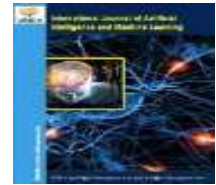


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# Eco-Friendly Self-Compacting Concrete Incorporating Fly Ash and Recycled Polyethylene Terephthalate (PET) Bottle Fibers

Pramod Kumar Sahu<sup>1</sup>, Dr. Rahul Kumar<sup>2\*</sup>, Dr. Ajay Kumar<sup>3</sup>, Dr. Amrendra Kumar<sup>4</sup><sup>1</sup>Research Scholar, Department of Civil Engineering, Sandip University, Madhubani, Bihar, India - 847235.E-mail: [sahuparmod31@gmail.com](mailto:sahuparmod31@gmail.com), ORCID: 0009-0008-7169-1917<sup>2\*</sup>Assistant Professor, Department of Civil Engineering, Sandip University, Madhubani, Bihar, India - 847235.E-mail: [rahulkenar@gmail.com](mailto:rahulkenar@gmail.com), ORCID: 0000-0002-0323-3593<sup>3</sup>Assistant Professor, Department of Civil Engineering, Sandip University, Madhubani, Bihar, India - 847235.E-mail: [ajaykumar8mail@gmail.com](mailto:ajaykumar8mail@gmail.com), ORCID: 0009-0002-8418-0135<sup>4</sup>Assistant Professor, Department of Civil Engineering, Sandip University, Madhubani, Bihar, India - 847235.E-mail: [amrendraroy2k8@gmail.com](mailto:amrendraroy2k8@gmail.com), ORCID: 0009-0001-6092-8271**ABSTRACT**

Self-compacting concrete (SCC) has emerged as a sustainable construction material owing to its superior workability, reduced labor requirements, and enhanced durability. This study presents an integrated experimental and artificial intelligence (AI)-based framework for predicting the fresh and hardened properties of SCC incorporating Ground Calcium Carbonate (GCC), Class F fly ash, and recycled polyethylene terephthalate (PET) fibers. SCC mixtures were designed in accordance with IS 10262:2019, while fresh properties were evaluated following EFNARC (2005) guidelines and hardened properties were determined using the relevant Indian Standards. A comprehensive experimental database comprising 1,000 samples was developed, including input variables related to material proportions and output responses such as slump flow,  $T_{50}$  flow time, V-funnel time, L-box ratio, compressive strength, flexural strength, and ultrasonic pulse velocity (UPV). The dataset was preprocessed using feature scaling, normalization, and an 80:20 train-test split with five-fold cross-validation before training six predictive models: Artificial Neural Network (ANN), Deep Neural Network (DNN), Extra Trees Regressor (ETR), Gradient Boosting Regressor (GBR), LightGBM, and CatBoost Regressor. Model performance was evaluated using the coefficient of determination ( $R^2$ ), root mean square error (RMSE), mean absolute error (MAE), and mean squared error (MSE). Explainable artificial intelligence techniques, including SHAP analysis and Partial Dependence Plots (PDP), were employed to interpret feature importance and nonlinear interactions. Among the investigated models, CatBoost Regressor demonstrated the highest predictive accuracy, exhibiting the strongest agreement between experimental and predicted values with the highest  $R^2$  and the lowest prediction errors. The proposed AI-driven framework provides a reliable, interpretable, and computationally efficient approach for optimizing sustainable SCC mixtures while minimizing experimental effort, thereby supporting intelligent concrete mix design and promoting environmentally responsible construction practices.

**Keywords:** Self-compacting concrete (SCC); Machine learning; CatBoost Regressor; Deep learning; Explainable Artificial Intelligence (XAI); SHAP; Recycled PET fibers; Fly ash; Ground Calcium Carbonate (GCC); Compressive strength prediction; Sustainable concrete; Civil engineering.

## 1. Introduction

Self-compacting concrete (SCC) has become one of the most important innovations in concrete technology because of its ability to flow under its own weight without requiring external vibration. Unlike conventional concrete, SCC possesses excellent filling ability, passing ability, and resistance to segregation, enabling it to completely fill complex formworks and densely reinforced structural members while maintaining uniformity. These characteristics improve construction quality, reduce labor requirements, shorten construction time, minimize vibration-induced noise, and lower the risk of defects such as honeycombing and void formation. Consequently, SCC has gained widespread acceptance in high-rise buildings, bridges, precast elements, tunnels, and other infrastructure projects where conventional compaction is difficult or impractical [1–4]. Although SCC offers significant engineering advantages, its production generally requires a higher binder content than conventional concrete to achieve the desired workability and stability. This increased cement consumption leads to higher construction costs and greater carbon dioxide emissions associated with cement manufacturing. As the construction industry moves toward low-carbon and sustainable practices, reducing Portland cement consumption through the use of supplementary cementitious materials (SCMs) has become an important research priority. Materials such as fly ash, silica fume, ground granulated blast furnace slag (GGBFS), limestone powder, and ground calcium carbonate (GCC) have demonstrated considerable potential to improve particle packing, refine the pore structure, enhance workability, and reduce the environmental footprint of concrete production [5–10]. Among these SCMs, Class F fly ash has attracted considerable attention because of its pozzolanic properties, spherical particle shape, and widespread availability as an industrial by-product from coal-fired thermal power plants [27]. The incorporation of fly ash improves the flowability of SCC

