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THE ROLE OF ARTIFICIAL INTELLIGENCE IN OPTIMIZATION AND PREDICTION OF CEMENT CONCRETE PROPERTIES

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Abstract

The integration of artificial intelligence (AI) into concrete technology represents a paradigm shift in construction materials engineering, enabling unprecedented capabilities in property prediction, mix optimization, and quality control. This comprehensive literature review synthesizes recent empirical and theoretical evidence on the application of AI techniques, including machine learning algorithms, neural networks, metaheuristic optimization, response surface methodology, and hybrid models, for predicting and optimizing the mechanical and durability properties of cement concrete. The analysis reveals that AI-based models consistently outperform traditional regression models in prediction accuracy, with hybrid approaches demonstrating superior performance through the synergistic combination of multiple algorithms. Statistical design methods including Scheffe's simplex lattice, Box-Behnken design, and central composite design have enabled efficient mix optimization with significantly reduced experimental runs. The integration of AI with waste-derived materials and supplementary cementitious materials has further advanced sustainable concrete production, enabling precise prediction of performance characteristics of alternative binders including geopolymers, recycled aggregates, and industrial by-products. However, challenges persist including model interpretability, data quality requirements, generalization across diverse material compositions, and computational complexity. This review identifies critical gaps in real-time quality control applications, lifecycle prediction models, standardized benchmarking frameworks, and multi-objective optimization approaches balancing performance, economics, and sustainability, providing actionable recommendations for researchers, practitioners, and policymakers.

Keywords: *Artificial intelligence, concrete properties, machine learning, compressive strength prediction, mix optimization, sustainable concrete, metaheuristic optimization*

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Introduction

Cement concrete remains the most widely used construction material globally, with annual production exceeding 30 billion tonnes. The performance of concrete structures depends critically on the complex interplay of constituent materials, including cement, aggregates, water, and admixtures, and the resulting mechanical and durability properties (Tiza et al., 2024a; Utsev et al., 2022; Okagbare et al., 2026). Traditional approaches to concrete mix design rely on empirical relationships, trial batching, and statistical regression models that often fail to capture the nonlinear interactions among constituent materials, leading to suboptimal performance and resource inefficiency (Agunwamba et al., 2024a; Tiza et al., 2025a).

The emergence of artificial intelligence (AI) and machine learning (ML) techniques has revolutionized concrete technology by enabling the development of predictive models that capture complex material behavior with unprecedented accuracy. AI-based approaches can identify hidden patterns in experimental data, optimize mix proportions for multiple performance criteria simultaneously, and predict long-term property evolution under various environmental conditions (Singh et al., 2025a). These capabilities are particularly valuable given the increasing complexity of concrete mixtures incorporating supplementary cementitious materials, recycled aggregates, and functional nanomaterials (Nsobundu & Tiza, 2025).

The application of AI in concrete technology has accelerated substantially in recent years, as evidenced by the proliferation of studies employing machine learning models for property prediction and optimization. Hafez et al. (2023) developed a data-driven optimization tool for blended cement concrete incorporating supplementary cementitious materials, demonstrating that AI-based approaches can simultaneously optimize functional, economic, and environmental performance criteria. Similarly, Parhi et al. (2024) applied metaheuristic optimization of machine learning models for strength prediction of high-performance self-compacting alkali-activated slag concrete, achieving superior prediction accuracy compared to conventional methods.

The significance of AI applications in concrete technology is further underscored by the growing emphasis on sustainability in the construction sector. As the industry seeks to reduce its environmental footprint through the utilization of waste-derived materials and supplementary cementitious materials, the ability to accurately predict the behavior of these alternative mixtures becomes essential (Nsobundu & Tiza, 2025; Okagbare et al., 2026). Bheel et al. (2024) demonstrated the application of response surface modeling for optimizing concrete incorporating human hair fiber and millet husk ash, while Maaze et al. (2025) employed central composite design for predicting alkaline ratios in waste cement concrete-based geopolymer.

Evolution of Modeling Approaches in Concrete Technology

Traditional Statistical and Empirical Models

The development of predictive models for concrete properties has evolved through several methodological generations. Early approaches relied on empirical relationships derived from extensive experimental databases, such as Abrams' law relating water-cement ratio to compressive strength and Bolomey's formula for mix design. While these models provided practical guidance, their limited scope and inability to capture nonlinear interactions constrained their accuracy for complex mixtures. Agunwamba et al. (2024a) applied Scheffe's simplex lattice model for concrete mixture design and performance enhancement, demonstrating that statistical mixture design approaches enable systematic exploration of the composition-property relationship. The Scheffe's

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simplex lattice model, represented in Equation (1), allows for the prediction of response variables based on mixture component proportions.

1. Scheffé's Simplex Lattice Model (Equation 1)

$$Y = \sum_{i=1}^{q} \beta_i X_i + \sum_{i<j}^{q} \beta_{ij} X_i X_j$$

Definitions:

- **Y:** Predicted response (e.g., compressive strength of concrete at 28 days).
- **X_i:** Proportion of the i^{th}component in the mixture (cement, water, sand, aggregate, admixtures, etc.), satisfying:

$$\sum_{i=1}^{q} X_i = 1$$

β_i: Linear effect of component $i$on the response. Measures the change in $Y$when only $X_i$changes.

- **β_{ij}:** Interaction effect between components $i$and j. Captures combined effects beyond individual contributions.
- **q:** Total number of mixture components.

Key Features:

- Designed specifically for mixture experiments where the sum of components is constrained to 1 (100%).
- Useful for predicting concrete properties while minimizing the number of experimental trials.
- Example application: Agunwamba et al. (2024a) used this model to predict compressive strength efficiently.

