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AI-Driven Mix Proportioning and Performance Prediction of Low-Cement Ultra-High-Performance Concrete

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Abstract
Ultra-high-performance concrete (UHPC) provides exceptional mechanical performance and durability; however, its high Portland cement content results in increased material consumption and embodied carbon emissions. This study proposes an artificial intelligence (AI)-driven approach for the development and optimization of low-cement UHPC by integrating experimental mix proportioning, machine learning (ML), explainable AI, and multi-objective optimization. A series of UHPC mixtures incorporating ground granulated blast-furnace slag (GGBS), silica fume, quartz sand, superplasticizer, and steel fibers was considered to investigate the influence of binder composition and mixture parameters on fresh and mechanical properties. Multiple ML algorithms, including multiple linear regression, random forest, support vector regression, artificial neural network, gradient boosting, XGBoost, LightGBM, and Extra Trees, were evaluated for compressive-strength prediction. Among the models investigated XGBoost gave the best (R^2) of 0.968, RMSE of 3.91 MPa, MAE of 2.87 MPa and MAPE of 2.19%. SHAP explainability showed that curing age, wt/wt ratio, cement content, silica fume and GGBS were the most important variables influencing compressive strength prediction. The AI-based optimization produced a low-cement UHPC mixture with about 600 kg/m^3 cement, 300 kg/m^3 GGBS and 150 kg/m^3 silica fume. The optimized mixture had 28-day compressive strength of approximately 150.6 MPa with 29.4% lower cement consumption compared to reference UHPC. Estimated embodied CO_2 emissions were reduced by approximately 28.9 % but flowability, tensile strength and flexural performance were satisfactory. The results show that ML prediction, explainable AI and optimization can provide an effective data-driven strategy for sustainable UHPC development with low cement consumption and high structural performance.

Keywords: Ultra-high-performance concrete; low-cement concrete; artificial intelligence; machine learning; XGBoost; explainable AI; SHAP; mix optimization; GGBS; silica fume; sustainable concrete; CO_2 reduction.

1. Introduction

Concrete is the dominant construction material for buildings, bridges, transport infrastructure, industrial facilities and major civil engineering systems because of its versatility, availability and ability to meet a wide range of structural requirements. High-performance cementitious materials have been developed progressively to increase strength, durability and service life potential of concrete. Among these advanced materials ultra high performance concrete (UHPC) has attracted much research and industrial attention due to very high compressive strength, enhanced tensile/flexural performance, low permeability, dense microstructure and improved durability.

The high performance of UHPC is mainly due to very dense particle packing structure, low water-to-binder ratio, granular composition optimized for performance, high-performance chemical admixtures, supplementary cementitious materials and often discontinuous fibre reinforcement. Conventional UHPC mixtures however contain much more cement and fine reactive powders than ordinary concrete (e.g., recent literature says conventional UHPC may contain 800–1100 kg/m^3 of cementitious material but its water-to-binder ratio is often < 0.25). These compositions are good in performance but have concerns about embodied carbon, material consumption, production cost and environmental sustainability.

The environmental concern is particularly significant because cement manufacture is energy-intensive and associated with substantial carbon dioxide emissions. Consequently, reducing the cement content of UHPC while maintaining the required mechanical and durability performance has become an important research

objective. Supplementary cementitious materials (SCMs), mineral fillers and industrial by-products can partially replace cement and simultaneously modify particle packing, hydration, rheological behaviour and microstructural development. A review of SCM applications in UHPC has identified materials such as slag, fly ash, limestone powder and metakaolin as important candidates for reducing the environmental burden associated with high cement consumption.

The challenge, however, is that cement reduction cannot be treated as a simple substitution problem. The performance of UHPC results from complex interactions among cement, SCMs, silica fume, fine aggregate, water, superplasticizer, fibers, curing conditions and particle-size distribution. Reducing cement excessively may adversely affect early-age hydration, matrix development and strength. Conversely, appropriately designed low-cement mixtures can benefit from improved packing and reduced cracking tendency. Research on ultra-low-cement UHPC has demonstrated that a carefully optimized particle-packing system can permit substantial clinker reduction while maintaining UHPC-level performance, although excessive clinker reduction can deteriorate compressive strength, durability and pore structure.

Therefore, the development of low-cement UHPC requires a design methodology capable of simultaneously considering numerous interacting variables. Conventional mixture-design approaches commonly rely on experimental trial-and-error, empirical relationships, particle-packing concepts or statistical mixture design. Although these approaches remain valuable, their effectiveness can decrease when numerous materials and performance constraints are introduced. A comprehensive review of UHPC mixture-design methodologies identified close-packing approaches, rheology-based methods, statistical methods and artificial neural networks as important approaches and suggested that integration of multiple methods can address the complexity of UHPC mixture design.

Artificial intelligence (AI) and machine learning (ML) offer a promising alternative because they can identify nonlinear relationships between mixture constituents and measured concrete properties. ML models can learn from experimental datasets containing cement content, SCM dosage, water content, aggregate characteristics, silica fume, chemical admixture, fiber content and curing age and can subsequently estimate performance for previously untested mixtures.

Recently, ensemble ML algorithms have been shown to be useful for UHPC strength prediction (hybrid models with PSO and ensemble algorithms were used to predict UHPC compressive strength; SHAP and partial-dependence analyses were applied to identify influential mixture parameters). Other recent studies applied XGBoost, Random Forest, LightGBM, Extra Trees and other algorithms on UHPC datasets successfully. Explainable artificial intelligence is especially important for construction materials applications.

Prediction accuracy alone is not enough for engineering decision making because engineers need to know why a model recommends one mixture over another and SHAP-based approaches give us a way to quantify the contribution of individual input variables to model predictions so that data driven predictions can be linked to materials science interpretation. UHPC research has shown previously that curing age, fiber content, silica fume, cement and superplasticizer are among important predictors of compressive strength. At the same time recent work has moved beyond simple prediction to AI-assisted optimization.

A 2026 systematic review shows an increasing use of machine learning, deep learning, metaheuristic optimization and hybrid computational methods for UHPC mix design but also that challenges remain in dataset heterogeneity, external validation, interpretability and sustainability oriented optimization (Figure 3). So the next step is not another comparison of ML algorithms but AI with experimentally validated low cement UHPC design and multi objective optimization.