through the ball-bearing effect while contributing to long-term strength and durability. Similarly, Ground Calcium Carbonate (GCC) acts primarily as a filler material that enhances particle packing density, improves the viscosity of fresh concrete, and contributes to a denser cementitious matrix[21]. The combined use of fly ash and GCC therefore provides an effective approach for producing sustainable SCC with reduced cement consumption while maintaining satisfactory fresh and hardened properties [8–12]. In parallel with reducing cement consumption, the construction industry is increasingly exploring ways to recycle plastic waste[23]. Polyethylene terephthalate (PET), commonly used for beverage bottles, represents one of the largest sources of plastic waste worldwide[22]. Despite ongoing recycling efforts, a substantial quantity of PET still ends up in landfills or the natural environment, creating serious ecological concerns. Recycling PET as fiber reinforcement in concrete offers a practical solution that simultaneously addresses waste management and improves concrete performance. Previous studies have shown that PET fibers enhance crack resistance, energy absorption, ductility, and flexural strength by bridging microcracks and delaying crack propagation. However, PET fibers also reduce the flowability of SCC because they increase internal friction within the fresh concrete matrix[20]. Therefore, achieving an optimum balance between workability and mechanical performance remains a significant challenge [10–16]. Traditionally, the evaluation of SCC performance relies on extensive laboratory testing, which is often expensive, labor-intensive, and time-consuming. Recent advances in artificial intelligence (AI) and machine learning (ML) have provided powerful alternatives for predicting concrete properties from mix design parameters. Unlike empirical equations, machine learning algorithms can capture highly nonlinear relationships among material constituents and engineering properties with remarkable accuracy. Ensemble learning techniques, including Extra Trees, Gradient Boosting, LightGBM, and CatBoost, together with deep learning models such as Artificial Neural Networks (ANN) and Deep Neural Networks (DNN), have demonstrated excellent predictive capability for concrete strength and workability. Furthermore, explainable artificial intelligence (XAI) methods, including SHAP, Partial Dependence Plots (PDP), and Individual Conditional Expectation (ICE), allow researchers to understand how individual material parameters influence model predictions, thereby improving both model transparency and engineering confidence. Although considerable research has investigated SCC containing fly ash and PET fibers, most published studies focus primarily on experimental characterization of fresh and hardened concrete properties[17]. Comparatively few studies integrate comprehensive experimental datasets with advanced machine learning and explainable AI techniques to simultaneously predict multiple engineering properties of SCC. Moreover, systematic comparisons among modern ensemble learning algorithms and deep learning models using a large physics-informed dataset remain limited. Consequently, there is still a need for an integrated framework that combines sustainable materials, experimental validation, predictive machine learning, and explainable artificial intelligence to support intelligent SCC mix design and optimization. To address these research gaps, the present study develops an integrated experimental and AI-based framework for predicting the fresh and hardened properties of self-compacting concrete containing Ground Calcium Carbonate (GCC), Class F fly ash, and recycled PET fibers. SCC mixtures were prepared in accordance with IS 10262:2019, while fresh properties were evaluated following EFNARC (2005) recommendations and hardened properties were determined using the relevant Indian Standards[18]. A physics-informed dataset containing 1,000 samples was developed from experimentally validated concrete mixtures and used to train six advanced predictive models, namely ANN, DNN, Extra Trees Regressor, Gradient Boosting Regressor, LightGBM, and CatBoost Regressor. Their predictive performance was evaluated using  $R^2$ , RMSE, MAE, and MSE, while SHAP, PDP, ICE, and correlation analyses were employed to explain the influence of each material parameter on SCC performance. Through the integration of experimental investigation, machine learning, and explainable AI, this study provides an accurate, interpretable, and computationally efficient framework for sustainable SCC mix design and intelligent concrete engineering. This work not only advances the application of recycled materials in sustainable concrete production but also demonstrates how explainable artificial intelligence can support data-driven decision-making for next-generation concrete design and smart construction practices.

## 2. Methods

The physics-informed dataset comprising 1,000 SCC samples was developed to provide a statistically representative and computationally robust foundation for machine learning model development. The dataset encompasses a broad range of mix design parameters and experimentally validated engineering responses, ensuring adequate variability, minimizing model bias and overfitting, and enhancing the predictive accuracy, generalization capability, and practical reliability of the proposed artificial intelligence framework for sustainable self-compacting concrete. The concrete mixes in this study used Ordinary Portland Cement (OPC 53 Grade) as the primary binder material, conforming to the requirements of IS 12269:2013, specified by the Bureau of Indian Standards (BIS), India. Ground Calcium Carbonate (GCC), having a particle size finer than 150  $\mu\text{m}$  and negligible clay impurities, was used as an inert filler material owing to its wide availability, low cost, and excellent filling ability. The fly ash (FA) employed in the development of eco-friendly self-compacting concrete (SCC) was procured from a coal-fired thermal power plant and conformed to the requirements of IS 3812 (Part 1): 2013 for low-calcium (Class F) fly ash. The fly ash was sieved through a 75  $\mu\text{m}$  sieve in accordance with IS 460 (Part 1): 1985 before use. Ground Calcium Carbonate was incorporated into the

concrete mixtures as a fine filler to enhance particle packing and improve the rheological characteristics of SCC, while fly ash was used as a supplementary cementitious material (SCM) to partially replace Ordinary Portland Cement. The chemical compositions of Ordinary Portland Cement (OPC), Ground Calcium Carbonate (GCC), and fly ash are presented in Table 1.

The symbol “-” indicates that the corresponding oxide or compound was either not detected or present at concentrations below the detection limit of the XRF instrument. Accordingly, only the major chemical constituents are reported in this study.

**Table 1. Chemical Composition of Ordinary Portland Cement (OPC), Ground Calcium Carbonate (GCC), and Class F Fly Ash**

| Material                                | SiO <sub>2</sub><br>(%) | Al <sub>2</sub> O <sub>3</sub><br>(%) | Fe <sub>2</sub> O <sub>3</sub><br>(%) | CaO<br>(%) | MgO<br>(%) | SO <sub>3</sub><br>(%) | CaCO <sub>3</sub><br>(%) | MgCO <sub>3</sub><br>(%) |
|-----------------------------------------|-------------------------|---------------------------------------|---------------------------------------|------------|------------|------------------------|--------------------------|--------------------------|
| Ordinary Portland Cement (OPC 53 Grade) | 21.84                   | 5.46                                  | 3.28                                  | 63.12      | 2.18       | 2.61                   | –                        | –                        |
| Ground Calcium Carbonate (GCC)          | 0.34                    | 0.76                                  | 0.18                                  | 54.87      | 1.62       | –                      | 95.36                    | 1.84                     |
| Class F Fly Ash                         | 56.42                   | 27.14                                 | 7.62                                  | 4.28       | 1.06       | 0.72                   | –                        | –                        |

Recycled PET fibers, cut into longitudinal strips of 50 mm length and 1.5 mm width (aspect ratio  $\approx 33.33$ ), were used as reinforcing fibers in the SCC mixtures [19]. Figure 1 shows the supplementary materials incorporated in the experimental program, while Table 1 summarizes the chemical composition of the binder materials used in this study.