2. Box-Behnken Design Quadratic Model (Equation 2)

$$Y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}^{k} \beta_{ij} x_i x_j + \varepsilon$$

Definitions:

Y: Predicted response (e.g., compressive strength).
x_i: Coded independent variable i(values usually normalized for RSM).
β_0: Intercept coefficient.
β_i: Linear coefficient for variable i.
β_{ii}: Quadratic coefficient for variable i. Captures curvature effects.
β_{ij}: Interaction coefficient between variables $i$and j.
k: Number of independent variables.
ε: Random error term.

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The Box-Behnken design is a widely used approach within Response Surface Methodology (RSM) that efficiently captures linear, interaction, and quadratic effects of multiple variables. By strategically selecting experimental points, it allows researchers to explore the combined influence of several factors on a response without the need to test all possible combinations, thereby reducing the number of experiments required. This approach has been effectively applied in concrete technology; for example, Tiza et al. (2025a) employed the Box-Behnken design to optimize the compressive strength of cement concrete, demonstrating its ability to provide reliable predictions while minimizing experimental effort. Agunwamba et al. (2024b) conducted an appraisal of statistical and probabilistic models in highway pavements, highlighting the evolution from deterministic empirical models to probabilistic approaches that account for variability in material properties and construction conditions. The authors noted that while traditional regression models have served the industry well, their limitations in handling complex nonlinear relationships have motivated the adoption of AI-based approaches.

Nguyen et al. (2023) employed dense packing theory combined with response surface methodology to optimize the engineering properties of cement concrete containing gravel and waste rock. Their approach, represented by the modified Fuller's equation shown in Equation (3), enabled efficient optimization of particle packing for enhanced concrete performance.

Equation (3): Modified Fuller's Equation for Dense Packing

The Modified Fuller's Equation is commonly used to achieve dense particle packing in concrete aggregates. It is expressed as:

$$P(d) = \left(\frac{d}{D_{\max}}\right)^{n}$$

where $P(d)$represents the cumulative percentage of aggregate passing a sieve of size d, $D_{\max}$is the maximum particle size in the aggregate, and $n$is the distribution modulus, typically ranging from 0.45 to 0.50 for dense packing. This equation helps engineers design aggregate gradations that maximize packing density, reduce voids, and improve the overall workability and strength of concrete.

Statistical Design of Experiments

Statistical design of experiments has emerged as a powerful tool for efficient exploration of concrete mixture properties. Central composite design (CCD), a response surface methodology approach, enables estimation of quadratic effects and interaction terms with fewer experimental runs than full factorial designs. Maaze et al. (2025) employed central composite design for predicting alkaline ratios in waste cement concrete-based geopolymer, demonstrating the effectiveness of this approach for optimizing geopolymer synthesis conditions. The central composite design model structure is presented in Equation (4).

Equation (4): Central Composite Design Model

$$Y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}^{k} \beta_{ij} x_i x_j$$

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The CCD approach enables the estimation of response surfaces with a relatively small number of experimental runs, making it particularly valuable for optimizing complex material systems with multiple variables. Ganasen et al. (2023) applied regression-based machine learning approaches for predicting the properties of raw rice husk concrete bricks, demonstrating that response surface methodology combined with machine learning can effectively model the behavior of sustainable construction materials. The authors compared multiple regression techniques, establishing that ensemble methods achieved superior prediction accuracy.

Machine Learning Algorithms for Concrete Property Prediction

Artificial Neural Networks

Artificial Neural Networks (ANNs) represent one of the most widely applied AI techniques in concrete technology. ANNs consist of interconnected layers of nodes (neurons) that process input information and learn patterns through iterative adjustment of connection weights. The general structure of an ANN can be represented by Equation (5).

Equation (5): Artificial Neural Network Forward Propagation

In an artificial neural network, the output of neuron j is given by

$$y_j = f\left(\sum_{i=1}^{n} w_{ij}\, x_i + b_j\right)$$

where x_i represents the input from neuron i, w_{ij} is the weight connecting neuron i to neuron j, and b_j is the bias term for neuron j. The function $f(\cdot)$ is an activation function, such as sigmoid, ReLU, or tanh, which introduces non-linearity and allows the network to model complex relationships. This equation essentially computes a weighted sum of inputs, adjusts it with a bias, and then transforms it via the activation function to produce the neuron's output, forming the building block of neural network computations. Siddiq et al. (2025) applied a hybrid Taguchi–Grey–ANN approach for AI-driven optimization of fly ash-based geopolymer concrete for sustainable high strength and CO_2 reduction. The Taguchi method was employed for experimental design, while Grey relational analysis enabled multi-objective optimization, and ANN provided predictive modeling capabilities.

Parhi et al. (2024) developed metaheuristic optimization of machine learning models for strength prediction of high-performance self-compacting alkali-activated slag concrete. The study compared multiple ANN architectures optimized using metaheuristic algorithms, demonstrating that the hybrid approach significantly improved prediction accuracy compared to conventional ANN models.

Table 1. *Artificial Neural Network Architectures for Concrete Property Prediction*

Network Type	Architecture	Applications	Advantages
Feedforward Neural Network	Input-hidden-output layers	Compressive strength, workability	Simple architecture; fast training

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Backpropagation Neural Network	Multiple hidden layers with error backpropagation	Strength prediction; durability	Captures complex patterns
Radial Basis Function Network	RBF hidden layer with linear output	Non-linear function approximation	Good interpolation capabilities
Deep Neural Network	Multiple hidden layers (≥3)	High-dimensional data; complex relationships	High accuracy; feature learning
Convolutional Neural Network	Convolution and pooling layers	Microstructure analysis; image-based prediction	Spatial feature extraction

Support Vector Machines and Kernel Methods

Support Vector Machines (SVMs) have been applied to concrete property prediction with demonstrated success. The ability of SVMs to handle high-dimensional data and avoid overfitting through regularization makes them valuable for modeling concrete properties from limited experimental data. The SVM regression model is expressed in Equation (6).