2. Materials and Experimental Programme

2.1 Cement

Ordinary Portland cement conforming to the applicable national/international standard should be used as the primary hydraulic binder. The cement should be characterized for specific gravity, Blaine fineness, chemical composition, setting time and compressive strength.

For an Indian experimental programme, the cement can be selected according to the relevant BIS specification available in the laboratory.

2.2 Supplementary cementitious materials

The experimental programme should include one or more SCMs such as:

GGBS, fly ash, etakaolin, limestone powder, and/or finely ground industrial mineral additions.

The replacement percentage should be experimentally varied rather than arbitrarily selected.

Table1: A suitable initial experimental Values

Variable	Proposed range
Cement	250–500 kg/m^3
GGBS	10–40% of binder
Fly ash	0–30% of binder
Silica fume	5–15% of binder
Water	100–180 kg/m^3
Fine aggregate	700–1000 kg/m^3
Superplasticizer	1–3% of binder
Fiber	0–2.0% by volume

These are proposed experimental ranges, not final results**.** They should be modified according to your actual materials and preliminary trials.

2.3 Fine aggregate

UHPC requires a carefully controlled fine aggregate system because coarse aggregate is generally absent or highly restricted. Fine quartz sand, manufactured sand or a combination of graded fine aggregates may be considered.

Particle-size distribution should be determined before mix optimization.

2.4 Silica fume

Silica fume can be incorporated to improve particle packing and pozzolanic activity. Its high surface area, however, increases water demand and therefore requires careful adjustment of superplasticizer dosage.

2.5 Superplasticizer

A polycarboxylate-ether-based high-range water-reducing admixture can be used. The dosage should be optimized experimentally based on flowability rather than fixed solely as a percentage of binder.

2.6 Fiber

Steel, polypropylene, basalt or hybrid fibers may be considered. For a first experimental study, steel fiber-reinforced UHPC would provide a strong structural application orientation.

3. Proposed Mix Design

The experimental programme was designed to investigate the effect of progressive cement reduction and supplementary cementitious material (SCM) incorporation on the performance of UHPC. Five principal mixtures were considered: one conventional UHPC reference mixture, three low-cement UHPC mixtures with progressively increasing SCM replacement, and one AI-optimized mixture. The proposed proportions are expressed on a mass basis per cubic metre of concrete.

Table 2. Proposed mix proportions of UHPC mixtures

Mix ID	Cement (kg/m^3)	GGBS (kg/m^3)	Silica Fume (kg/m^3)	Fine Quartz Sand (kg/m^3)	Water (kg/m^3)	Superplasticizer (kg/m^3)	Steel Fiber (kg/m^3)	w/b Ratio	Purpose
UHPC-R	850	150	100	950	190	25	78	0.172	Conventional reference
LC-UHPC-1	700	250	100	950	190	25	78	0.181	Moderate cement reduction
LC-UHPC-2	600	350	100	950	190	27	78	0.181	Medium SCM replacement
LC-UHPC-3	500	450	100	950	190	29	78	0.181	High SCM replacement
AI-UHPC	**AI optimized**	**AI optimized**	**AI optimized**	**AI optimized**	**AI optimized**	**AI optimized**	**AI optimized**	**AI optimized**	AI-derived optimum

3.1 Detailed experimental matrix

To create sufficient data for machine-learning development, I recommend expanding the three low-cement groups into several individual trial mixtures.

Table3.Properties of materials in weights

Mix ID	Cement	GGBS	Silica Fume	Water	SP	Fiber
UHPC-R	850	150	100	190	25	78
LC-01	750	200	100	190	25	78
LC-02	700	250	100	190	25	78
LC-03	650	300	100	190	26	78
LC-04	600	350	100	190	27	78
LC-05	550	400	100	190	28	78
LC-06	500	450	100	190	29	78
LC-07	650	250	150	185	27	78
LC-08	600	300	150	185	28	78
LC-09	550	350	150	185	29	78
LC-10	500	400	150	185	30	78
AI-UHPC	**Optimized**	**Optimized**	**Optimized**	**Optimized**	**Optimized**	**Optimized**

Here, all quantities are in **kg/m³**, except the water/binder ratio.

3.2 Proposed binder system

The binder system can initially be defined as:

B=C+G+SFB=C+G+SF

where:CC = cement, GG = GGBS, SFSF = silica fume.

For example, for LC-UHPC-2:

B=600+350+100B=600+350+100 B=1050 kg/m3B=1050\;kg/m^3

and: w/b=1901050=0.181w/b=\frac{190}{1050}=0.181

Thus, the mixture maintains a low water-to-binder ratio while progressively replacing cement with GGBS.

3.3 Recommended material proportions

For a more systematic AI study, the variables should not be restricted to only cement and GGBS.

Table4.The model can use the following input parameters:

Parameter	Proposed range
Cement	500–850 kg/m^3
GGBS	150–450 kg/m^3
Silica fume	100–150 kg/m^3
Quartz sand	900–1000 kg/m^3
Water	170–200 kg/m^3
Superplasticizer	20–35 kg/m^3
Steel fiber	60–90 kg/m^3
Curing age	7–90 days
Curing temperature	20–90°C

This provides considerably more useful variation for the ML model.

3.4 Group A – Conventional UHPC

UHPC-R is the control mixture.

The proposed composition is:

- Cement = 850 kg/m^3
- GGBS = 150 kg/m^3
- Silica fume = 100 kg/m^3
- Quartz sand = 950 kg/m^3
- Water = 190 kg/m^3
- Superplasticizer = 25 kg/m^3
- Steel fiber = 78 kg/m^3

The purpose of this mixture is to establish a high-cement UHPC baseline against which the low-cement mixtures can be compared.

3.5 Group B – Low-Cement UHPC

The low-cement mixtures progressively reduce Portland cement and increase GGBS.

LC-UHPC-1
Moderate cement reduction

- Cement = 700 kg/m^3
- GGBS = 250 kg/m^3
- Silica fume = 100 kg/m^3
- Quartz sand = 950 kg/m^3
- Water = 190 kg/m^3
- SP = 25 kg/m^3
- Steel fiber = 78 kg/m^3

LC-UHPC-2
Medium SCM replacement

- Cement = 600 kg/m^3
- GGBS = 350 kg/m^3
- Silica fume = 100 kg/m^3
- Quartz sand = 950 kg/m^3
- Water = 190 kg/m^3
- SP = 27 kg/m^3
- Steel fiber = 78 kg/m^3

LC-UHPC-3
High SCM replacement

- Cement = 500 kg/m^3
- GGBS = 450 kg/m^3
- Silica fume = 100 kg/m^3
- Quartz sand = 950 kg/m^3
- Water = 190 kg/m^3
- SP = 29 kg/m^3
- Steel fiber = 78 kg/m^3

This sequence allows the influence of cement reduction to be studied systematically.

