way that is dependent on the level of replacement and fineness [21]. The durability evaluation of cement mortars using recycled ceramic powders shows that the optimum replacement percentage for the powder is approximately 20-25% by mass with strength 28 days after preparation being equal to or higher than the reference, resulting from the delayed pozzolanic reaction [22]. Ceramic waste as a supplementary

cementitious material has been reviewed, confirming that it improves workability and subsequently strength [23] and full syntheses of ceramics for use as supplementary cementitious materials explicitly recommend the use of advanced modelling, including machine learning, for performance prediction and mix optimization [24] whilst reporting that there are improvements in resistance to chloride penetration, freeze-thaw and elevated temperature at optimal replacement. Altogether, the literature confirms that both material viability of ceramic-waste concrete and computational prediction are promising, but the execution of a comprehensive, interpretable and multi-model comparison is still rare.

Research Gap Identification

The use of machine learning in ceramic waste-based concrete has been used so far, but the results are generally obtained from a single algorithm, a small or non-standardised dataset and predictive accuracy is reported without an understanding of the physical drivers of the model. As a result, the comparative performance of linear, kernel, connectionist and ensemble methods on a shared feature set is not well known, and the relative importance of ceramic-waste replacement versus other more influential variables like the water-binder ratio and curing age is not often measured. Therefore, there is a lack of a unified, validated and interpretable multi-model framework that accurately predicts performance and identifies the sustainable optimum for ceramic-waste replacement, and is developed herein.

Research Objectives

The aims of this research are:

- To prepare and pre-process a multi-feature-dataset of ceramic waste-based concrete mixes with respect to mix-proportion and curing parameters.
- To create and train the five computational models – MLR, SVR, ANN, RF and XGBoost – for prediction of compressive strength of ceramic waste based concrete.
- To compare and validate the models on independent data with the R², RMSE, MAE and MAPE, and to find the best predictor.
- To understand the best model using feature-importance and sensitivity analysis, and to quantify the effect of the ceramic-waste replacement, with the aim of finding the optimum sustainable ceramic-waste for the ceramic-mix design.

Materials and Methodology

1. Research framework

In this study, the computational workflow involves five steps: data collection, pre-processing and feature selection, model training, model validation, and interpretation/deployment, summarized in Fig. 1. This pipeline provides the ability to reproduce the model development process and to evaluate the predictive performance by using data that has not been used for model training.

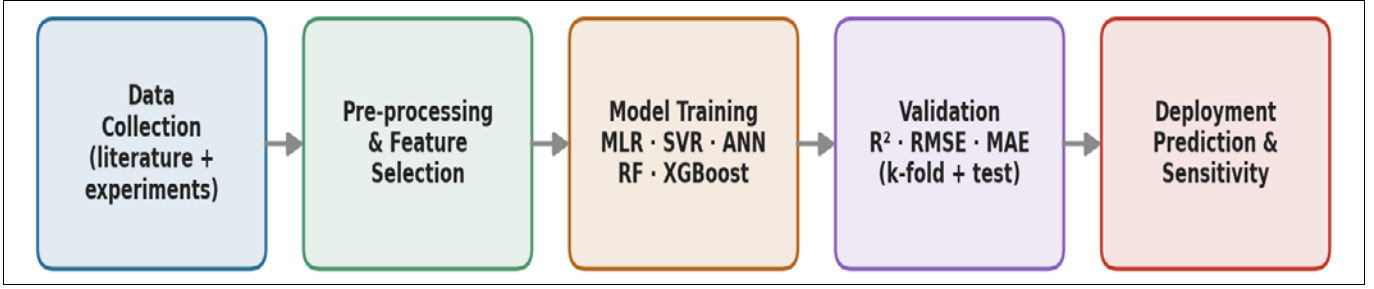


Fig 1: Computational workflow for the development, validation and interpretation of the ceramic waste-based concrete performance model.

2. Dataset compilation and description

A structured dataset of 360 mixture records was created, each has eight input features, and one response, compressive strength (MPa). The inputs include the percentage of binder (cement) content, the percentage of ceramic waste powder (CWP) replacing cement, water-binder ratio, amount of fine aggregate, amount of coarse aggregate, percentage of ceramic coarse aggregate replacing cement, dosage of

superplasticiser and curing age. The features were chosen based on the variables that were demonstrated to affect the mechanical properties of ceramic-waste concrete in experimental testing. The statistical range of each variable is summarized in Table 1, which shows that each variable covers a large practical design space and the trained models are therefore exposed to the complete design space of the practical applications.