Equation (6): Support Vector Regression

$f(x)$ =In Support Vector Machine (SVM) regression, the predicted output for a given input $x$is expressed as,

$$y = \sum_{i=1}^{n} (\alpha_i - \alpha_i^*) K(x_i, x) + b$$

where $\alpha_i$and $\alpha_i^*$are Lagrange multipliers obtained during model training, $K(x_i, x)$is a kernel function that maps input data into a higher-dimensional space, $b$is the bias term, and $n$is the number of support vectors. Common kernel functions used in concrete technology applications include the linear kernel $K(x_i, x_j) = x_i^T x_j$, the polynomial kernel $K(x_i, x_j) = (x_i^T x_j + r)^d$, and the radial basis function (RBF) kernel $K(x_i, x_j) = \exp(-\gamma \parallel x_i - x_j \parallel^2)$. By using these kernels, SVM models can capture linear and non-linear relationships between input variables, such as mix proportions or curing conditions, and output properties like compressive strength, making them highly effective for predictive modeling in concrete mix optimization.

Khan et al. (2024) developed predictive modeling for compressive strength of blended cement concrete using hybrid machine learning models, demonstrating that SVM combined with optimization algorithms achieved superior prediction accuracy compared to standalone models. The hybrid approach integrated feature selection and hyperparameter optimization to enhance model performance.

Ensemble Methods

Ensemble methods, including random forests, gradient boosting machines, and extreme gradient boosting (XGBoost), combine multiple models to improve prediction accuracy and robustness. The general principle of ensemble learning is represented in Equation (7).

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Equation (7): Ensemble Prediction

In ensemble modeling, the overall predicted output $\hat{y}$is computed as a weighted combination of predictions from multiple base models. It is expressed as

$$\hat{y} = \sum_{m=1}^{M} w_m f_m(x)$$

where $f_m(x)$represents the prediction from the m^{th}base model, $w_m$is the weight assigned to that model based on its relative importance or performance, and $M$is the total number of base models in the ensemble. This approach leverages the strengths of individual models while mitigating their weaknesses, often resulting in improved predictive accuracy and robustness. In concrete technology, ensemble models can combine outputs from neural networks, SVMs, and other predictive models to more accurately estimate properties such as compressive strength or workability under varying mix conditions.

Mali et al. (2025) developed a deep learning enhanced framework for multi-objective optimization of cement-slag concrete for balancing performance, economics, and sustainability. The study employed ensemble methods to predict multiple performance indicators simultaneously, enabling comprehensive optimization of concrete mixtures. Kaveh et al. (2025) applied metaheuristic-optimized machine learning for mechanical property prediction in eco-friendly rubberized concrete. The study demonstrated that ensemble methods combined with metaheuristic optimization achieved higher prediction accuracy than single-model approaches.

Table 2. *Ensemble Methods for Concrete Property Prediction*

Ensemble Method	Mechanism	Strengths	Limitations
Random Forest	Bootstrap aggregation (bagging) of decision trees	Robust to outliers; feature importance	Less interpretable than single trees
Gradient Boosting	Sequential tree building with residual correction	High accuracy; handles nonlinearity	Computationally intensive
XGBoost	Regularized gradient boosting	Fast training; handles missing data	Parameter tuning required
AdaBoost	Adaptive boosting with weighted samples	Simple implementation; interpretable	Sensitive to noisy data
Stacking	Meta-learner combining multiple models	Leverages strengths of diverse models	Increased complexity

Deep Learning Approaches

Deep learning models, characterized by multiple hidden layers, have demonstrated superior performance for complex prediction tasks in concrete technology. Gazi et al. (2025) developed machine learning models for predicting and classifying tensile strength of concrete, employing deep neural networks to capture complex relationships between mixture composition and mechanical properties. The forward propagation through a deep neural network with L layers can be represented recursively by Equation (8).

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WIJSITAR Volume 1 Number 1, 2025
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Equation (8): Deep Neural Network Forward Propagation

In a multi-layer neural network, the output of each hidden layer is computed by applying an activation function to a linear combination of inputs and layer-specific weights and biases. For the first hidden layer, this is expressed as

$\mathbf{h}^{(1)} = \sigma\left(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}\right)$ and for subsequent hidden layers $l = 2, \dots, L-1$, the activations are
$\mathbf{h}^{(l)} = \sigma(\mathbf{W}^{(l)}\mathbf{h}^{(l-1)} + \mathbf{b}^{(l)})$

where $\mathbf{h}^{(l)}$is the activation vector of layer l, $\mathbf{W}^{(l)}$and $\mathbf{b}^{(l)}$are the weight matrix and bias vector for that layer, respectively, and $\sigma(\cdot)$is the activation function such as ReLU, sigmoid, or tanh. The final output prediction $\hat{y}$is obtained by applying the last layer weights and biases to the final hidden layer activations:
$\hat{y} = \mathbf{W}^{(L)}\mathbf{h}^{(L-1)} + \mathbf{b}^{(L)}$

This framework allows the network to learn complex, non-linear relationships between input variables, such as concrete mix proportions or curing conditions—and target outputs like compressive strength or durability, making deep neural networks highly effective for predictive modeling in concrete technology. Deif et al. (2025) explored optimizing concrete mix designs with synthetic data generation and machine learning prediction models, demonstrating that deep learning approaches combined with data augmentation techniques can overcome limitations associated with small experimental datasets.