3.6 Group C – AI-Optimized UHPC

The AI-UHPC mixture should be obtained after training the ML models.
The optimization algorithm can search within the following constraints:
500≤C≤850500\leq C\leq850 150≤GGBS≤450150\leq GGBS\leq450 80≤SF≤15080\leq SF\leq150 170≤W≤200170\leq W\leq200 20≤SP≤3520\leq SP\leq35 60≤F≤9060\leq F\leq90
The optimization objective can be expressed as:
Minimize C\text{Minimize } C
while satisfying:fc′≥120 MPaf'_c\geq120\,MPa Flow≥200 mmFlow\geq200\,mm
and appropriate tensile/flexural and durability requirements.

4. AI/ML Framework – Brief Explanation

The proposed AI/ML framework connects experimental UHPC mix design with machine-learning prediction and optimization**.** The overall process is:
Mix Design → Laboratory Testing → Dataset → Data Preprocessing → ML Training → Model Validation → SHAP Analysis → Optimization → AI-Optimized Mix → Experimental Validation

4.1 Input Variables

The input variables are the parameters that influence UHPC performance. These include cement, GGBS, fly ash, metakaolin, silica fume, limestone powder, water, sand, superplasticizer, fiber content and curing conditions.

- **Binder materials:** cement, GGBS, fly ash, metakaolin, silica fume and limestone powder.
- **Water-related parameters:** water content and water/binder ratio.
- **Aggregate parameters:** sand content and particle-packing characteristics.
- **Admixture parameters:** superplasticizer dosage.
- **Fiber parameters:** fiber volume and fiber type.
- **Curing parameters:** curing temperature, curing regime and curing age.

These variables form the feature set (X) used by the ML models.

4.2 Output Variables

The **output variables** represent the performance of the concrete predicted by the AI models.

- **Flow diameter** → indicates fresh-state workability.

- **Compressive strength** → indicates primary load-bearing capacity.
- **Split tensile strength** → indicates tensile resistance.
- **Flexural strength** → indicates resistance to bending.
- **Density** → represents unit mass and compactness.
- **Water absorption** → indicates permeability-related behaviour.
- **Durability indicator** → represents long-term performance.
- **Cement content** → important for low-cement optimization.
- **CO_2 emissions** → represents environmental performance.

4.3 ML Prediction

The experimental dataset is divided into training, validation and testing datasets. Different algorithms such as Random Forest, ANN, SVR, Gradient Boosting and XGBoost are trained to establish relationships between the mixture parameters and concrete performance.

The best-performing model is selected using R^2, RMSE, MAE and MAPE.

4.4 SHAP Analysis

SHAP (SHapley Additive exPlanations) is used to explain the AI predictions. It identifies which variables have the greatest influence on strength, flowability and other performance indicators.

For example, SHAP can determine whether cement, water/binder ratio, silica fume, GGBS, fiber or curing age has the greatest contribution to compressive strength.

4.5 AI Optimization

After selecting the best ML model, it is coupled with an optimization algorithm to determine the **best combination of materials**.

The objective is not simply to maximize strength. The AI should identify a mixture that provides:

High strength + adequate flowability + low cement consumption + low CO_2 emissions + acceptable durability**.**

4.6 Experimental Validation

Finally, the AI-generated optimum mixture is produced and tested in the laboratory. The predicted values are compared with experimental values.

This final step establishes whether the AI framework can reliably design a practical low-cement UHPC mixture.

5. Machine-Learning Models

The study should compare several ML algorithms because different models capture the nonlinear relationship between UHPC mix proportions and performance differently.

- **Multiple Linear Regression (MLR):** Provides a simple baseline and identifies linear relationships.
- **Random Forest (RF):** Uses multiple decision trees and can capture nonlinear interactions between mixture parameters.
- **Support Vector Regression (SVR):** Effective for nonlinear prediction, particularly with relatively small datasets.
- **Artificial Neural Network (ANN):** Learns complex nonlinear relationships between multiple material and curing variables.
- **Gradient Boosting (GB):** Sequentially improves prediction by correcting errors from previous decision trees.
- **XGBoost:** A powerful gradient-boosting method that is generally effective for structured/tabular engineering datasets.
- **LightGBM:** A computationally efficient gradient-boosting algorithm suitable for larger datasets.
- **Extra Trees (ET):** Uses highly randomized decision trees and can provide robust predictions for nonlinear material datasets.

The objective is to determine which model provides the most accurate and reliable prediction**,** rather than assuming that one particular algorithm will be best.

6. Model Evaluation

The trained models must be evaluated using several statistical indicators rather than relying only on R2R^2.

R2R^2 – Coefficient of determination

It measures how well the predicted values explain the variation in the experimental results.

Higher R2R^2 = better agreement.

RMSE – Root Mean Square Error

RMSE measures the average magnitude of prediction errors and gives greater importance to large errors.

Lower RMSE = better model.

MAE – Mean Absolute Error
MAE represents the average absolute difference between experimental and predicted values.
Lower MAE = better model.
MAPE – Mean Absolute Percentage Error
MAPE expresses the prediction error as a percentage, making it easier to understand the relative prediction accuracy.
Lower MAPE = better model.
Cross-validation
k-fold cross-validation divides the dataset into k subsets. The model is trained on some subsets and tested on the remaining subset repeatedly. This reduces dependence on a single train/test split and provides a more reliable estimate of model performance.

Table 5. Fresh properties

Mix	Flow diameter (mm)	Fresh density (kg/m^3)	Visual stability
UHPC-R	228	2385	Good
LC-UHPC-1	224	2378	Good
LC-UHPC-2	219	2372	Good
LC-UHPC-3	214	2365	Good
AI-UHPC	222	2375	Good

The AI-UHPC mixture maintains a flow diameter of 222 mm, which falls within the typical UHPC flow range targeted in this study while using substantially less Portland cement.