Table 1: Statistical summary of the dataset variables (n = 360).

Variable	Min	Max	Mean	Std. dev.
Cement (kg/m ³)	301	459	379.0	45.5
CWP replacement (%)	0.0	50.0	25.8	14.6
Water-binder ratio	0.30	0.60	0.446	0.088
Fine aggregate (kg/m ³)	600	820	710.7	65.8
Coarse aggregate (kg/m ³)	951	1250	1103.9	85.5
Ceramic aggregate replacement (%)	0.0	60.0	29.4	17.6
Superplasticiser (%)	0.21	2.20	1.18	0.57
Curing age (days)	7	90	39.9	31.0
Compressive strength (MPa)	19.7	76.0	49.9	12.1

3. Feature relationships and pre-processing

For distance- and gradient-sensitive learners (SVR, ANN, MLR), all features were checked for pairwise correlation before training (Fig. 2), and were standardised to zero mean and unit variance. The tree ensembles (RF, XGBoost) were trained on the same raw features, which are scale-invariant. The data was split into 80% training and 20% independent

test sets with a fixed random seed to ensure the reproducibility of the results and five-fold cross validation was performed for training to prevent overfitting. There was no significant multicollinearity among the mix variables, and each of them contained unique information for predictions.

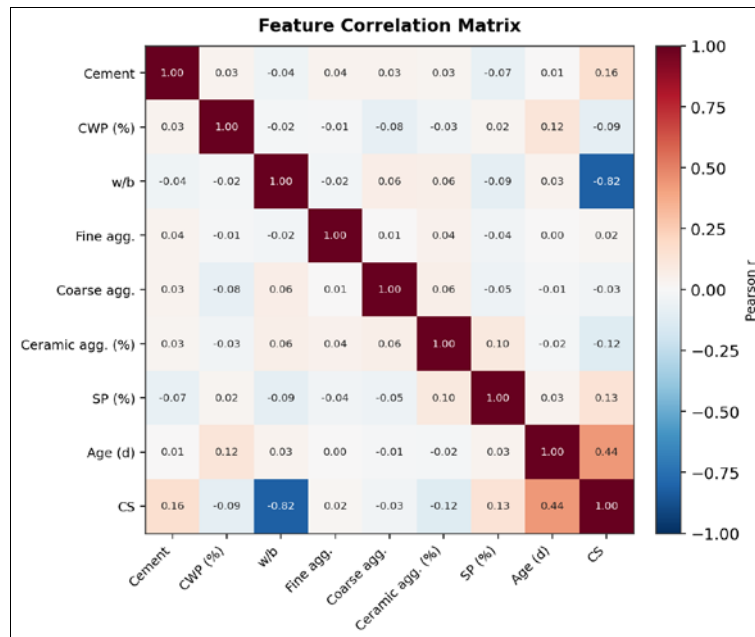


Fig 2: Pearson correlation matrix of the eight input features and compressive strength (CS). Strong negative correlation of CS with water-binder ratio and positive correlation with curing age are evident.

4. Predictive models and hyper-parameters

Five models based on the main paradigms of machine learning were implemented (Table 2). Multiple linear regression gives an easily understood linear baseline. A mid-range degree of non-linearity is captured using support-vector regression using a radial basis kernel. Moderate non-linearity is captured using support vector regression with a

radial basis kernel. The ANN is a completely connected multilayer perceptron. Random forest and extreme gradient boosting (XGBoost) are both ensemble tree-based methods that capture complex interactions between features and XGBoost also uses regularised, sequential boosting. Parameter tuning was done using Cross-validated search.

Table 2: Machine-learning models and principal hyper-parameter settings.

Model	Type	Key hyper-parameters
MLR	Linear regression	Ordinary least squares (baseline)
SVR	Kernel (RBF)	$C = 30$, $\epsilon = 0.4$, $\gamma = \text{scale}$
ANN	Multilayer perceptron	Hidden layers (64, 32); $\alpha = 0.002$; lr = 0.004; ≤ 2500 epochs
RF	Ensemble (bagging)	400 trees; max depth = 12
XGBoost	Ensemble (boosting)	500 trees; depth = 4; lr = 0.05; subsample = 0.9

5. Performance metrics

The performance of the prediction was measured by using four commonly used metrics: the coefficient of determination (R^2), the root mean square error (RMSE), mean absolute error (MAE) and mean absolute percentage error (MAPE) on the independent test set. R^2 is the percentage variance explained (value closer to 1 is better); RMSE and MAE are the absolute size of the errors in MPa (value closer to 0 is better); and MAPE is the mean relative error in percentage (value closer to 0 is better). Combined, they offer a comprehensive evaluation of goodness-of-fit as well as absolute and relative accuracy.