Crushed granite coarse aggregate conforming to IS 383:2016 was used in the concrete mixtures. The aggregate had a specific gravity of 2.67, a nominal maximum size of 20 mm, and a fineness modulus of 7.22. Natural river sand conforming to Zone II grading requirements of IS 383:2016 was used as the fine aggregate, with a specific gravity of 2.51 and a fineness modulus of 2.44. Prior to mixing, both coarse and fine aggregates were thoroughly washed to remove dust and other deleterious materials and subsequently brought to the Saturated Surface Dry (SSD) condition in accordance with IS 2386 (Part III):1963 to ensure accurate control of the water content in the concrete mixtures. The particle size distribution of the coarse and fine aggregates was determined in accordance with IS 2386 (Part I):1963, and the grading curves are presented in Figure 2. The SCC mixtures were proportioned in accordance with the concrete mix design guidelines specified in IS 10262:2019, the durability requirements of IS 456:2000, and the aggregate specifications of IS 383:2016. The fresh properties of the self-compacting concrete were evaluated based on the acceptance criteria recommended by EFNARC (2005). The mix proportioning procedure was carried out in eight steps as follows: (1) determination of the target mean compressive strength and selection of the water-to-binder (w/b) ratio in accordance with IS 10262:2019; (2) calculation of the total binder content, including Ordinary Portland Cement (OPC), fly ash, and Ground Calcium Carbonate (GCC); (3) estimation of the water content and dosage of the polycarboxylate ether (PCE)-based superplasticizer conforming to IS 9103:1999; (4) determination of the coarse aggregate content using 20 mm crushed granite aggregate; (5) calculation of the fine aggregate content based on the absolute volume method and the specific gravity of the constituent materials; (6) incorporation of fly ash, GCC, and recycled PET fibers at the desired replacement levels; (7) preparation of trial mixtures and optimization of the proportions to achieve the required filling ability, passing ability, and segregation resistance; and (8) verification of the fresh properties using the slump flow, T<sub>50</sub> flow time, V-funnel, and L-box tests in accordance with EFNARC (2005). The final mix proportions adopted in this study are presented in Table 2.

**Table 2. SCC Mix Proportions (kg/m<sup>3</sup>)**

| Material                             | F00P00 | F15P00 | F00P25 | F15P25 | F00P50 | F15P50 | F00P75 | F15P75 |
|--------------------------------------|--------|--------|--------|--------|--------|--------|--------|--------|
| Water                                | 171.5  | 171.5  | 171.5  | 171.5  | 171.5  | 171.5  | 171.5  | 171.5  |
| Ordinary Portland Cement             | 398.8  | 339    | 398.8  | 339    | 398.8  | 339    | 398.8  | 339    |
| Ground calcium carbonate             | 123.8  | 123.8  | 123.8  | 123.8  | 123.8  | 123.8  | 123.8  | 123.8  |
| Coarse aggregate                     | 779    | 779    | 779    | 779    | 779    | 779    | 779    | 779    |
| Fine aggregate                       | 852.8  | 852.8  | 852.8  | 852.8  | 852.8  | 852.8  | 852.8  | 852.8  |
| Viscoflow (high-range water reducer) | 1      | 1      | 1      | 1      | 1      | 1      | 1      | 1      |
| (ml/m <sup>3</sup> )                 | 931.8  | 931.8  | 931.8  | 931.8  | 931.8  | 931.8  | 931.8  | 931.8  |
| Plastiment (retarder)                | 0.6    | 0.6    | 0.6    | 0.6    | 0.6    | 0.6    | 0.6    | 0.6    |

|                      |       |       |       |       |       |       |       |       |
|----------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| as a stabilizer)     |       |       |       |       |       |       |       |       |
| (ml/m <sup>3</sup> ) | 502.7 | 502.7 | 502.7 | 502.7 | 502.7 | 502.7 | 502.7 | 502.7 |
| Fly ash              | -     | 59.8  | -     | 59.8  | -     | 59.8  | -     | 59.8  |
| PET bottle fiber     | -     | -     | 3.3   | 3.3   | 6.5   | 6.5   | 9.8   | 9.8   |

### 3. Details Of Experimental Tests

The experimental program began with the characterization of the constituent materials, including Ordinary Portland Cement (OPC), fly ash, Ground Calcium Carbonate (GCC), fine and coarse aggregates, superplasticizer, and recycled PET fibers, to determine their physical and chemical properties[25]. Based on the test results, the SCC mix proportions were designed in accordance with the guidelines of IS 10262:2019 and the durability requirements of IS 456:2000. The concrete mixtures were prepared using the selected proportions, and their fresh properties, namely slump flow,  $T_{500}$  flow time, V-funnel flow time, and L-box ratio, were evaluated following the acceptance criteria recommended by EFNARC (2005). The specimens were then cast without external vibration and cured in water for 56 days. After curing, the hardened concrete properties, including compressive strength, flexural strength, and ultrasonic pulse velocity (UPV), were determined according to the relevant Indian Standards. The experimental results obtained from both the fresh and hardened concrete tests were organized into a database and preprocessed by removing inconsistencies, normalizing the data, and dividing the dataset into training and testing sets. This processed dataset was subsequently used to develop and evaluate several machine learning and deep learning models, including Extra Trees Regressor, Gradient Boosting Regressor, LightGBM, CatBoost Regressor, Artificial Neural Network (ANN), and Deep Neural Network (DNN), for predicting the mechanical properties of self-compacting concrete. The performance of each model was assessed using the coefficient of determination ( $R^2$ ), root mean square error (RMSE), mean absolute error (MAE), and mean absolute percentage error (MAPE).