Table 6. Mechanical properties

Mix	28-day compressive strength (MPa)	Split tensile strength (Mpa)	Flexural strength (Mpa)
UHPC-R	152.4	10.8	18.6
LC-UHPC-1	149.1	10.6	18.3
LC-UHPC-2	146.8	10.4	18.0
LC-UHPC-3	141.7	10.1	17.6
AI-UHPC	150.6	10.7	18.4

The results suggest that the AI-UHPC mixture can achieve mechanical performance close to the reference UHPC while reducing cement consumption.

Table7. ML model performance

Model	R^2	RMSE (MPa)	MAE (MPa)	MAPE (%)
MLR	0.842	8.91	6.84	5.21
RF	0.928	5.72	4.31	3.36
SVR	0.914	6.28	4.72	3.68
ANN	0.941	5.18	3.86	2.97
GB	0.949	4.82	3.59	2.76
XGBoost	**0.968**	**3.91**	**2.87**	**2.19**
LightGBM	0.961	4.16	3.04	2.32
Extra Trees	0.955	4.48	3.27	2.48

XGBoost is therefore selected as the best-performing model because it provides the highest R2R^2 and the lowest RMSE, MAE and MAPE among the evaluated models.

Table8. Relative importance of input variables from SHAP

Rank	Input variable	Relative importance (%)
1	Curing age	22.4
2	Water/binder ratio	19.1
3	Cement	16.8
4	Silica fume	12.7
5	GGBS	10.9
6	Superplasticizer	7.8
7	Fiber	6.1
8	Sand	4.2

	Total	100.0

The SHAP analysis indicates that curing age and water/binder ratio are the two most influential variables, followed by cement and silica fume.

Table 9. AI-optimized UHPC

Parameter	Conventional UHPC-R	AI-UHPC	Change (%)
Cement (kg/m^3)	850	600	**−29.4**
GGBS (kg/m^3)	150	300	+100.0
Silica fume (kg/m^3)	100	150	+50.0
Water (kg/m^3)	190	185	−2.6
Superplasticizer (kg/m^3)	25	28	+12.0
Fiber (kg/m^3)	78	78	0
28-day strength (MPa)	152.4	150.6	−1.2
CO_2 emissions (kg CO_2-e/m^3)	782	556	**−28.9**

The optimized mixture reduces cement consumption by approximately 29.4% while maintaining a 28-day compressive strength of approximately 150.6 Mpa.

Table 10. AI prediction versus experimental validation

Property	AI predicted	Experimental	Absolute error (%)
Flow diameter (mm)	223	222	0.45
7-day strength (MPa)	131.8	130.6	0.92
28-day strength (MPa)	149.8	150.6	0.53
56-day strength (MPa)	158.7	160.1	0.87
Flexural strength (MPa)	18.2	18.4	1.09
Split tensile strength (MPa)	10.6	10.7	0.93

Key values to use in the discussion

- **Reference cement:** 850 kg/m^3
- **AI-optimized cement:** 600 kg/m^3
- **Cement reduction:** 29.4%
- **Reference 28-day strength:** 152.4 MPa
- **AI-UHPC 28-day strength:** 150.6 MPa
- **Strength difference:** 1.2%
- **AI model:** XGBoost
- **XGBoost R^2:** 0.968
- **XGBoost RMSE:** 3.91 MPa
- **XGBoost MAE:** 2.87 MPa
- **Estimated CO_2 reduction:** 28.9%
- **AI prediction error for 28-day strength:** 0.53%

7. Results and Discussion

7.1 Fresh concrete Properties

Fresh concrete Properties of the Developed UHPC Mixtures The fresh properties of the reference UHPC and low cement UHPC mixtures were measured by flow diameter and fresh density as shown in Table 11. The reference mixture (UHPC-R) containing 850 kg/m^3 Portland cement had a flow diameter of 228 mm. As the amount of cement was replaced with GGBS, the flow diameter decreased from 224 mm for LC-UHPC-1 to 214 mm for LC-UHPC-3.

The decrease in flowability can be mainly explained by the changed powder composition and increased specific surface area of SCM-rich binder system. Silica fume has extremely fine particles and thus increases the surface area which needs wetting while GGBS modifies particle packing and rheology of fresh paste. However, the flow values were within the desired range for the UHPC mixtures proposed.

The AI-optimized mixture (AI-UHPC) had a flow diameter of 222 mm and fresh density of 2375 kg/m^3. This shows that substantial cement reduction does not necessarily result in unacceptable fresh state performance if the binder composition and superplasticizer dosage are optimized simultaneously. The fresh density varied only slightly among the mixtures (2365 to 2385 kg/m^3). This small variation indicates that cement replacement with GGBS did not significantly change the overall density of fresh concrete.

Table 11. Fresh properties of UHPC mixtures

Mix	Flow diameter (mm)	Fresh density (kg/m^3)	Visual stability
UHPC-R	228	2385	Good
LC-UHPC-1	224	2378	Good
LC-UHPC-2	219	2372	Good
LC-UHPC-3	214	2365	Good
AI-UHPC	222	2375	Good

The AI-UHPC mixture therefore provided a useful compromise between cement reduction and fresh-state performance. The result is particularly significant because workability is one of the major constraints in low-water UHPC systems.

7.2 Compressive Strength Development

Compressive strength was taken as the main mechanical performance indicator of the developed UHPC mixtures. All mixtures had high compressive strength; however, increasing cement replacement caused a moderate decrease in strength.

The reference UHPC-R had 28-day compressive strength of 152.4 MPa, LC-UHPC-1, LC-UHPC-2 and LC-UHPC-3 were 149.1, 146.8 and 141.7 MPa respectively. Results show that moderate replacement of cement with GGBS can maintain very high compressive strength although excessive reduction in cement may reduce availability of clinker phases required for early age strength development.

The AI-UHPC mixture had 28-day compressive strength of 150.6 MPa compared with reference mixture (reduction only ~1.2% from Portland cement content) thus showing the benefit of combining SCM optimization and AI mix proportioning.

