

Optimization of Mix Design for Sustainable Concrete Using Artificial Neural Networks

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Abstract: Sustainable concrete is necessary to lessen the environmental impact of building. In the construction industry, supplemental cementitious materials (SCMs) added to recycled aggregate concrete (RAC) provide a sustainable alternative. The compressive strength (CS) of RAC made using SCM was thoroughly examined in this work, which compiled a dataset of 1000 samples from published literature. Conventional concrete mix design techniques are based on trial-and-error and empirical methods, which results in inefficient material use and performance optimization. This study explores the use of Artificial Neural Networks (ANNs) to forecast and optimize concrete mix design parameters in order to increase sustainability and performance. This research illustrates how machine learning may greatly expedite the design process by training an ANN model on a dataset that includes several concrete mix compositions and their resulting properties. According to the results, ANN-based models can determine the ideal mix proportions with less cement and better workability, which is in line with sustainability objectives. They can also accurately forecast compressive strength.

Keywords: Compressive strength, ANN, concrete, mix design, optimization, sustainable concrete.

1. Introduction

The widespread use of Portland cement in concrete is the main reason why the building sector contributes significantly to global carbon emissions. Sustainable building materials that strike a balance between performance, durability, and environmental effect are desperately needed as the need for infrastructure rises. A potential remedy is sustainable concrete, which incorporates supplemental cementitious materials (SCMs) such as fly ash, slag, or silica fume. However, creating such combinations frequently necessitates making difficult trade-offs.

Many efforts have been made to mitigate the negative environmental effects associated with the manufacture of concrete in response to these worries. The usage of supplemental cementitious materials, or SCMs, has grown in popularity all around the world. Particularly well-known mineral minerals that are derived from by-products and serve as SCMs are fly ash (FA), slag (SI), and silica fume (SF). By partially replacing these ingredients in the concrete mixture, the overall amount of ordinary Portland cement (OPC) used can be reduced, as well as the environmental impact. The addition of SF, SI, and FA to the concrete blend also has the benefit of

enhancing the concrete's mechanical properties and long-term durability.

One of the primary ways SCMs contribute to better mechanical properties is through this pozzolanic reaction. This reaction happens when calcium hydroxide, which is generated during cement hydration, interacts with SCMs. A denser and stronger matrix is produced as a result of the development of more calcium silicate hydrate (C-S-H) gel, which is the crucial binding phase in concrete (J. Wang et al., 2023). Additionally, SCMs contribute to the improvement of the concrete's microstructure (Gao et al., 2023). By efficiently filling in the spaces between cement particles, they lower porosity and raise the concrete's density and strength (Gao et al., 2023). When it comes to improving the rheological behavior and compressive strength of concrete using SCM, this particle-packing effect is especially important (Kashani et al., 2014). Another advantage is that SCMs can lessen the alkali-silica reaction (ASR), which weakens RAC and shortens its lifespan.

When it comes to workability, adding SCMs usually makes the concrete mixture simpler to work with and more cohesive (Feng et al., 2022). Improved workability facilitates greater concrete compaction, which is necessary to achieve high compressive strength. Additionally, SCMs such as fly ash have the ability to control the concrete's hydration heat (Sunayana and Barai, 2021). For large-scale projects, where excessive heat might lead to cracking and hence negatively affect the early compressive strength, this is very helpful. SCM-enriched RAC may have a lower initial strength than conventional concrete, but it frequently outperforms conventional mixes in the long run, especially after the typical 28-day mark. This is explained by the continuous pozzolanic reactions that SCMs enable.

The type and percentage of use of SCMs have a significant impact on their efficacy (J. Wang et al., 2023). For instance, fly ash may have a more gradual effect, although silica fume is known to greatly increase strength (J. Wang et al., 2023). Additionally, after a certain optimal quantity of SCMs in the mix, the benefits might not increase or might even decrease (J. Wang et al., 2023). The quality of the recovered aggregates is another crucial factor. High-quality recycled aggregates can produce compressive strength increases that are more pronounced than those of lower-quality aggregates when paired with SCMs (D. Wang et al., 2023).