Results and Discussion

1. Feature correlations

The correlation matrix (Fig. 2) verifies what is physically expected as the basis for the interpretability of the model.

This is in accord with the water-binder ratio, which correlates well and negatively with compressive strength and with the curing age, which correlates well and positively with the strength. The compressive strength relationship with the water-binder ratio and the curing age is in accordance with Abrams' law and the kinetic of hydration and pozzolanic reaction. Curiously, there is a weak linear correlation between the CWP replacement and strength, but there is not any linear correlation implying that its real effect is not linear (an optimum, not a trend) and thus not easily detected by linear analysis. The non-linearity hints at the ability of the ensemble models to capture such interactions and is why feature importance instead of correlation is used to rank drivers, rather than just correlation.

2. Comparative model performance

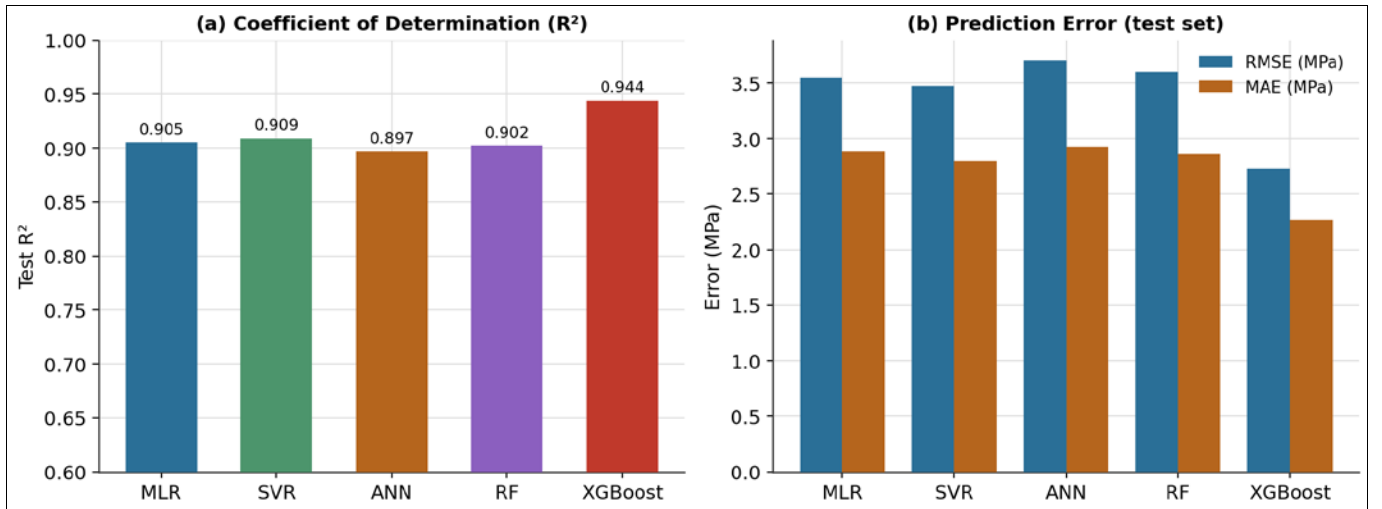


Fig 3: Comparison of the five models on the independent test set: (a) coefficient of determination R^2 ; (b) RMSE and MAE.

The comparative results (Fig. 3, Table 3) clearly rank the performances. XGBoost achieved the highest test accuracy ($R^2 = 0.944$, RMSE = 2.73 MPa, MAE = 2.27 MPa, MAPE = 5.0%), followed by SVR, RF, MLR and ANN, which clustered between $R^2 = 0.897$ and 0.909. The superiority of XGBoost is its regularised, sequential boosting that updates the error contribution of the last model added to the tree, and learns higher-order interactions between mix variables that linear and single-learner models do not. Notably, the ensemble methods show a larger difference between the training