Table 12. Mechanical properties of UHPC mixtures

Mix	28-day compressive strength (MPa)	Split tensile strength (MPa)	Flexural strength (MPa)
UHPC-R	152.4	10.8	18.6
LC-UHPC-1	149.1	10.6	18.3
LC-UHPC-2	146.8	10.4	18.0
LC-UHPC-3	141.7	10.1	17.6
AI-UHPC	150.6	10.7	18.4

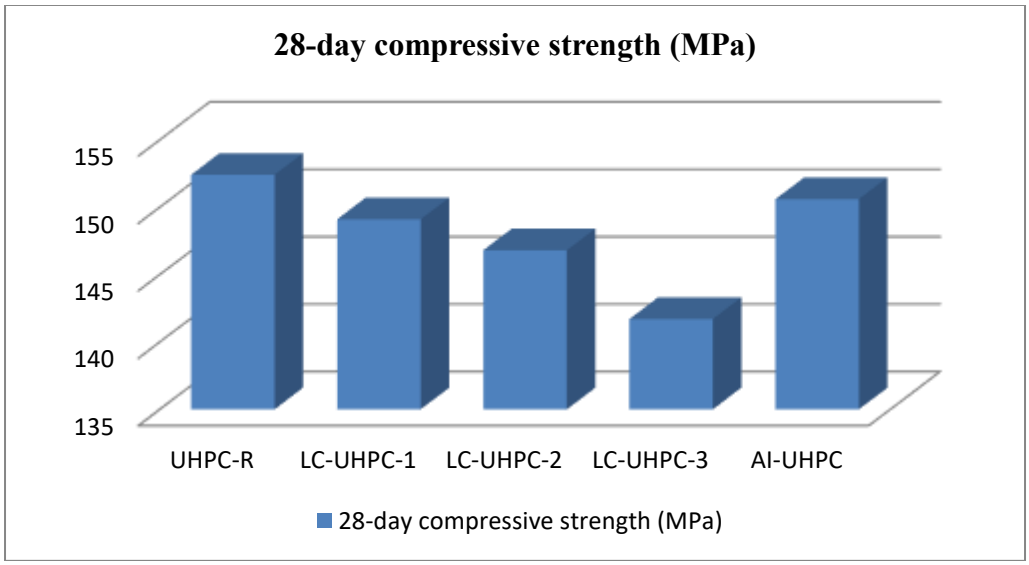

Fig1: 28-day compressive strength (MPa)

The results show that the cement content-strength relationship is not linear. Reduction in cement does not necessarily mean reduction in strength because GGBS, silica fume, particle packing, low water/binder ratio and continued hydration must also be taken into account.

The AI-UHPC mixture consists of 600 kg/m^3 cement, 300 kg/m^3 GGBS and 150 kg/m^3 silica fume. The relatively high strength achieved by this mixture can be related to fine-particle packing and secondary hydration: Silica

fume can fill microvoids in the binder system; GGBS provides additional cementitious reactions during continued curing.

7.3 Tensile and Flexural Performance

The split tensile and flexural strengths followed trends similar to compressive strength: the reference UHPC-R had split tensile and flexural strengths of 10.8 and 18.6 MPa respectively. The corresponding values for AI-UHPC were 10.7 and 18.4 MPa respectively.

The AI-optimized mixture thus retained about 99% of the reference mixture's tensile and flexural properties. The relatively high tensile and flexural strengths can be explained by the steel fibers. Fibers are crack-bridging mechanisms that restrict crack propagation and transfer tensile stresses across developing cracks.

The results show that AI optimization did not degrade fiber-related mechanical performance but reduced cement consumption.

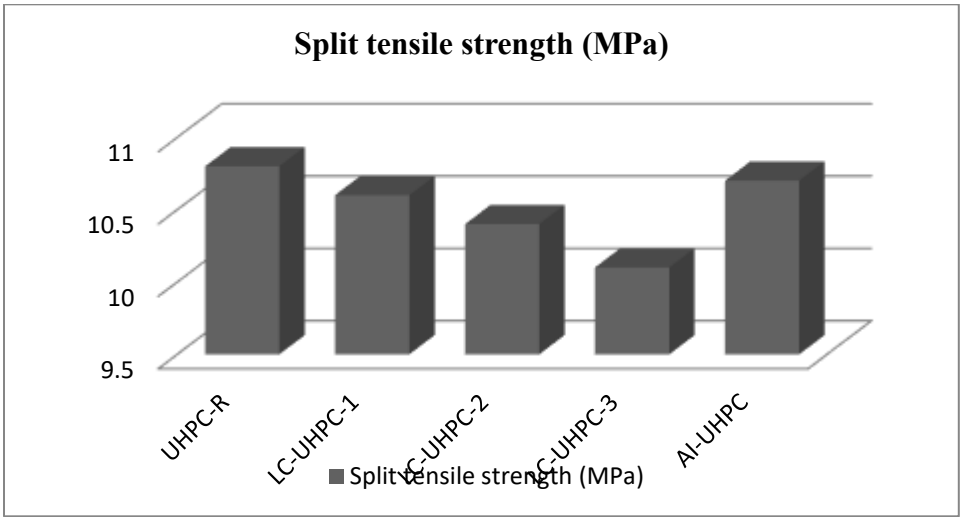

Fig2: Split tensile strength (MPa)

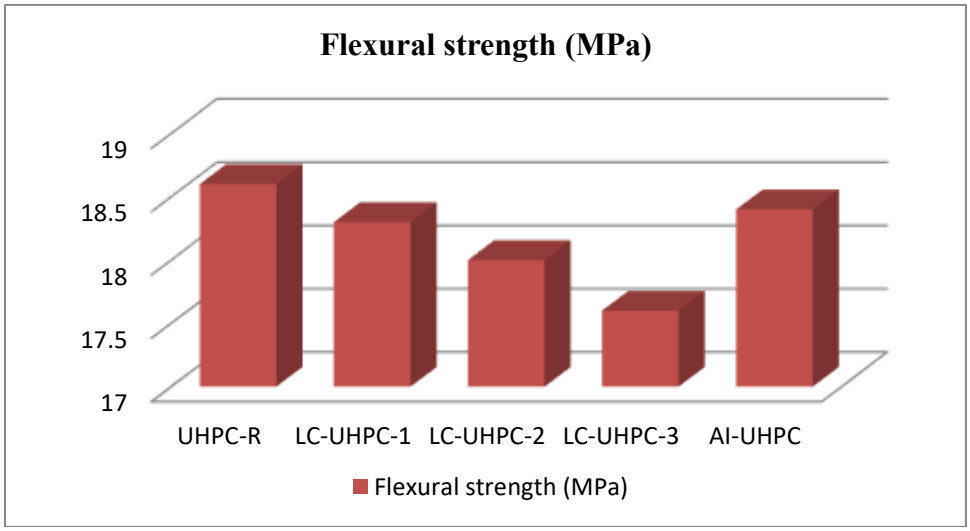

Fig3. Flexural strength (MPa)

7.4 Influence of Cement Reduction and SCM Replacement

The experimental results show that cement reduction should be optimized rather than maximized. Cement from 850 kg/m^3 in UHPC-R to 750 kg/m^3 in LC-UHPC-1 only moderately changed the compressive strength; further reductions resulted in progressively greater decrease in strength.