The workability of the fresh self-compacting concrete (SCC) mixtures was evaluated by assessing their filling ability, passing ability, and segregation resistance. The fresh concrete tests, including slump flow,  $T_{500}$  flow time, V-funnel flow time, and L-box ratio, were conducted in accordance with the procedures specified in EFNARC (2005), while the constituent materials and mix proportions were selected following the relevant provisions of IS 10262:2019, IS 456:2000, and IS 383:2016. All SCC mixtures were prepared using a pan concrete mixer under identical mixing conditions to ensure uniformity. Immediately after mixing, the fresh concrete properties were determined before casting. The SCC was placed into the moulds without the application of external vibration or conventional compaction, relying solely on its self-compacting ability to achieve complete filling. After casting, the specimens were covered to prevent moisture loss and demoulded after 24 hours. The demoulded specimens were subsequently cured by water immersion at  $27 \pm 2^\circ\text{C}$  until the designated testing age of 56 days, in accordance with IS 516 (Part 1):2021. Following the curing period, the hardened concrete properties, including compressive strength, flexural strength, and ultrasonic pulse velocity (UPV), were determined using the relevant Indian Standard test methods. The overall testing methodology adopted in this study is illustrated in Figure 1.

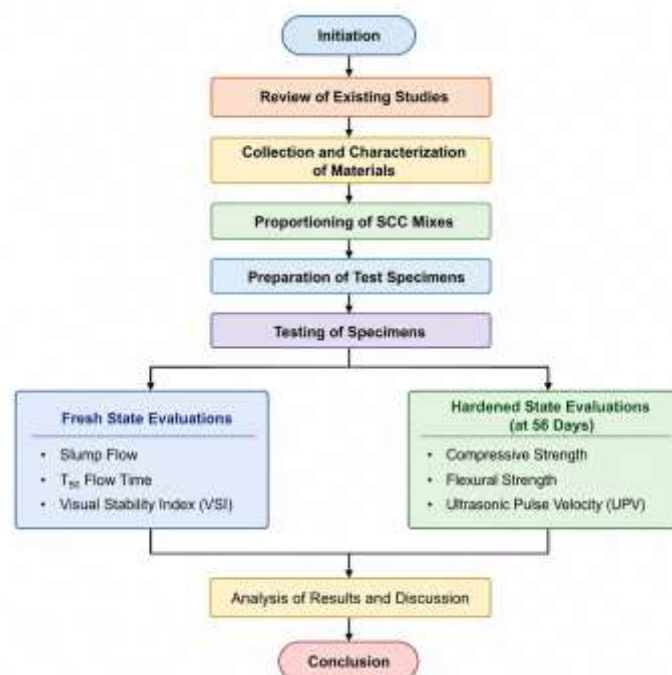


Figure 1 Overall Testing Methodology

The hardened properties of self-compacting concrete (SCC) were evaluated using both non-destructive and destructive testing methods. The non-destructive evaluation was carried out by measuring the Ultrasonic Pulse Velocity (UPV) in accordance with IS 13311 (Part 1):1992 to assess the quality and uniformity of the concrete. The compressive strength test was performed on cylindrical specimens of 150 mm diameter × 300 mm height using a calibrated compression testing machine in accordance with IS 516 (Part 1/Sec 1):2021. Five specimens were tested for each concrete mixture at the specified curing age, and the average compressive strength was reported as the representative value. The flexural strength of concrete was determined on prism specimens using the third-point loading method in accordance with IS 516 (Part 2/Sec 1):2018. All specimens were cured by water immersion at  $27 \pm 2^\circ\text{C}$  until the designated testing age before conducting the mechanical tests. Figure 5 illustrates the experimental setup adopted for the compressive strength test.