Hybrid and Metaheuristic Optimization Models

Genetic Algorithm-Based Optimization

Genetic Algorithms (GAs) are metaheuristic optimization techniques inspired by natural selection processes. GAs have been widely combined with machine learning models for optimizing concrete mixtures. The general structure of a genetic algorithm is presented in Equation (9).

Equation (9): Genetic Algorithm Representation

In genetic algorithm (GA)-based optimization, a potential solution is represented as a chromosome $\mathbf{x} = \{x_1, x_2, \dots, x_n\}$, where each $x_i$is an individual gene corresponding to a design variable. The quality or suitability of a chromosome is evaluated using a fitness function defined as,

$$F(\mathbf{x}) = \sum_{i=1}^{m} w_i f_i(\mathbf{x})$$

where $f_i(\mathbf{x})$represents the i^{th}objective function, $w_i$is the weight assigned to that objective, and $m$is the total number of objectives considered. By combining multiple objectives into a single weighted fitness value, the genetic algorithm can iteratively evolve the population of chromosomes toward optimal solutions. In the context of concrete mix design, $\mathbf{x}$could represent proportions of cement, water, aggregates, and admixtures, while the objectives $f_i(\mathbf{x})$might include maximizing

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compressive strength, minimizing cost, or improving workability, allowing simultaneous optimization of multiple performance criteria.

Lee and Wong (2023) applied multi-objective Taguchi optimization of cement concrete incorporating recycled mixed plastic fine aggregate using modified Fuller's equation. The Taguchi method was employed for experimental design, while genetic algorithm optimization enabled simultaneous optimization of multiple performance criteria. Mandal et al. (2024) studied the use of different machine learning techniques for prediction of concrete properties from their mixture proportions with deterministic and robust optimization. The study employed genetic algorithm optimization to identify optimal mixture proportions that satisfy multiple performance constraints simultaneously.

Particle Swarm Optimization

Particle Swarm Optimization (PSO) is a population-based metaheuristic inspired by social behavior of bird flocks. The velocity and position update equations for PSO are presented in Equations (10) and (11).

In Particle Swarm Optimization (PSO), each particle represents a candidate solution that "flies" through the search space by updating its velocity and position iteratively. The velocity of particle $i$at iteration $t+1$is updated according to

$$v_i^{(t+1)} = wv_i^{(t)} + c_1r_1(p_{best,i} - x_i^{(t)}) + c_2r_2(g_{best} - x_i^{(t)})$$

where $v_i^{(t)}$is the current velocity, $w$is the inertia weight controlling the influence of the previous velocity, $c_1$and $c_2$are cognitive and social acceleration coefficients guiding the particle toward its personal best $p_{best,i}$and the global best g_{best}, respectively, and $r_1, r_2$are random numbers in [0,1] that introduce stochastic behavior. The particle's position is then updated as

$$x_i^{(t+1)} = x_i^{(t)} + v_i^{(t+1)}$$

allowing it to move through the solution space. In concrete mix optimization, each particle can represent a set of mixture proportions, and the PSO algorithm iteratively adjusts these to maximize properties such as compressive strength or durability while satisfying constraints, efficiently searching for optimal or near-optimal mix designs.

Farouk et al. (2025) applied machine learning and swarm intelligence approaches for optimizing ultra-high-performance concrete with recycled fine and CO_2 reduction strategies. The study demonstrated that PSO-optimized machine learning models achieved superior prediction accuracy compared to standalone approaches.

Grey Wolf Optimization

Grey Wolf Optimization (GWO) is a metaheuristic algorithm inspired by the hunting behavior of grey wolves. Mei et al. (2026) developed a machine learning-driven multi-objective optimization model for enhancing the mechanical properties of silica fume-modified magnesium phosphate cement concrete, employing GWO for hyperparameter optimization.

The hierarchical structure of grey wolf optimization is represented in Equation (12).

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WIJSITAR Volume 1 Number 1, 2025
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Equation (12): Grey Wolf Optimization Position Update

In the Grey Wolf Optimizer (GWO), the position of each grey wolf is updated based on the position of the prey, mimicking the social hierarchy and hunting strategy of wolves. The distance between a grey wolf and the prey is computed as

$$\mathbf{D} = \mid \mathbf{C} \cdot \mathbf{X}_p(t) - \mathbf{X}(t) \mid$$

where $\mathbf{X}_p(t)$is the prey's position vector, $\mathbf{X}(t)$is the grey wolf's current position vector, and $\mathbf{C}$is a coefficient vector that introduces randomness in the search. The grey wolf then updates its position using

$$\mathbf{X}(t+1) = \mathbf{X}_p(t) - \mathbf{A} \cdot \mathbf{D}$$

where $\mathbf{A}$is another coefficient vector controlling the step size toward the prey. This mechanism enables the wolves to balance exploration and exploitation of the search space. In concrete mix optimization, each wolf can represent a candidate mix, and the GWO algorithm iteratively adjusts the mixtures to improve target properties such as compressive strength, workability, or durability, effectively searching for optimal or near-optimal solutions.

Hybrid Optimization Frameworks

The combination of multiple optimization and machine learning techniques has emerged as a powerful approach for concrete property prediction and optimization. Hafez et al. (2023) developed a data-driven optimization tool for the functional, economic, and environmental properties of blended cement concrete using supplementary cementitious materials. The hybrid framework integrated machine learning prediction models with multi-objective optimization algorithms. Mendhe et al. (2025) developed multifunctional property predictions of nano-engineered cementitious composites for high-performance concrete structures using hybrid machine learning techniques. The hybrid approach combined multiple AI algorithms to achieve superior prediction accuracy across diverse property types.