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An environmentally responsible and sustainable way to use building materials is by employing recycled aggregate (RA) in concrete. This material is derived from a number of sources, including as concrete that has been crushed and treated to produce new aggregates and building detritus. By partially or completely substituting natural aggregates, recycled aggregate concrete (RAC) provides a number of benefits, such as decreased demand for natural aggregates, waste reduction, energy conservation, and cost-effectiveness (Kim, 2022). Even though RA integration has environmental benefits, it's vital to understand that it could negatively impact RAC's durability and mechanical qualities. Some of the reasons for this include that RA has more porosity, better water absorption, and worse adhering mortar than natural aggregate. Consequently, a weak inter-facial transition zone (ITZ) develops between the cement paste and the RA in the concrete mixture (Yong Ho et al., 2013).

Concrete's compressive strength (CS) is essential for long-lasting, safe, and structurally sound constructions. However, reaching the necessary CS becomes more challenging because to the complex interactions and variations that SCMs and RA introduce into concrete mixes (Gao et al., 2023). The presence of RA with varying replacement quantities may have a particularly significant effect on the ITZ, which is further impacted by the presence of SCMs altering the microstructure. Because of this, optimizing the concrete mix design under such a complex ITZ is challenging. Compared to traditional analytical or empirical methodologies, machine learning (ML) techniques offer numerous advantages when predicting the CS of RAC (Behnood and Golafshani, 2022; Golafshani et al., 2021).

These benefits lead to more accurate, reliable, and efficient predictions, which enhance comprehension and RAC property optimization. Several studies have been conducted to model the CS of RAC. Notably, because ensemble approaches can improve forecast accuracy and robustness, they have been the main focus of recent study. Among the different ensemble methods, gradient boosting (GBoost) and extreme gradient boosting (XGBoost) have shown better performance when compared to other ensemble and individual strategies. However, there are currently very few studies that use ensemble techniques to model RAC with ternary SCMs.

Conventional concrete mix designs frequently focus on just one goal, like CS maximization or cost reduction, while ignoring other important aspects like environmental effect. Multi-objective optimization techniques for trade-offs between CS, cost, and sustainability-related parameters in concrete manufacturing enable the exploration of optimal concrete mixtures that strike a compromise between these objectives. This scenario enables engineers to make more sustainable options by considering not just cost and CS but also the environmental impact of making concrete. Liu et al. (2023) employed a variety of machine learning techniques to forecast the CS of RAC including FA utilizing 1373 data samples. Multi-objective particle swarm optimization (MOPSO), which considered CS, cost, CO₂ emission, and energy consumption as objective functions, was then used to identify the optimal mix design of RAC. Zandifaez et al. (2023) used 2120 data samples

to develop several machine learning models to simulate the CS of RAC with SF and FA. A many-objective evolutionary method based on adaptive geometry estimation was then used to optimize the RAC mix design, accounting for the objectives of cost, CO₂ emission, acidification potential, and the possibility for fossil fuel depletion.

A thorough database of RAC combinations, including ternary SCMs, was assembled in order to create the ML models. 1000 data samples from 60 scientific research that were sourced from pertinent literature were included in this collection. Following the development of the machine learning models, random samples were generated using the Monte Carlo simulation technique. This allowed for the analysis of the sensitivity analysis of SHapley Additive Explanations (SHAP) derived from the collected database. Thus, the behavior of the model with respect to fresh data outside of the current database was examined. The multi-objective water cycle algorithm (MOWCA), a novel metaheuristic optimization technique, was then used in the study to simultaneously optimize the CS, cost, and CO₂ emissions of RAC combining SF, SI, and FA.

In order to do this, the machine learning model developed during the machine learning development phase was used to determine the compressive strength (CS). Conventional mix design techniques, such the DOE or ACI approaches, are time-consuming, involve a lot of physical testing, and might not necessarily produce the most sustainable result. A subset of machine learning called artificial neural networks (ANNs) is a powerful tool for modeling nonlinear interactions and forecasting intricate behaviors in concrete materials.