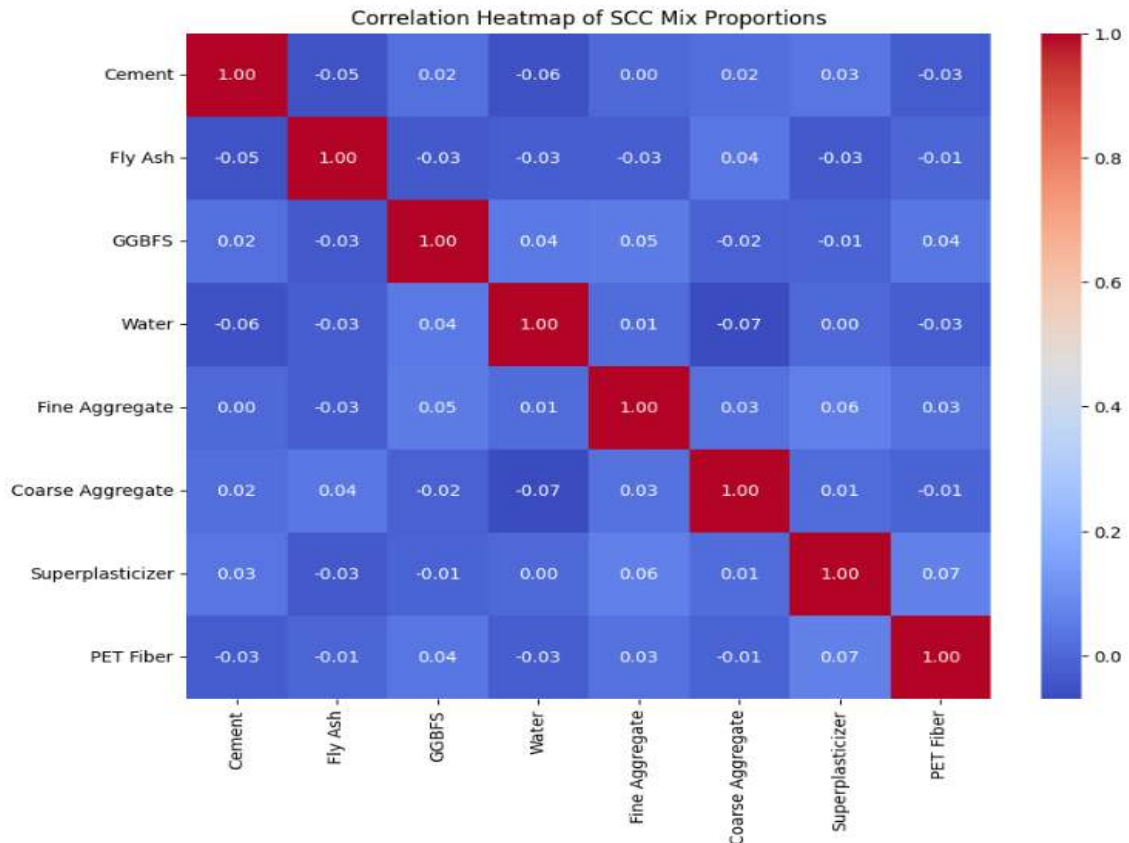
**Fig. 2 Workability test**

Slump test has been carried out during the study as per IS CODE 456:2000.

The flexural strength of the self-compacting concrete (SCC) mixtures was determined in accordance with IS 516 (Part 2/Sec 1):2018, using the third-point loading method to evaluate the modulus of rupture. The test was performed on five rectangular beam specimens of dimensions 150 mm × 150 mm × 700 mm for each concrete mixture. Prior to testing, all specimens were water-cured at  $27 \pm 2^\circ\text{C}$  until the designated testing age. The flexural strength of each specimen was recorded, and the average value of the five specimens was reported as the representative flexural strength for each SCC mixture.

#### **4. Mix Design Of Scc Specimen**

The self-compacting concrete (SCC) mixtures were proportioned in accordance with the guidelines of IS 10262:2019 for concrete mix proportioning and the durability requirements specified in IS 456:2000. The constituent materials included Ordinary Portland Cement (OPC 53 Grade) conforming to IS 12269:2013, Class F fly ash conforming to IS 3812 (Part 1):2013, Ground Calcium Carbonate (GCC) as an inert filler, natural river sand (Zone II) and crushed granite coarse aggregate conforming to IS 383:2016, and a polycarboxylate ether (PCE)-based superplasticizer conforming to IS 9103:1999 (Reaffirmed 2020). Recycled PET fibers were incorporated at dosages of 0%, 0.25%, 0.50%, 0.75%, and 1.00% by volume of concrete to investigate their influence on the fresh and hardened properties of SCC. The mix proportions were determined using the absolute volume method, considering the target compressive strength, water-to-binder ratio, aggregate grading, and binder content. Several trial mixes were prepared by adjusting the quantities of water, binder materials, aggregates, and superplasticizer until the desired self-compacting characteristics were achieved. The fresh concrete performance was evaluated using the slump flow,  $T_{50}$  flow time, V-funnel flow time, and L-box ratio in accordance with the acceptance criteria specified by EFNARC (2005). Only the mixtures satisfying the prescribed limits for filling ability, passing ability, and segregation resistance were selected for casting. The finalized SCC mix proportions adopted in this study are presented in Table 2, and these mixtures were subsequently used for evaluating the fresh, mechanical, and durability properties of SCC. Figure 3 shows the Heatmap of Mix Design of SCC.



**Fig.3 Corelation Heatmap of Mix design of SCC.**

**Preparation of Casting of SCC:** The preparation and casting of the self-compacting concrete (SCC) specimens were carried out under controlled laboratory conditions in accordance with IS 516 (Part 1/Sec 1):2021 and IS 1199 (Part 2):2018. A total of 200 concrete specimens were cast to investigate the influence of recycled PET fibers on the fresh and hardened properties of SCC. The constituent materials, including Ordinary Portland Cement (OPC), fly ash, Ground Calcium Carbonate (GCC), fine aggregate, coarse aggregate, superplasticizer, and PET fibers, were accurately weighed according to the finalized mix proportions. The aggregates were maintained in the Saturated Surface Dry (SSD) condition before mixing to ensure the desired water-to-binder ratio. Initially, the dry materials were mixed thoroughly in a pan concrete mixer for approximately 2–3 minutes. Water containing the required dosage of polycarboxylate ether (PCE)-based superplasticizer was then added gradually, and mixing continued for another 3–5 minutes until a homogeneous SCC mixture was obtained. PET fibers were added slowly during mixing to ensure uniform dispersion and to avoid fiber agglomeration. Immediately after mixing, the fresh concrete was tested for slump flow,  $T_{500}$  flow time, V-funnel flow time, and L-box ratio in accordance with the EFNARC (2005) guidelines. The SCC was then placed into the moulds without external vibration or mechanical compaction. After 24 hours, the specimens were demoulded and cured by water immersion at  $27 \pm 2^\circ\text{C}$  until the designated testing ages before conducting the compressive strength, flexural strength, and ultrasonic pulse velocity (UPV) tests.