Table 3. *Hybrid Optimization Frameworks for Concrete Mixture Design*

Framework	Components	Application	Key Findings
Taguchi-Grey-ANN	Taguchi design + Grey relational analysis + ANN	Fly ash geopolymer concrete	Improved multi-objective optimization; 15% CO_2 reduction
Metaheuristic-ML	PSO + XGBoost + Random Forest	Ultra-high-performance concrete	$R^2 > 0.95$ for strength prediction
GA-ML	Genetic algorithm + ANN	Cement-slag concrete	Balanced performance, economics, sustainability
Bayesian-ML	Bayesian inference + Gaussian process	High-fluidization cement grout	Uncertainty quantification; robust predictions
Hybrid Ensemble	Stacking + metaheuristic optimization	Rubberized concrete	Improved prediction accuracy; reduced variance

Optimization of Sustainable Concrete Mixtures

Recycled and Waste-Derived Materials

The utilization of recycled and waste-derived materials in concrete has gained significant attention due to sustainability imperatives. Tiza et al. (2024a) conducted energy dispersive X-ray fluorescence (EDXRF) oxide composition analysis of coarse aggregates and reclaimed asphalt pavement (RAP) as construction materials, providing fundamental data for modeling the behavior of RAP-containing concrete. Alwathaf et al. (2024) investigated the enhancement and optimization of mechanical properties in cement concrete with recycled asphalt pavement (RAP). The study demonstrated that optimized RAP incorporation can achieve satisfactory mechanical performance while reducing environmental impact. Ghazy et al. (2021) examined the characteristics and optimization of cement concrete mixes with recycled asphalt pavement aggregates. The study employed response surface methodology to optimize RAP content and establish relationships between mixture variables and mechanical properties.

Table 4. *Optimization of Sustainable Concrete Incorporating Recycled Materials*

Recycled Material	Optimization Method	Key Parameters	Optimal Content	Performance Outcome
Reclaimed Asphalt Pavement	Scheffe's simplex lattice	RAP content; cement content; water-cement ratio	20–30%	15–20% strength reduction; 25% cost reduction
Recycled Mixed Plastic	Multi-objective Taguchi	Plastic content; particle size; Fuller's modulus	10–15%	12% strength reduction; improved ductility
Waste Rock	Dense packing + RSM	Gradation; packing density; cement content	30–40% of coarse aggregate	Enhanced packing; 10% strength improvement
Human Hair Fiber + Millet Husk Ash	Response surface methodology	Fiber content; ash content; water-cement ratio	1% fiber; 10% ash	22% flexural strength improvement
Textile Sludge + Glass Powder	Machine learning optimization	Sludge content; glass powder content; curing time	15% sludge; 20% glass powder	18% strength improvement; reduced embodied carbon
Biomedical Waste Ash	Machine learning optimization	Ash content; binder composition; curing conditions	5–10% replacement	8% strength reduction; 15% CO_2 reduction

Geopolymer and Alkali-Activated Materials

Geopolymer concrete, produced through alkali activation of aluminosilicate precursors, represents a sustainable alternative to ordinary Portland cement concrete. Maaze et al. (2025) conducted economic-environmental and multi-criteria optimization for predicting alkaline ratios in waste cement concrete-based geopolymer using central composite design.

Equation (13): Geopolymer Compressive Strength Prediction Model

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The compressive strength of geopolymer concrete can be empirically estimated using the relationship

$$f_c = \alpha \cdot \left(\frac{SiO_2}{Al_2O_3}\right)^{\beta} \cdot \left(\frac{Na_2O}{SiO_2}\right)^{\gamma} \cdot \left(\frac{H_2O}{Na_2O}\right)^{\delta}$$

where f_c is the compressive strength, and $\alpha, \beta, \gamma, \delta$ are empirical constants determined from experimental data. The ratios SiO_2/Al_2O_3, Na_2O/SiO_2, and H_2O/Na_2O represent the silica-to-alumina, alkali-to-silica, and water-to-alkali ratios, respectively, which strongly influence the geopolymerization reaction and resulting mechanical properties. This model allows engineers to predict the strength of geopolymer concrete based on the chemical composition of the binder and activator solution, providing a valuable tool for mix design and optimization.

Dhawan and Verma (2025) conducted optimization of geopolymer concrete mix design using machine learning for enhanced sulphate and chloride resistance. The study employed machine learning models to predict durability properties, enabling the development of geopolymer mixtures with superior resistance to aggressive environments.

Parhi et al. (2024) developed metaheuristic optimization of machine learning models for strength prediction of high-performance self-compacting alkali-activated slag concrete, demonstrating that optimized mixtures achieved both high strength and excellent workability.

Supplementary Cementitious Materials

The incorporation of supplementary cementitious materials (SCMs) such as fly ash, slag, silica fume, and calcined clay has become standard practice for enhancing concrete sustainability and performance. Hafez et al. (2023) developed a data-driven optimization tool for blended cement concrete using supplementary cementitious materials, enabling simultaneous optimization of functional, economic, and environmental properties.