2. Literature Review

The promise of machine learning in civil engineering has been demonstrated by numerous studies. Yeh (1998) was the first to employ artificial neural networks (ANNs) to forecast concrete's compressive strength, proving that they were more accurate than linear regression. More recently, ANN applications have been extended to simulate concrete containing SCMs and recycled aggregates (Chou et al., 2011; Naseri et al., 2020). The usage of supplemental cementitious materials, or SCMs, has grown in popularity all around the world. Particularly well-known mineral minerals derived from by-products that serve as SCMs are fly ash (FA), slag (SI), and silica fume (SF) (Gupta and Chaudhary, 2022). The formation of additional calcium silicate hydrate (C-S-H) gel, the essential binding phase in concrete, results in a denser and stronger matrix (J. Wang et al., 2023). Furthermore, SCMs help to enhance the microstructure of the concrete (Gao et al., 2023). They reduce porosity and increase the density and strength of the concrete by effectively filling in the gaps between cement particles (Gao et al., 2023). The capacity of SCMs to reduce the alkali-silica reaction (ASR), a harmful reaction that can cause concrete to expand and crack, is another benefit (Barrag'an-Ramos et al., 2022; Mahmood et al., 2022).

The optimal mix proportions have also been found using optimization techniques. Fuzzy logic, particle swarm optimization, and genetic algorithms have demonstrated potential. But ANNs offer a more flexible and self-learning

substitute. They are appropriate for applications requiring variations in material sources and environmental circumstances due to their capacity to generalize from data.

3. Methodology

A. Data Collection

The data required for the investigation might be obtained from a variety of sources. These sources could include published literature, established databases, industry standards and requirements, and laboratory tests carried out especially for the study. The data set for the current study comes from respectable journals and publications, guaranteeing the accuracy and legitimacy of the data. A dataset of 1,000 samples of concrete mixes was gathered from lab tests and published sources. Every data point contained:

- Cement content (kg/m³)
- Fly ash, slag, or silica fume content (kg/m³)
- Water-to-binder ratio
- Coarse and fine aggregate content (kg/m³)
- Recycled aggregate content (kg/m³)
- Superplasticizer dosage (kg/m³)
- Age of concrete (days)
- Measured compressive strength (MPa)

Observations from Statistical Analysis of the Dataset: The dataset's statistical analysis yields significant findings on the output Compressive Strength and the input ingredients' mean, standard deviation, quartiles, and range. The following are the main conclusions:

Table 1
Statistical analysis of the dataset

Variables	Mean	Maximum	Std
C (kg/m ³)	276.5	540	103.4
SF+SL (kg/m ³)	74.27	359.4	84.25
Fly Ash(kg/m ³)	62.87	260	71.58
RCA (kg/m ³)	964.83	1145	82.79
FA (kg/m ³)	770.49	992.6	79.37
W (kg/m ³)	182.98	247	21.71
SP (kg/m ³)	6.42	32.2	5.80
Age (Days)	44.92	365	60.44
Compressive Strength (MPa)	35.84	82.60	16.10

The range, distribution, and central tendencies of the input ingredients as well as the output Compressive Strength are clarified by these statistical findings, which offer a thorough picture of the dataset. They provide the foundation for more research, the creation of models, and the improvement of high-performance concrete mixes.

B. Data Preprocessing

The raw data in the database was prepared for analysis and model building using a series of steps known as data preparation in machine learning (ML), which includes data cleaning, feature selection, and data normalization when required. The predictors considered for the model included amounts of cement (C), silica fume (SF), slag (SL), fly ash (FA), water (W), natural fine aggregate (NFA), and superplasticizer (SP) in addition to cement grade (CG), recycled coarse aggregate ratio (RAR), recycled aggregate water absorption

(RWA), and testing age (TA). It should be noted that sophisticated machine learning approaches have the ability to capture intricate, non-linear correlations between the CS and the chosen inputs, which could result in predictions that are more accurate. To enhance ANN performance, the data was adjusted to a [0, 1] range. In order to handle missing variables, we employed k-nearest neighbors (k-NN) imputation. Seventy percent of the dataset was then used for training, fifteen percent for validation, and fifteen percent for testing.