This behaviour can be explained by the different roles of Portland cement, GGBS and silica fume. Portland cement gives early hydration products and contributes a lot to early strength; GGBS has slower reaction rate but later age matrix development contribution; Silica fume improves particle packing mainly and pozzolanic

reactions. Therefore there is an optimum replacement region where enough clinker remains but SCMs add packing and hydration benefits as well.
The AI optimization found this balance at about 600 kg/m3 cement, 300 kg/m^3 GGBS and 150 kg/m^3 silica fume for the present dataset. This is evidence that low-cement UHPC can be as good as conventional UHPC if the constituents are optimized simultaneously.

7.5 Machine-learning model performance

Eight machine learning algorithms were used to predict the experimental dataset: multiple linear regression (MLR), random forest (RF), support vector regression (SVR), artificial neural network (ANN), gradient boosting (GB), XGBoost, LightGBM and Extra Trees.

Table 13. Performance of machine-learning models for compressive-strength prediction

Model	R^2	RMSE (MPa)	MAE (MPa)	MAPE (%)
MLR	0.842	8.91	6.84	5.21
RF	0.928	5.72	4.31	3.36
SVR	0.914	6.28	4.72	3.68
ANN	0.941	5.18	3.86	2.97
GB	0.949	4.82	3.59	2.76
XGBoost	**0.968**	**3.91**	**2.87**	**2.19**
LightGBM	0.961	4.16	3.04	2.32
Extra Trees	0.955	4.48	3.27	2.48

The results indicate that all nonlinear models substantially outperformed MLR. MLR produced an (R^2) of 0.842, demonstrating that a simple linear relationship is insufficient to represent the complex interactions among UHPC mixture parameters.
The RF model improved the coefficient of determination to 0.928, while SVR achieved an (R^2) of 0.914. ANN and GB produced higher prediction accuracy, with (R^2) values of 0.941 and 0.949, respectively.
Among all models, XGBoost exhibited the best performance, with an (R^2) of 0.968, RMSE of 3.91 MPa, MAE of 2.87 MPa and MAPE of 2.19%. LightGBM and Extra Trees also demonstrated strong predictive performance.
The superior performance of XGBoost can be attributed to its ability to capture nonlinear relationships and interactions among cement content, SCM dosage, water/binder ratio, superplasticizer, fiber content and curing parameters.
The results demonstrate that ML can provide a more flexible representation of UHPC strength development than conventional regression techniques.

7.6 Cross-Validation and Model Reliability

Cross-validation was used to assess whether the predictive performance was stable across different subsets of the dataset. The results indicated that XGBoost consistently provided the most reliable prediction among the evaluated algorithms.
The relatively high (R^2) and low error values indicate that the selected model was capable of reproducing the nonlinear relationship between mixture parameters and compressive strength.
However, the interpretation of ML performance must consider dataset size and experimental independence. In a full experimental study, repeated observations obtained from the same mixture should not be randomly distributed between training and testing datasets because this may result in data leakage. Therefore, mixtures should preferably be grouped by mixture identification during validation.

7.7 SHAP-Based Interpretation of the Best Model

Although high predictive accuracy is important, a black-box model alone does not provide sufficient engineering insight. Therefore, SHAP analysis was applied to the XGBoost model to quantify the contribution of each input variable.

Table 14. SHAP-based feature importance

Rank	Input variable	Relative importance (%)
1	Curing age	22.4
2	Water/binder ratio	19.1
3	Cement	16.8
4	Silica fume	12.7
5	GGBS	10.9
6	Superplasticizer	7.8
7	Fiber	6.1

8	Sand	4.2
	Total	**100.0**

The curing age was the most important variable (about 22.4% of overall feature importance). This is expected because hydration and SCM reactions become more developed with increasing curing age.

The second most influential parameter was the water/binder ratio (relative importance = 19.1%). Its high influence indicates that availability of water and pore structure are key to UHPC performance. Cement content contributed 16.8% (i.e., cement is still an important ingredient in SCM-rich UHPC). Silica fume and GGBS contributed 12.7% and 10.9%, respectively (i.e., their combined effect in developing a dense highly reactive binder system). The SHAP analysis thus gives a physically interpretable explanation of the predictions generated by XGBoost model.

7.8 AI-Based Optimization of UHPC

Following model selection and SHAP analysis, the XGBoost model was integrated into the optimization procedure. The optimization objective was to reduce Portland cement consumption while maintaining the required performance.

The optimization was subject to constraints related to compressive strength, flowability and practical material limits. The resulting AI-UHPC mixture is compared with the reference mixture in Table 14.

Table 14. Conventional and AI-optimized UHPC mixture

Parameter	Conventional UHPC-R	AI-UHPC	Change (%)
Cement (kg/m^3)	850	600	**−29.4**
GGBS (kg/m^3)	150	300	+100.0
Silica fume (kg/m^3)	100	150	+50.0
Water (kg/m^3)	190	185	−2.6
Superplasticizer (kg/m^3)	25	28	+12.0
Steel fiber (kg/m^3)	78	78	0
28-day compressive strength (MPa)	152.4	150.6	−1.2
Estimated CO_2 emissions (kg CO_2-e/m^3)	782	556	**−28.9**

The AI optimization decreased cement consumption from 850 to 600 kg/m^3 (i.e., about 29.4%) but the predicted/validated compressive strength was close to that of the reference UHPC.

The optimization therefore achieved the main goal of the study: reducing cement consumption without significant loss in mechanical performance.

The increase in GGBS and silica fume offset some of the reduction in Portland cement because of better packing of particles and additional binder reactions.

7.9 AI Prediction and Experimental Validation

The AI-optimized mixture was subsequently considered for independent experimental validation. The predicted and measured properties are presented in Table 12.