Equation (14): Multi-Criteria Optimization Function for SCM Concrete

In sustainable concrete mix design, a common approach is to formulate a weighted multi-objective function that simultaneously considers cost, environmental impact, and performance. This can be expressed as

$$\text{Minimize } F = w_1 \cdot \frac{C}{C_0} + w_2 \cdot \frac{E}{E_0} - w_3 \cdot \frac{S}{S_0}$$

where C is the cost of the concrete mixture, E is the embodied carbon, and S is the compressive strength. The parameters C_0, E_0, S_0 are reference values for normalization, and w_1, w_2, w_3 are weighting factors assigned to each objective such that their sum equals 1. By minimizing F, the optimization process seeks concrete mixtures that reduce cost and environmental impact while maximizing strength. This formulation is particularly useful in integrating sustainability considerations into concrete mix optimization using metaheuristic or AI-based algorithms. Naukhez et al. (2025) optimized ultra-high performance concrete with coarse aggregate for enhanced sustainability, employing a comprehensive assessment of slump flow and mechanical

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properties. The study demonstrated that AI-based optimization can achieve ultra-high performance concrete with reduced cement content and improved sustainability metrics.

Multi-Objective Optimization Frameworks

Performance-Economics-Sustainability Optimization

The simultaneous optimization of multiple conflicting objectives—performance, economics, and sustainability, represents a critical challenge in concrete mixture design. Mali et al. (2025) developed a deep learning enhanced framework for multi-objective optimization of cement-slag concrete for balancing performance, economics, and sustainability.

Equation (15): Multi-Objective Optimization Formulation

In multi-objective concrete mix optimization, the design problem can be formulated as minimizing a vector of objectives

$$\mathbf{F}(\mathbf{x}) = [f_1(\mathbf{x}), f_2(\mathbf{x}), f_3(\mathbf{x})]$$

where $f_1(\mathbf{x})$represents the cost of the mixture, $f_2(\mathbf{x})$represents the environmental impact (e.g., embodied carbon), and $f_3(\mathbf{x})$represents performance metrics such as compressive strength. The optimization is subject to inequality constraints $g_j(\mathbf{x}) \leq 0$for $j = 1, \dots, m$, equality constraints $h_k(\mathbf{x}) = 0$for $k = 1, \dots, p$, and bound constraints $\mathbf{x}_L \leq \mathbf{x} \leq \mathbf{x}_U$, where $\mathbf{x}$is the vector of design variables, such as proportions of cement, water, aggregates, and admixtures. This formulation allows simultaneous consideration of multiple objectives while ensuring feasibility with respect to material, structural, and sustainability constraints, making it suitable for advanced optimization using metaheuristic algorithms, AI models, or hybrid approaches.Siddiq et al. (2025) applied the hybrid Taguchi–Grey–ANN approach for AI-driven optimization of fly ash-based geopolymer concrete, demonstrating that the multi-objective optimization framework effectively balanced strength, cost, and CO_2 reduction objectives.

Pareto Frontier Analysis

Pareto frontier analysis enables visualization of trade-offs between competing objectives, allowing designers to select optimal solutions based on project-specific priorities. The concept of Pareto dominance is defined in Equation (16).

Equation (16): Pareto Dominance Definition

In multi-objective optimization, a solution $\mathbf{x}^{(1)}$is said to dominate another solution $\mathbf{x}^{(2)}$if it is no worse in all objectives and strictly better in at least one objective. Formally, $\mathbf{x}^{(1)}$dominates $\mathbf{x}^{(2)}$if

1. $f_i(\mathbf{x}^{(1)}) \leq f_i(\mathbf{x}^{(2)})$for all objectives i, and
2. $f_j(\mathbf{x}^{(1)}) < f_j(\mathbf{x}^{(2)})$for at least one objective j.

This concept underpins Pareto-based optimization, where the goal is to identify a set of non-dominated solutions, known as the Pareto front, representing trade-offs among competing objectives. In concrete mix optimization, dominance allows selection of mixtures that simultaneously balance cost, environmental impact, and performance without strictly prioritizing

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a single objective. Hafez et al. (2023) employed Pareto frontier analysis to visualize the trade-offs between cost, embodied carbon, and compressive strength for blended cement concrete mixtures, enabling identification of optimal mixtures across the performance spectrum.

Table 5. *Multi-Objective Optimization Studies for Concrete Mixtures*

Objectives	Optimization Method	Pareto Front Size	Key Trade-offs
Cost, CO_2, Strength	Genetic algorithm + ANN	15–25 solutions	Cost vs. CO_2; 5–10% trade-off
Workability, Strength	Taguchi-Grey-ANN	8–12 solutions	Workability vs. strength; 8% trade-off
Cost, Durability, Strength	NSGA-II + machine learning	20–30 solutions	Durability vs. cost; 12% trade-off
Strength, Slump, Carbon	Central composite design	10–15 solutions	Slump vs. carbon; 5% trade-off
Flexural Strength, Cost	Multi-objective Taguchi	6–10 solutions	Flexural vs. cost; 7% trade-off

Uncertainty Quantification and Robust Optimization

Bayesian Methods for Uncertainty Quantification

Uncertainty quantification is essential for reliable prediction and optimization of concrete properties, given the inherent variability in constituent materials and construction processes. Ren et al. (2022) developed an uncertainty-based performance prediction and optimization approach for high-fluidization cement grouting material using machine learning and Bayesian inference.

Equation (17): Bayesian Inference Framework

Bayes' theorem provides a framework for updating the probability of model parameters θbased on observed data D. It is expressed as

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)}$$

where $P(\theta \mid D)$is the posterior probability of the parameters given the data, $P(D \mid \theta)$is the likelihood of observing the data given specific parameter values, $P(\theta)$is the prior probability reflecting existing knowledge about the parameters, and $P(D)$is the marginal likelihood or evidence, which normalizes the posterior distribution. In concrete technology, Bayesian approaches can be applied to estimate uncertain parameters in mix design models, machine learning predictions, or durability assessments, allowing integration of prior knowledge with experimental data to improve predictive reliability and quantify uncertainty. Gaussian process regression (GPR) has emerged as a powerful tool for uncertainty quantification in concrete property prediction. The GPR predictive distribution is expressed in Equation (18).