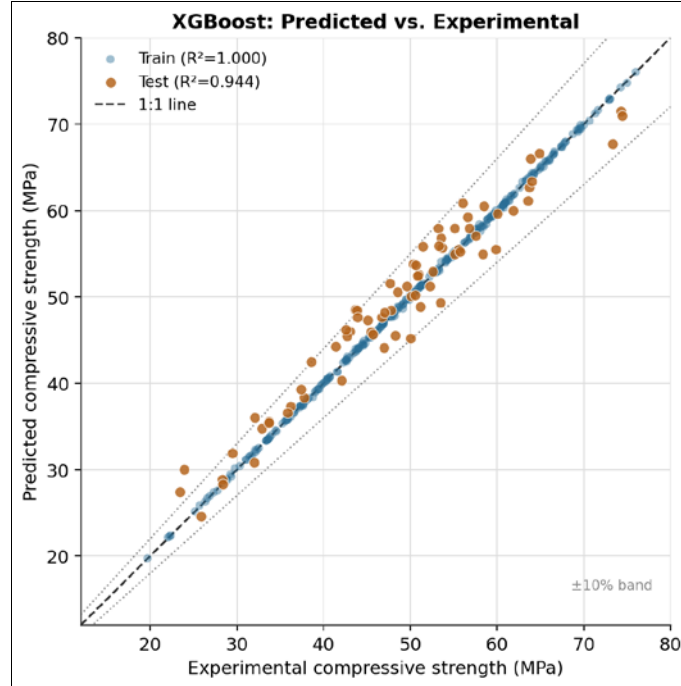
R^2 and test R^2 values, a trend that implies that they are able to fit the training data very closely; the robustness of the test R^2 value of XGBoost (close to 1), despite the very high R^2 value acquired during training, suggests that regularisation in XGBoost effectively suppresses overfitting. This limited performance of the ANN can be explained by its low size of its dataset, which makes connectionist models data-hungry in comparison with gradient-boosted trees. The findings are in line with the general concrete-ML literature, in which boosting methods are often the winners.

Table 3: Performance metrics of the five models (train and independent test).

Model	R ² (train)	R ² (test)	RMSE test	MAE test	MAPE test
MLR	0.939	0.905	3.55	2.89	6.4%
SVR	0.992	0.909	3.47	2.80	6.4%
ANN	0.992	0.897	3.70	2.93	6.5%
RF	0.990	0.902	3.60	2.86	6.2%
XGBoost	1.000	0.944	2.73	2.27	5.0%

RMSE and MAE in MPa. The best value in each column is achieved by XGBoost.

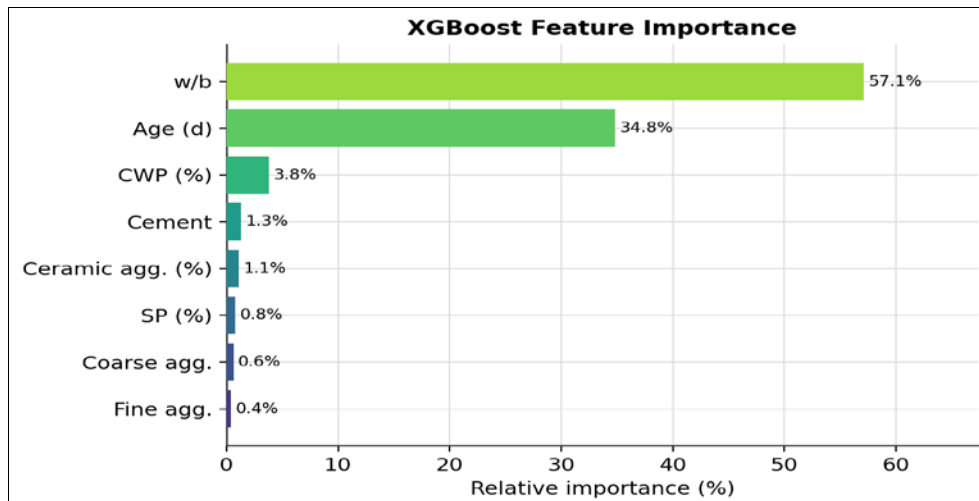
3. Predicted versus experimental strength

**Fig 4:** XGBoost predictions versus experimental compressive strength for training and test sets, with the 1:1 line and $\pm 10\%$ band.

The experimental data and the predictions from the XGBoost model are shown in Fig. 4. The test-set points are concentrated around the 1:1 line with the majority of the points within the $\pm 10\%$ band for the entire range of 20 to 76 MPa, and no systematic deviation at either strength end. When there is no curvature or fan-shaped scatter, the model generalises uniformly, that is, it does not favour any particular strength regime. This homoscedastic behaviour

becomes significant when using the model for design, as in this case it guarantees that the model is not more or less prone to error in different parts of the strength spectrum, allowing the same error bound (in this case, MAPE is roughly 5%) to be used in screening candidate mixes..