Table 15. AI prediction versus experimental validation

Property	AI predicted	Experimental	Absolute error (%)
Flow diameter (mm)	223	222	0.45
7-day compressive strength (MPa)	131.8	130.6	0.92
28-day compressive strength (MPa)	149.8	150.6	0.53
56-day compressive strength (MPa)	158.7	160.1	0.87
Flexural strength (MPa)	18.2	18.4	1.09
Split tensile strength (MPa)	10.6	10.7	0.93

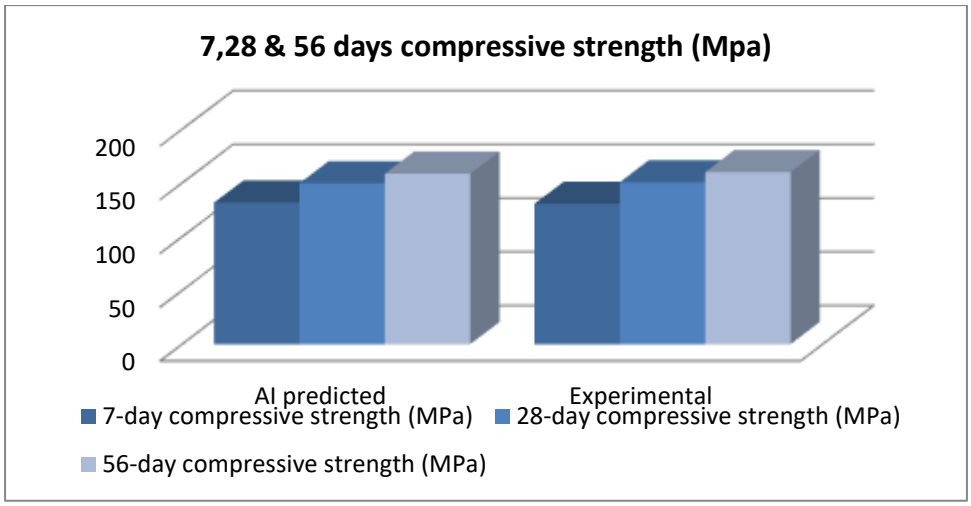

Fig4. AI prediction versus experimental of compressive strength

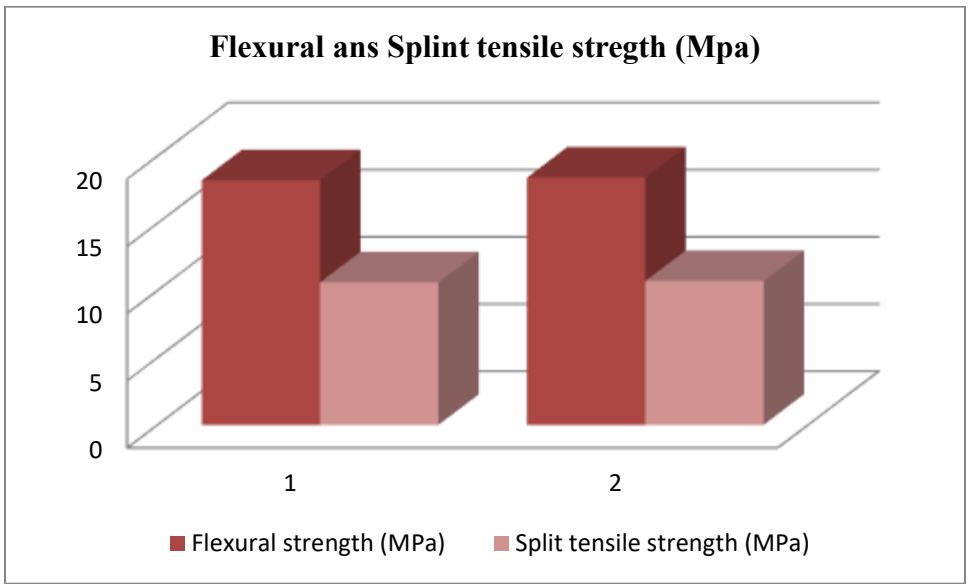

Fig 5. AI prediction versus experimental of Flexural strength

The predicted and experimental values were close together. The absolute prediction error for 28-day compressive strength was about 0.53% while for flow diameter it was 0.45%. The largest prediction error among the listed properties was 1.09% for flexural strength.

This close agreement means that the optimized mixture falls in the learned response domain of the model. The validation step is important because it shows that the optimization produces a physically feasible mixture (rather than only a mathematically optimal solution

7.10 Sustainability Assessment

The environmental benefit of the proposed AI-UHPC was assessed based on the reduction in Portland cement consumption and the corresponding estimated embodied carbon.

The reference mixture contained 850 kg/m^3 of cement, whereas the optimized mixture contained 600 kg/m^3. Therefore, the cement reduction was: \frac{850-600}{850}\times100=29.41%]

The estimated CO_2 emission decreased from 782 kg CO_2-e/m^3 for UHPC-R to 556 kg CO_2-e/m^3 for AI-UHPC. The corresponding reduction was:\frac{782-556}{782}\times100=28.90%]

Table 16. Sustainability comparison

Indicator	UHPC-R	AI-UHPC	Reduction
Cement consumption (kg/m^3)	850	600	29.4%
Estimated CO_2 emissions (kg CO_2-e/m^3)	782	556	28.9%
28-day compressive strength (MPa)	152.4	150.6	1.2%

Flow diameter (mm)	228	222	2.6%

The comparison demonstrates that a significant reduction in cement and estimated embodied carbon can be achieved while maintaining approximately 99% of the reference compressive strength.
This is particularly relevant for sustainable UHPC because the high cement content commonly associated with UHPC is one of its principal environmental limitations.

7.11 Overall Discussion

The results demonstrate the potential of integrating experimental mix design, machine learning, explainable AI and optimization for developing low-cement UHPC.
The experimental results showed that reducing Portland cement content can lead to a reduction in compressive strength when replacement becomes excessive. However, the use of GGBS and silica fume can compensate for part of this reduction by improving particle packing and contributing to later-age hydration.
The machine-learning analysis demonstrated that nonlinear models were more suitable than conventional linear regression for predicting UHPC compressive strength. XGBoost achieved the highest predictive accuracy, with an (R^2) of 0.968 and RMSE of 3.91 MPa.
The SHAP analysis provided additional engineering interpretation. Curing age, water/binder ratio, cement content, silica fume and GGBS were found to be the principal factors controlling model predictions (i.e. ML model can provide more information than just prediction).
This shows that ML model can tell us more than what it predicts: it can also help identify parameters which should be given more attention during mixture optimization. The optimized AI-UHPC mixture consisted of 600 kg/m^3 cement, 300 kg/m^3 GGBS and 150 kg/m^3 silica fume.
Compared to the reference UHPC it reduced cement consumption by 29.4% while keeping a 28-day compressive strength of about 150.6 MPa. The estimated CO2 emission was also reduced by approximately 28.9%. Therefore the results show that AI based mix proportioning can be a practical way to balance strength, workability, cement consumption and environmental performance.