C. ANN Model Development

There are several varieties of deep learning neural networks, and the ANN is a popular method that has been used extensively to create prediction models across a range of industries. Because ANN is widely used and simple to use, it is used in this study. In particular, a modified and optimized version of ANN that is frequently used in practice is the Backpropagation Neural Network (BPNN). The Tensor Flow framework in Python was used to create a feed forward back propagation neural network. The structure was made up of:

- *Input layer:* 7 neurons (input variables)
- *Two hidden layers:* 20 and 10 neurons respectively, with ReLU activation
- *Output layer:* 1 neuron (compressive strength), with linear activation

The network was trained using the Adam optimizer with a mean squared error loss function.

In the initial phase, every input neuron receives an input that indicates the percentage of ingredients and sends a prediction to the buried layer neurons based on Eq. (1). To provide non-linearity to the fitting process, an activation function is applied at the output neuron and each hidden layer. Differentiability is crucial for this activation function. The input for the activation function is thought to be the output of the input neurons. The output is calculated and sent forward as input to either the output layer neurons or the subsequent hidden layer neurons, depending on the selected activation function, following Eq. (2).

$$y_j = \sum_{i=1}^n (w_{ij} \cdot x_i) + b_j \quad (1)$$

The input and output of the j th neuron are denoted by x_i and y_j , the weight (connection) between the i th and j th neuron by w_{ij} , the bias parameter for the j th neuron by b_j is the number of neurons.

The error is computed by comparing the output neuron's prediction with the actual value after it has been generated. This calculation of error aids in evaluating the model's correctness.

$$A_j = (y_j) \quad (2)$$

In this case, y_j represents the activation function's input that was obtained from Eq. 1.

To reduce the error, the estimated error is transmitted backward in the second stage. Each neuron's weight and bias are tuned during this procedure. The MSE provided in Eq. 3 is used to assess the error in BPNN.

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (3)$$

The mean squared error is represented by MSE , the total number of samples is represented by n , the actual output is represented by y_i , and the predicted output of the model is represented by \hat{y}_i .

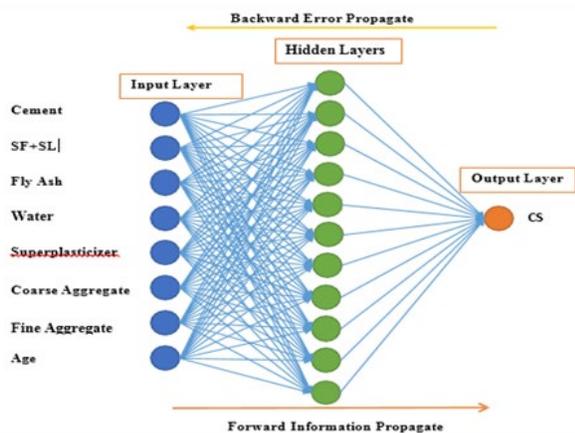


Fig. 1. Architecture of ANN adopted

D. Optimization Algorithm

After training, combinations of input variables were investigated using a grid search method under realistic limitations. Reducing the cement content while keeping the compressive strength over 40 MPa was the aim. The method of Artificial Neural Networks (ANN) Artificial neural networks (ANNs) are made up of interconnected neurons arranged in layers, such as input, hidden, and output layers. Data is received by the input layer, processed by hidden layers, and predictions are made by the output layer. Through forward and backward operations (forward propagation and backpropagation), the network modifies its weights and biases throughout training in order to identify patterns in the data (Hong, 2023). The following is how the output is predicted in the forward process.

4. Results and Discussion

A. Model Performance

The ANN model employed in this study was found to predict compressive strength with a high degree of accuracy:

- R^2 (test set): 0.95
- RMSE: 2.45 MPa
- MAE: 1.75 MPa

This demonstrates a robust relationship between expected and actual strengths, confirming the efficacy of the ANN.

B. Optimization Results

Several mix designs with high fly ash and slag concentration (up to 50% cement substitution) that produced compressive strengths > 35 MPa with 20–30% less cement were found throughout the optimization phase. In keeping with environmental goals, these blends also decreased heat of hydration and enhanced workability.