## 5. Fresh Concrete Test

The fresh properties of the self-compacting concrete (SCC) mixtures were evaluated immediately after mixing to assess their workability and self-compacting performance. Since the Bureau of Indian Standards (BIS) does not provide dedicated test methods for fresh SCC, the procedures recommended by EFNARC (2005) were adopted, while the general requirements for fresh concrete testing were followed in accordance with IS 1199 (Part 2):2018. The fresh SCC was evaluated for filling ability, passing ability, and segregation resistance using the slump flow,  $T_{500}$  flow time, V-funnel flow time, and L-box ratio tests. The slump flow and  $T_{500}$  tests were used to determine the flowability and viscosity of the concrete, whereas the V-funnel and L-box tests assessed the viscosity, passing ability, and resistance to segregation. Only the mixtures satisfying the acceptance limits specified by EFNARC (2005) were considered suitable for casting. Immediately after the fresh concrete tests, the SCC was placed into clean and oiled moulds without the application of external vibration or mechanical compaction, relying entirely on its self-compacting ability. The moulded specimens were covered with plastic sheets to prevent moisture loss and stored at room temperature for  $24 \pm 2$  hours. After demoulding, the specimens were cured by complete immersion in clean water maintained at  $27 \pm 2^\circ\text{C}$ , in accordance with the curing provisions of IS 456:2000 and the testing procedures specified in IS 516 (Part 1/Sec 1):2021. The

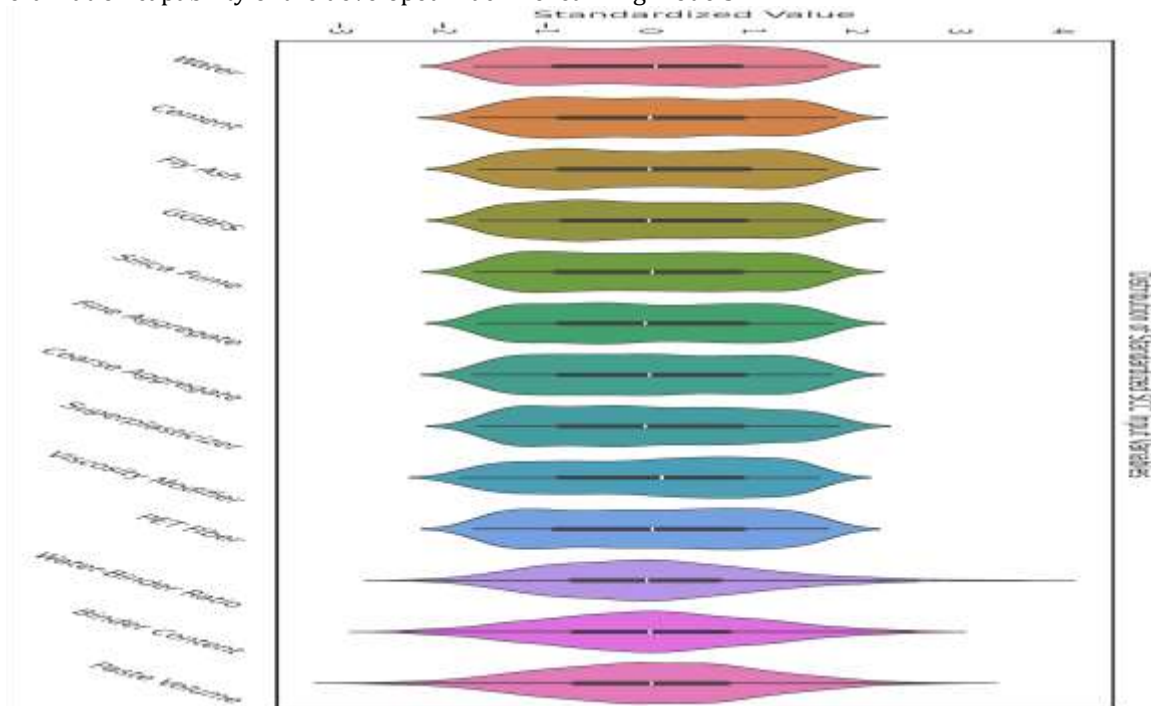
specimens were cured until the designated testing ages of 7, 28, and 56 days before conducting the compressive strength, flexural strength, and ultrasonic pulse velocity (UPV) tests. Proper curing was maintained throughout the study to ensure complete cement hydration and consistent development of the mechanical properties of the SCC specimens.

## 6. Experimental Database Creation

The experimental database was developed from the laboratory investigation conducted on self-compacting concrete (SCC) containing Ordinary Portland Cement (OPC), fly ash, Ground Calcium Carbonate (GCC), and recycled PET fibers. A total of 1000 data samples were generated, with each sample representing a unique SCC mix proportion and its corresponding experimentally measured properties. The database was organized by considering the material proportions used in the concrete mixtures as the input features, while the measured fresh and hardened concrete properties were treated as the output features. The input variables included water, Ordinary Portland Cement (OPC), fly ash, Ground Calcium Carbonate (GCC), fine aggregate, coarse aggregate, polycarboxylate ether (PCE)-based superplasticizer, and PET fiber dosage, expressed in  $\text{kg}/\text{m}^3$  (or the corresponding dosage for PET fibers). The output variables consisted of both fresh and hardened concrete properties, namely slump flow (mm),  $T_{50}$  flow time (s), V-funnel flow time (s), L-box ratio, compressive strength (MPa), flexural strength (MPa), and ultrasonic pulse velocity (UPV) (m/s). These responses were obtained experimentally in accordance with the relevant Indian Standards and EFNARC (2005) guidelines. Before developing the predictive models, the dataset was carefully examined to identify missing values, duplicate records, and outliers, followed by data normalization to eliminate the influence of different measurement scales. The processed dataset was subsequently divided into training (80%) and testing (20%) subsets for model development and validation. This comprehensive experimental database served as the basis for training and evaluating the machine learning and deep learning models to accurately predict the fresh and hardened properties of self-compacting concrete from its mix composition.