Equation (18): Gaussian Process Regression Predictive Distribution

WIJSITAR Volume 1 Number 1, 2025
ISSN: 3141-3765 Peer-Reviewed/Open Access/https://wijitars.fedpolywannune.edu.ng/

In Gaussian Process (GP) modeling, the prediction at a new test point $\mathbf{x}_*$is treated as a random variable with a Gaussian distribution, expressed as

$$f(\mathbf{x}_*) \sim \mathcal{N}(\mu(\mathbf{x}_*), \sigma^2(\mathbf{x}_*))$$

where $\mu(\mathbf{x}_*)$is the predictive mean, representing the model's best estimate of the output at $\mathbf{x}_*$, and $\sigma^2(\mathbf{x}_*)$is the predictive variance, quantifying the uncertainty of the prediction. This approach allows not only estimation of concrete properties, such as compressive strength or durability, but also provides a measure of confidence in the predictions, making Gaussian Processes particularly useful for surrogate modeling, optimization, and decision-making under uncertainty in concrete mix design and performance evaluation.Ren et al. (2022) demonstrated that Bayesian inference combined with Gaussian process regression enables robust prediction of grout properties with quantified uncertainty, facilitating risk-informed decision-making in concrete construction.

Robust Optimization

Robust optimization approaches account for uncertainty in material properties and processing conditions, identifying solutions that perform well across a range of possible scenarios. Mandal et al. (2024) studied the use of different machine learning techniques for prediction of concrete properties with deterministic and robust optimization.

Equation (19): Robust Optimization Formulation

In risk-averse optimization, the objective function is modified to account not only for the expected value but also for uncertainty in predictions, and is expressed as

$$\min_{\mathbf{x}} [\mu_f(\mathbf{x}) + \kappa\, \sigma_f(\mathbf{x})]$$

where $\mu_f(\mathbf{x})$is the predictive mean of the objective function, $\sigma_f(\mathbf{x})$is the standard deviation representing uncertainty, and $\kappa$is a risk-aversion parameter that balances the trade-off between expected performance and risk. By minimizing this formulation, the optimization process favors solutions that achieve good expected outcomes while reducing the probability of poor performance. In concrete mix design, this approach can be applied to models such as Gaussian Processes or other predictive frameworks to identify mixtures that are not only strong and durable but also robust under variability in material properties or environmental conditions. The robust optimization approach identifies solutions that minimize not only the expected performance but also the sensitivity to uncertainty, leading to more reliable concrete mixtures.

Comparative Performance Analysis

AI Models vs. Traditional Statistical Models

The comparative performance of AI-based models against traditional statistical approaches has been extensively evaluated in the literature. Khan et al. (2024) conducted a comprehensive comparison of hybrid machine learning models for predicting compressive strength of blended cement concrete, demonstrating that AI-based approaches consistently outperformed traditional regression models.

Equation (20): Model Performance Metrics

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WIJSITAR Volume 1 Number 1, 2025
ISSN: 3141-3765 Peer-Reviewed/Open Access/https://wijitars.fedpolywannune.edu.ng/

To evaluate the accuracy of predictive models in concrete property estimation, several statistical metrics are commonly used. The Root Mean Square Error (RMSE) measures the square root of the average squared differences between predicted and actual values:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

The Mean Absolute Error (MAE) calculates the average absolute differences between predicted and actual values:

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n} | y_i - \hat{y}_i |$$

Finally, the coefficient of determination (R^2) quantifies the proportion of variance in the actual values explained by the predictions:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

where $y_i$is the actual value, $\hat{y}_i$is the predicted value, $\bar{y}$is the mean of actual values, and $n$is the number of samples. Together, these metrics provide a comprehensive assessment of model performance, capturing both average deviations and overall goodness-of-fit in predicting concrete properties.

Table 6. *Comparative Performance of AI vs. Traditional Models for Concrete Property Prediction*

Model Type	R^2 Range	RMSE Range (MPa)	MAE Range (MPa)	Advantages	Limitations
Linear Regression	0.65–0.75	4.5–6.5	3.2–4.8	Simple; interpretable	Poor for nonlinear relationships
Response Surface	0.75–0.85	3.2–5.0	2.4–3.6	Captures quadratic effects	Limited to low-order interactions
Artificial Neural Network	0.85–0.94	1.8–3.5	1.4–2.8	Captures complex nonlinearity	Black-box; requires large datasets
Support Vector Machine	0.87–0.93	2.0–3.8	1.6–2.9	Good generalization	Parameter tuning required
Random Forest	0.88–0.95	1.6–3.2	1.3–2.5	Robust; feature importance	Computationally intensive

XGBoost	0.90–0.96	1.4–2.8	1.1–2.2	High accuracy; efficient	Overfitting with noisy data
Hybrid Models	0.92–0.98	1.0–2.2	0.8–1.8	Best overall performance	Complex; requires expertise

Performance by Property Type

The prediction accuracy of AI models varies depending on the property being predicted. Gazi et al. (2025) developed machine learning models for predicting and classifying tensile strength of concrete, achieving high accuracy for this challenging property. Similarly, Dhawan and Verma (2025) applied machine learning to predict durability properties including sulphate and chloride resistance.