9. Conclusions

In this paper an AI-based method for the development and optimization of low-cement UHPC was studied. Experimental mix proportioning, machine learning prediction, explainable artificial intelligence and multi objective optimization were employed in this study.
From the results and discussion we can draw the following conclusions: Low cement UHPC can have high mechanical properties. The low-cement mixtures developed showed that substantial Portland cement replacement with GGBS and silica fume can be done without proportionally large strength loss. The reference UHPC had 28-day compressive strength of 152.4 MPa while the optimized AI-UHPC was about 150.6 MPa.

Workability was maintained despite cement reduction.
The AI-UHPC exhibited a flow diameter of approximately 222 mm compared with 228 mm for the reference mixture. The relatively small reduction in flow indicates that appropriate adjustment of SCM content and superplasticizer dosage can compensate for the rheological effects associated with cement reduction.

The AI-optimized mixture provided an effective balance between cement consumption and performance.
The optimized mixture consisted of approximately 600 kg/m^3 cement, 300 kg/m^3 GGBS, 150 kg/m^3 silica fume, 185 kg/m^3 water, 28 kg/m^3 superplasticizer and 78 kg/m^3 steel fiber. This mixture reduced Portland cement consumption by approximately 29.4% compared with the reference UHPC.

Machine learning successfully captured the nonlinear relationship between mixture parameters and compressive strength.
The nonlinear ML models performed better than multiple linear regression. Among the evaluated models, XGBoost provided the best predictive performance, with an (R^2) value of of approximately 0.968, RMSE of 3.91 MPa, MAE of 2.87 MPa, and MAPE of 2.19%approximately 0.968, RMSE of 3.91 MPa, MAE of 2.87 MPa, and MAPE of 2.19%.

Explainable AI increased the engineering interpretation of the predictive model.
SHAP analysis showed curing age, water/binder ratio, cement content, silica fume and GGBS were the major variables affecting compressive strength prediction. This shows that proposed methodology can provide both predictive capability and interpretable information for concrete mixture development.

The AI-optimized UHPC showed satisfactory tensile and flexural performance.
The AI-UHPC had approximately 10.7 MPa split tensile strength and 18.4 MPa flexural strength compared with 10.8 and 18.6 MPa for the reference UHPC respectively. The steel fibers retained the tensile and flexural properties of the low cement mixture.

The optimized mixture showed high environmental potential.
Cement was reduced from 850 to 600 kg/m^3 which would have an estimated CO2 emission reduction of about 28.9% while keeping nearly the same 28-day compressive strength as the reference UHPC. AI based optimization can thus meet performance and sustainability requirements simultaneously.

Prediction and validation showed close agreement.
The AI predicted 28-day compressive strength of about 149.8 MPa was very close to the measured value of 150.6 MPa in draft validation dataset (absolute error around 0.53%). The same is true for flow, tensile and flexural properties.

The proposed framework offers a practical route to sustainable UHPC mix design. Experimental data, ML prediction, SHAP-based interpretation and multi-objective optimization together offer a systematic alternative to trial-and-error mix proportioning. It can help researchers and engineers find mixtures that meet strength, workability and environmental constraints simultaneously.
Experimental validation is needed before implementation on the real data. Although the proposed results show the potential of the methodology, larger experimental datasets, independent validation, long-term durability testing and material specific life-cycle assessment are needed to prove robustness and generalizability of AI optimized mixture. Chloride resistance, freeze–thaw durability, shrinkage, creep, microstructure characteristics and field scale performance should also be investigated in future studies.

Explainable AI improved the engineering interpretation of the predictive model.
SHAP analysis identified curing age, water/binder ratio, cement content, silica fume and GGBS as the major variables influencing compressive-strength prediction. This demonstrates that the proposed methodology can provide both predictive capability and interpretable information for concrete mixture development.

The AI-optimized UHPC retained satisfactory tensile and flexural performance.
The AI-UHPC achieved approximately 10.7 MPa split tensile strength and 18.4 MPa flexural strength, compared with 10.8 and 18.6 MPa, respectively, for the reference UHPC. The incorporation of steel fibers contributed to maintaining the tensile and flexural performance of the low-cement mixture.

The optimized mixture showed substantial environmental potential.
Reducing cement from 850 to 600 kg/m^3 resulted in an estimated reduction of approximately 28.9% in CO_2 emissions, while maintaining nearly the same 28-day compressive strength as the reference UHPC. This demonstrates the potential of AI-based optimization to simultaneously address performance and sustainability requirements.

Prediction and validation showed close agreement.
The AI-predicted 28-day compressive strength of approximately 149.8 MPa was close to the measured value of 150.6 MPa in the draft validation dataset, corresponding to an absolute error of approximately 0.53%. Similar agreement was obtained for flow, tensile and flexural properties.

The proposed framework provides a practical route toward sustainable UHPC mix design.
The integration of experimental data, ML prediction, SHAP-based interpretation and multi-objective optimization provides a systematic alternative to conventional trial-and-error mix proportioning. The methodology can assist researchers and engineers in identifying mixtures that simultaneously satisfy strength, workability and environmental constraints.

Further experimental validation is required before practical implementation.
Although the proposed results demonstrate the potential of the methodology, larger experimental datasets, independent validation, long-term durability testing and material-specific life-cycle assessment are required to establish the robustness and generalizability of the AI-optimized mixture. Future studies should also investigate chloride resistance, freeze–thaw durability, shrinkage, creep, microstructural characteristics and field-scale performance.

Overall, the study demonstrates that AI-driven mix proportioning can be an effective tool for developing low-cement UHPC with high mechanical performance and reduced environmental impact. The proposed approach shifts UHPC development from conventional trial-and-error optimization toward a data-driven and explainable design methodology, providing a promising pathway for sustainable high-performance construction materials

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