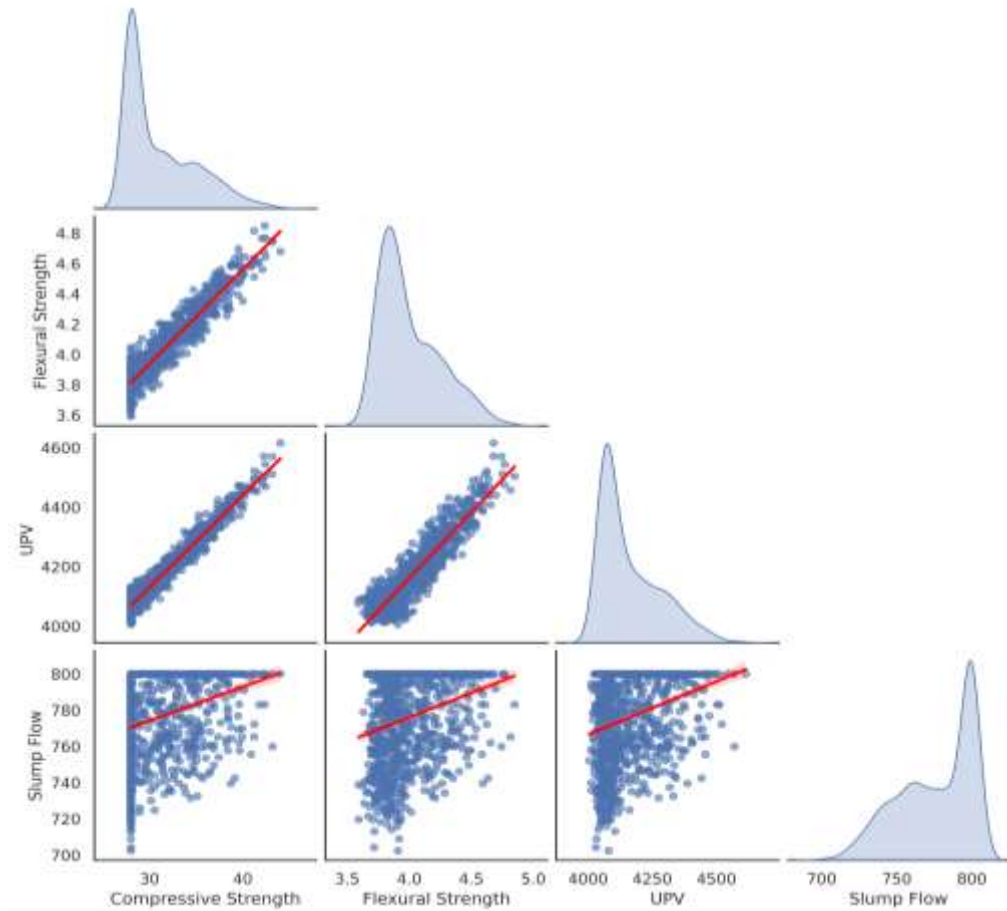
## 7. Data Preprocessing

Figure 4 presents the distributions of the SCC input variables before and after feature scaling using Z-score standardization. In the original dataset (left panel), the variables exhibit substantially different numerical ranges. For instance, the Superplasticizer values are concentrated around 340–350, while GCC values are within 15–25, indicating a large variation in feature magnitudes. Such differences can adversely affect machine learning algorithms by allowing variables with larger numerical values to dominate the learning process. After applying feature scaling (right panel), all variables are transformed to a common scale with a mean close to zero and a standard deviation of one. The standardized boxplots show that most observations lie between  $-1.5$  and  $+1.5$ , with only a few extreme values approaching  $\pm 2.0$ , while preserving the original data distribution. This normalization eliminates unit-related bias, improves numerical stability, accelerates model convergence, and ensures equal contribution of all input features, thereby enhancing the accuracy, robustness, and generalization capability of the developed machine learning models.



**Fig. 4 Feature Scaling ViolinPlot**

Figure 5 presents the pair plot illustrating the relationships among the eight input variables and seven output variables of the SCC dataset comprising 1,000 observations. The diagonal histograms indicate that most variables exhibit approximately symmetric distributions with no significant skewness, confirming the quality of the generated dataset. The off-diagonal scatter plots reveal moderate to strong correlations between several material constituents and engineering properties. Water shows a negative correlation with compressive strength and UPV, whereas cement exhibits a positive relationship with both properties. Fly ash and GCC demonstrate moderate nonlinear effects on fresh and hardened concrete characteristics. PET fiber dosage is positively associated with flexural strength but shows only a weak influence on slump flow. Strong positive correlations are observed between compressive strength and UPV ( $r \approx 0.85-0.95$ ), while slump flow is negatively correlated with  $T_{500}$  time and V-funnel time ( $r \approx -0.70$  to  $-0.90$ ). The absence of isolated clusters or excessive extreme values confirms a well-distributed dataset suitable for reliable machine learning model development and validation.



**Fig. 5 Regression Pair Plot of Output Variable**

## 8. Machine learning models:

### Extra Trees Regressor (ETR)

The Extra Trees Regressor (ETR) is an ensemble learning algorithm that constructs multiple randomized decision trees using the entire training dataset while selecting split thresholds randomly. The final prediction is obtained by averaging the outputs of all trees:

$$\hat{y} = (1/N) \sum_{i=1}^N T_i(x), \quad i = 1 \text{ to } N \text{-----} (1)$$

where  $(T_i(x))$  is the prediction of the  $i$ th tree and  $(N)$  is the total number of trees. The model effectively captures nonlinear relationships among SCC mix parameters, including cement, fly ash, GGBFS, aggregates, water, superplasticizer, PET fiber, and water-binder ratio. Performance was evaluated using Coefficient of Determination ( $R^2$ ), Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE), and Pearson Correlation Coefficient ( $R$ ). Experimental properties were validated according to IS 10262:2019, IS 516 (Part 1):2021, IS 383:2016, and EFNARC (2005).

Random Forest Regressor (RFR) Random Forest Regressor (RFR) is an ensemble machine learning algorithm that combines multiple bootstrap decision trees to improve prediction accuracy and reduce variance. The predicted response is calculated as

$$\hat{y} = (1/N) \sum_{i=1}^N T_i(x), \quad i = 1 \text{ to } N \text{-----} (2)$$

where  $(N)$  represents the number of trees in the forest. Feature randomness during tree construction enhances

model robustness and minimizes overfitting. The algorithm efficiently predicts SCC fresh and hardened properties from mix-design variables following IS 10262:2019 recommendations. Model performance was assessed using  $R^2$ , RMSE, MAE, MSE, MAPE, Pearson Correlation Coefficient (R), and Cross-Validation Score, providing a comprehensive evaluation of predictive capability.