Table 7. *AI Model Performance by Concrete Property Type*

Property	Best Model Type	Typical R^2	Key Influencing Variables	Challenges	References
Compressive Strength	Ensemble (XGBoost)	0.94–0.98	Cement content; w/c; curing age	High nonlinearity	Khan et al. (2024); Farouk et al. (2025)
Split Tensile Strength	Deep Neural Network	0.88–0.93	Compressive strength; aggregate type	Limited data	Gazi et al. (2025)
Flexural Strength	Hybrid (GA-ANN)	0.85–0.91	Fiber content; beam dimensions	Complex failure modes	Lee & Wong (2023)
Slump/Workability	Response Surface	0.82–0.89	Water content; admixtures	Non-linear rheology	Naukhez et al. (2025)
Durability (Chloride)	Support Vector Machine	0.86–0.92	Permeability; exposure conditions	Long-term testing	Dhawan & Verma (2025)
Carbonation Depth	Random Forest	0.83–0.90	CO_2 concentration; relative humidity	Time-dependent	Maaze et al. (2025)

Challenges and Limitations

Data Quality and Availability

The performance of AI models for concrete property prediction is critically dependent on the quality and quantity of training data. Deif et al. (2025) addressed this challenge through synthetic data generation techniques, demonstrating that data augmentation can enhance model performance when experimental data are limited. Key data-related challenges include small dataset sizes as many studies employ fewer than 100 experimental mixtures; incomplete characterization due to missing data on constituent properties; inconsistent testing protocols due to variation in

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WIJSITAR Volume 1 Number 1, 2025
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curing conditions, specimen geometry, and testing procedures; and imbalanced data due to underrepresentation of certain mixture types or property ranges.

Model Interpretability

The black-box nature of many AI models limits their acceptance in engineering practice, where mechanistic understanding is valued. Tiza et al. (2023a) noted that while neural networks achieve high prediction accuracy, their internal workings remain difficult to interpret, constraining their utility for fundamental understanding of material behavior. Efforts to enhance model interpretability include feature importance analysis (e.g., random forest variable importance); SHAP (SHapley Additive exPlanations) values for explaining individual predictions; partial dependence plots for visualizing marginal effects; and rule extraction from trained models.

Generalization Across Diverse Mixtures

The ability of AI models to generalize beyond their training data remains a significant challenge. Models trained on specific material systems may not perform well when applied to mixtures with different constituent types or proportions. Mei et al. (2026) addressed this challenge by developing machine learning-driven multi-objective optimization models that incorporated diverse training data from multiple sources, enhancing model generalization. Similarly, Mandal et al. (2024) employed robust optimization approaches to identify solutions that perform well across a range of possible scenarios.

Computational Complexity

Advanced AI models, particularly deep learning and hybrid optimization approaches, can be computationally intensive, requiring significant resources for training and optimization. Parhi et al. (2024) noted that while metaheuristic optimization of machine learning models achieves superior accuracy, the computational cost may be prohibitive for routine applications.

Looking to the Future of Research

Real-Time Quality Control

The integration of AI models with sensor technologies and Internet of Things (IoT) platforms enables real-time quality control during concrete production. Future research should focus on developing predictive models that can adjust mix proportions in real-time based on constituent material variability, ensuring consistent concrete quality.

Lifecycle Prediction Models

Extending AI models to predict long-term performance evolution under environmental exposure conditions represents a critical research need. Ren et al. (2022) developed uncertainty-based prediction models for grouting materials, but comprehensive lifecycle prediction models for structural concrete remain underdeveloped.

Standardized Benchmarking Frameworks

The development of standardized benchmarking frameworks would facilitate comparison of AI models across studies and enable identification of best practices. Potential components of such

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WIJSITAR Volume 1 Number 1, 2025
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frameworks include, standardized datasets for model training and testing, common evaluation metrics and protocols, benchmark model implementations, and performance reporting guidelines.

Multi-Scale Modeling Integration

Integrating AI-based property prediction with multi-scale modeling approaches—from molecular dynamics to continuum mechanics, offers potential for enhanced mechanistic understanding and predictive capability. Mendhe et al. (2025) explored this direction through multifunctional property predictions of nano-engineered cementitious composites, but comprehensive multi-scale frameworks remain an area for future development.

Generative Design and Optimization

The application of generative AI techniques, including Generative Adversarial Networks (GANs) and diffusion models, to concrete mixture design represents an emerging frontier. These approaches can generate novel mixture compositions optimized for multiple performance criteria, potentially discovering mixtures beyond those considered in traditional experimental designs.

Conclusion

The study examined recent empirical and theoretical evidence on the application of artificial intelligence for optimization and prediction of cement concrete properties. The synthesis of peer-reviewed academic scholarship reveals that AI-based approaches have fundamentally transformed concrete technology, enabling unprecedented capabilities in property prediction, mix optimization, and quality control. The evidence demonstrates that AI models consistently outperform traditional statistical approaches, with ensemble methods and hybrid models achieving the highest prediction accuracy. Statistical design approaches including Scheffe's simplex lattice, Box-Behnken design, and central composite design have enabled efficient mix optimization with significantly reduced experimental runs. The integration of AI with waste-derived materials and supplementary cementitious materials has advanced sustainable concrete production, enabling precise prediction of performance characteristics of alternative binders including geopolymers, recycled aggregates, and industrial by-products.

Multi-objective optimization frameworks have enabled simultaneous optimization of performance, economics, and sustainability, with Pareto frontier analysis providing valuable insights into trade-offs between competing objectives. Uncertainty quantification through Bayesian methods and robust optimization approaches has enhanced the reliability of AI-based predictions, facilitating risk-informed decision-making. However, challenges persist including model interpretability, data quality requirements, generalization across diverse material compositions, and computational complexity. Future research should focus on real-time quality control applications, lifecycle prediction models, standardized benchmarking frameworks, multi-scale modeling integration, and generative design approaches.

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WIJSITAR Volume 1 Number 1, 2025
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