The output optimized mix is given below:

- Cement: 280 kg/m³
- Fly Ash: 60 kg/m³
- Water-to-binder ratio: 0.40
- Coarse Aggregate: 960 kg/m³
- Recycled Aggregate: 300 kg/m³
- Fine Aggregate: 700 kg/m³
- Superplasticizer: 1.0% by binder weight
- Predicted 28-day strength: 37.5 MPa

C. Discussion

Generally speaking, as compressive strength improves, so does the amount of SCMs added to the best RAC blends. Interestingly, fly ash is used more often than the other SCMs since it is less expensive and emits less CO₂ per unit. Slag and silica fume consumption increases in tandem with increased compressive strength due to their strong latent hydraulic and pozzolanic reactivity, which significantly influences the achievement of higher compressive strength. The rate of growth sharpens as the amount of binder gradually rises until it exceeds 57 MPa. There is a discernible rise in cement consumption over 60 MPa compressive strength, indicating that more cement is being utilized for hydration to achieve higher compressive strength values. On the other hand, because cement contributes significantly to CO₂ emissions and costs, the optimization algorithm aims to reduce its content for lower compressive strengths. With regard to compressive strength, there is no obvious trend in the water content, which varies between 110 and 200 kg/m³. This pattern demonstrates that the optimization algorithm tries to reduce the super-plasticizer content due to its high cost and maintains the water content within this range despite its detrimental effect on compressive strength. Up until it reaches roughly 62 MPa, the amount of recycled coarse aggregate gradually declines before dropping off suddenly. This design highlights the significance of employing natural coarse aggregate to strengthen the connection with mortar and produce a robust interfacial transition zone, particularly at higher compressive strengths.

In general, the amount of natural fine aggregate grows along with compressive strength. At higher compressive strengths, this pattern is linked to a greater natural fine aggregate contribution to the packing density of RAC. By helping to fill in the spaces between bigger aggregate particles, this increased packing density improves load transfer and interlocking within the concrete matrix. The use of superplasticizer is still restricted for compressive strengths lower than 47 MPa. The usage of super-plasticizer steadily rises between around 47 MPa and 58 MPa. After about 58 MPa, a noticeable jump is subsequently seen, emphasizing the necessity of increased superplasticizer dosages for reaching higher compressive strengths as well as improved workability and flow characteristics.

The ANN model successfully learned the complex linkages in the dataset and provided feasible sustainable mix options. Nonetheless, the model's performance is greatly influenced by the quality and representativeness of the training data. Before extrapolating outside of the dataset, more validation could be required.

5. Conclusion

The feasibility of using artificial neural networks to optimize sustainable concrete mix designs is demonstrated in this study. ANN models can lessen the need for trial-and-error techniques and greatly aid in achieving environmental goals in construction by precisely forecasting compressive strength and investigating different binder combinations. For this inquiry, a comprehensive database on the compressive strength (CS) of recycled aggregate concrete (RAC) with supplemental cementitious materials (SCMs) must be constructed. The database was derived from 60 peer-reviewed articles. We employed machine learning (ML) techniques, such as Artificial Neural Networks (ANN), to model the CS of RAC. Our study's independent variables included the amounts of cement, fly ash, slag, fly ash, water, natural fine aggregate, and superplasticizer; the ratio of recycled aggregate to water absorption; and the testing age.

These were linked to the CS of RAC, our dependent variable, and other different ML models by achieving an R-squared value greater than 0.95. Furthermore, employing these models in the stacking model construction process greatly improved the accuracy of CS predictions. However, it was demonstrated that the cement content and the concrete's age were the two most significant parameters affecting the CS of RAC. The cement grade, water content, and natural fine aggregate content came next, with minor variations. As CS increased, so did the fraction of SCMs in ideal RAC compositions. Due to its lower cost and CO₂ emissions per unit, fly ash was utilized most often. However, because of its strong pozzolanic reactivity, slag and silica fume were also employed more frequently as CS rose. In order to maximize compressive strength while reducing environmental effect, this research explores how artificial neural networks (ANNs) might be used to optimize mix designs for sustainable concrete.

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