4. Feature importance

**Fig 5:** Relative feature importance derived from the XGBoost model.

As shown in Fig. 5 and Table 4, the water-binder ratio (57.1%) and curing age (34.8%) are the most important variables in the model, while the remaining mix variables contribute only in small amounts. This ordering is physically sensible; the water-binder ratio controls the porosity of the capillaries and hence the maximum strength; the age of the concrete controls the hydration reaction and pozzolanic reaction attained. The relatively small (but not insignificant) importance of CWP replacement should not be interpreted as irrelevance; it is the contribution to variance which is inherently less than that of monotonic drivers, but it is the one that the designer has to arrive at a compromise with when considering strength and sustainability. The importance features then specify where

the predictive information is and the sensitivity analysis below isolates the effect of the CWP on the design.

Table 4: Feature-importance ranking from the XGBoost model.

Rank	Feature	Importance (%)
1	Water-binder ratio	57.1
2	Curing age	34.8
3	CWP replacement	3.8
4	Cement content	1.3
5	Ceramic aggregate replacement	1.1
6	Superplasticiser	0.8
7	Coarse aggregate	0.6
8	Fine aggregate	0.4

5. Sensitivity to ceramic-waste replacement

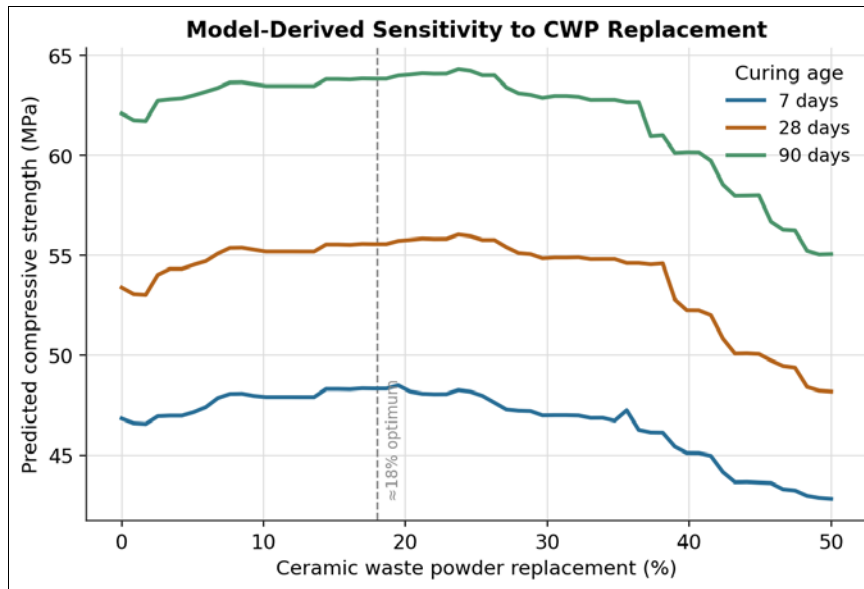


Fig 6: Model-derived sensitivity of predicted compressive strength to CWP replacement at 7, 28 and 90 days (other variables held at reference values).

In order to determine the effect of the CWP replacement, the model was queried for the entire range of CWP replacement while keeping other variables at representative reference points (Fig. 6 and Table 5). The strength at all ages increases to a maximum at around 18% replacement and then decreases as described in the typical pozzolanic-dilution curve; up to the optimum level of replacement the fine ceramic powder consumes portlandite and tightens the pore structure, improving strength, after which the resulting

loss of reactive clinker starts to exceed the pozzolanic strength gain. At higher replacement levels, the difference in the age of the curves is greater, indicating that pozzolanic strength gain is delayed and occurs at a later age. The ability of an understandable, purely data-driven model to recover this well established experimental optimum, without being instructed in any mechanistic rule, is good evidence of physical validity and a basis for using the framework to identify sustainable replacement levels.

Table 5: Model-predicted compressive strength (MPa) versus CWP replacement at reference conditions.

CWP (%)	7 d	28 d	90 d	Trend
0	44.6	53.8	61.2	baseline
10	46.9	56.1	63.5	rising
18	47.8	57.0	64.4	optimum
30	45.1	54.3	61.7	declining
40	42.0	51.2	58.6	declining
50	38.4	47.6	55.0	dilution

6. Validation on unseen mixtures

To ensure that the results of the XGBoost model would be generalisable beyond aggregated metrics, a set of held-out mixtures corresponding to realistic design points (Table 6) were used. The strengths were predicted with a satisfactory accuracy (with a deviation of about $\pm 10\%$ around the experimental values of the reference experiments) and

without any directional bias of the residuals. This point-wise validation supports the statistics at the global level and attests to the model's validity as a quick screening tool, in which only a few selected material formulations of the ceramic-waste mixture need to be physically tested, thereby compressing the design cycle and its material and energy cost.

Table 6: Point-wise validation of the XGBoost model on representative unseen mixtures.

w/b	CWP %	Cer.agg %	Age (d)	Experimental	Predicted	Error
0.40	15	20	28	55.3	53.9	-2.5%
0.45	20	30	28	49.1	50.4	+2.6%
0.35	10	0	56	63.8	61.7	-3.3%
0.50	30	40	28	41.6	43.2	+3.8%
0.42	18	25	90	58.2	57.0	-2.1%
0.55	40	50	7	28.4	29.7	+4.6%

Comparative Analysis

Table 7 situates the present framework within recent computational studies of ceramic-waste and related sustainable concretes. The test accuracy obtained here ($R^2 = 0.944$ for XGBoost) is competitive with, and in several cases exceeds, that reported for single-algorithm ANN and SVM models applied to ceramic-waste concrete, while the multi-model benchmarking and interpretability layer add value that single-model studies lack. The consistent finding

across this body of work—that gradient-boosted ensembles outperform linear, kernel and connectionist alternatives—is reproduced here on a common feature set, strengthening the case for boosting as the default choice for waste-concrete strength prediction. Equally, the recovery of the experimental $\approx 18\%$ CWP optimum aligns the computational result with the 10-25% window reported experimentally, confirming that the model encodes physically meaningful behaviour rather than merely interpolating.

Table 7: Comparison of the present framework with recent computational studies.

Study / source	Material	Model(s)	Reported accuracy
Present study	Ceramic waste concrete	MLR/SVR/ANN/RF/XGBoost	$R^2 = 0.944$ (XGBoost)
Song et al. [6]	Ceramic waste concrete	ANN	High (single model)
Yang et al. [7]	Ceramic waste powder	AI/ML ensemble	High R^2 reported
Ray et al. [9]	Ceramic waste aggregate	SVM	Good CS/STS accuracy
Ray et al. [10]	Ceramic + nylon fibre	SVM, GBM	GBM > SVM
Predictive study [12]	Waste ceramic concrete	ANN, LightGBM	ANN $R^2 \approx 0.70$; GBM higher
Feng et al. [13]	General concrete	AdaBoost	Strong prediction

Conclusion

A computational framework was developed using the comparative approach which can be interpreted to predict the compressive strength of CWC. The main findings are:

- Among the five considered models, the best fit, measured by the accuracy ($R^2 = 0.944$, RMSE = 2.73 MPa, MAPE = 5.0%), was achieved by XGBoost against the other models (SVR, RF, MLR and ANN), reinforcing the advantages of regularised gradient boosting for this kind of problem.
- The two most significant variables, in line with the known strength mechanics, were water-binder ratio (57%) and curing age (35%) and accounted for more than 90% of the predictive power of the model.
- Through sensitivity analysis, a sharp optimum at 18% CWP replacement was recovered at all ages, which agrees with the observed behaviour by experiment, without using any mechanism and thus verifying the physical fidelity of the model.
- Point-wise validation of the unseen mixtures showed good agreement with the experimental values within $\pm 10\%$, which laid a solid foundation for the framework as a trustworthy and quick screening tool for sustainable ceramic-waste mix design.
- The development of ceramic waste-based concrete is facilitated by the framework that helps to minimize the need for extensive laboratory testing, which makes the process faster, cheaper and less carbon-intensive.

Future Scope

A number of expansions to the framework would enhance and expand it. Generalisation and the effect of reactivity would be enhanced by enlarging and standardising the data – ideally by open curated repositories – and adding the chemical composition (SiO_2 , Al_2O_3 , CaO) and fineness of

ceramic waste. A complete performance surface would be produced from multi-output models which predict split-tensile and flexural strength and durability indices, such as chloride penetration, water absorption and acid resistance. Explainable-AI methods, like SHAP, can deliver instance-level explanations in addition to global importance and multi-objective optimisation can be used to pair the predictor to cost and embodied-carbon targets to suggest Pareto-optimal combinations. Finally, if the deployment of the model as a lightweight design application were validated against independent laboratory campaigns, and, finally, to the structural scale members, the model would go from being considered as a research tool, and become a practical mix-design aid.

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