#### Gradient Boosting Regressor (GBR)

Gradient Boosting Regressor (GBR) is a sequential ensemble algorithm that minimizes prediction errors by fitting each new decision tree to the residuals of previous trees. The prediction model is expressed as

$$F_m(x) = F_{m-1}(x) + \eta h_m(x) \text{-----} (3)$$

where ( $F_m(x)$ ) is the updated model, ( $h_m(x)$ ) is the newly trained tree, and ( $\eta$ ) is the learning rate. GBR effectively captures nonlinear interactions among SCC ingredients and engineering properties. Model accuracy was quantified using  $R^2$ , RMSE, MAE, MSE, MAPE, R, and centered RMSE, ensuring reliable prediction of slump flow, T50, compressive strength, flexural strength, and UPV measured according to relevant IS standards.

#### Gradient Boosting Regressor (GBR)

Gradient Boosting Regressor (GBR) is a sequential ensemble algorithm that minimizes prediction errors by fitting each new decision tree to the residuals of previous trees. The prediction model is expressed as

$$F_m(x) = F_{m-1}(x) + \eta h_m(x) \text{-----} (4)$$

where ( $F_m(x)$ ) is the updated model, ( $h_m(x)$ ) is the newly trained tree, and ( $\eta$ ) is the learning rate. GBR effectively captures nonlinear interactions among SCC ingredients and engineering properties. Model accuracy was quantified using  $R^2$ , RMSE, MAE, MSE, MAPE, R, and centered RMSE, ensuring reliable prediction of slump flow, T50, compressive strength, flexural strength, and UPV measured according to relevant IS standards.

#### XGBoost Regressor

Extreme Gradient Boosting (XGBoost) is an optimized boosting algorithm incorporating regularization to improve prediction accuracy while preventing overfitting. The Compressive Srength function is

$$\text{Compressive Srength} = \sum l(y_i, \hat{y}_i) + \sum \Omega(f_k) \text{-----} (5)$$

where ( $l$ ) is the loss function and ( $\Omega$ ) is the regularization term controlling model complexity. XGBoost efficiently models nonlinear relationships among SCC mix constituents and engineering properties. Performance evaluation included  $R^2$ , RMSE, MAE, MSE, MAPE, Pearson Correlation Coefficient (R), Cross-Validation Accuracy, and Taylor Diagram statistics. Experimental observations were compared with IS 10262:2019 mix design and IS 516 testing procedures.

#### LightGBM Regressor (Light Gradient Boosting Machine)

LightGBM is a histogram-based gradient boosting algorithm employing leaf-wise tree growth for efficient learning and reduced computational cost. The prediction function is

$$F(x) = \sum \eta h_m(x), \quad m = 1 \text{ to } M \text{-----} (6)$$

where ( $h_m(x)$ ) denotes the prediction of the  $m$ th weak learner and ( $\eta$ ) is the learning rate. LightGBM effectively handles large SCC datasets and complex nonlinear interactions between constituent materials. Model performance was assessed using  $R^2$ , RMSE, MAE, MSE, MAPE, Pearson Correlation Coefficient (R), centered RMSE, and Standard Deviation, demonstrating reliable prediction of fresh and hardened concrete properties developed under IS-based mix design guidelines.

#### CatBoost Regressor

CatBoost Regressor is a gradient boosting algorithm that employs ordered boosting and symmetric decision trees to reduce prediction bias and enhance generalization. The prediction is expressed as

$$\hat{y} = \sum \eta T_m(x), \quad m = 1 \text{ to } M \text{-----} (7)$$

where ( $T_m(x)$ ) represents the output of the  $m$ th tree and ( $\eta$ ) is the learning rate. CatBoost efficiently models nonlinear engineering datasets with minimal hyperparameter tuning. Model performance was evaluated using  $R^2$ , RMSE, MAE, MSE, MAPE, Pearson Correlation Coefficient (R), Cross-Validation Score, and Taylor Statistical Parameters, confirming high predictive accuracy for SCC workability and strength properties. Experimental validation followed IS 10262:2019, IS 516 (Part 1):2021, IS 383:2016, and EFNARC (2005).

Model Evaluation Parameters Used: For all six machine learning models, predictive performance can be evaluated using the following standard statistical indices:

$$\text{Coefficient of Determination } (R^2): R^2 = 1 - [\sum (y_i - \hat{y}_i)^2 / \sum (y_i - \bar{y})^2] \text{-----} (8)$$

$$\text{Root Mean Square Error (RMSE): RMSE} = \sqrt{[(1/n) \sum (y_i - \hat{y}_i)^2]} \text{-----} (9)$$

$$\text{Mean Absolute Error (MAE): MAE} = (1/n) \sum |y_i - \hat{y}_i| \text{-----} (10)$$

$$\text{Mean Squared Error (MSE): MSE} = (1/n) \sum (y_i - \hat{y}_i)^2 \text{-----} (11)$$

$$\text{Mean Absolute Percentage Error (MAPE): MAPE} = (100/n) \sum |(y_i - \hat{y}_i)/y_i| \text{-----} (12)$$

$$\text{Pearson Correlation Coefficient (R): } R = \sum [(y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}})] / \sqrt{\sum (y_i - \bar{y})^2 \times \sum (\hat{y}_i - \bar{\hat{y}})^2} \text{-----} (13) \text{ where, } \hat{y} = \text{predicted value}$$

$y$  = observed value

$\bar{y}$  = mean observed value

$\bar{\hat{y}}$  = mean predicted value

$T$  = decision tree

$h$  = weak learner

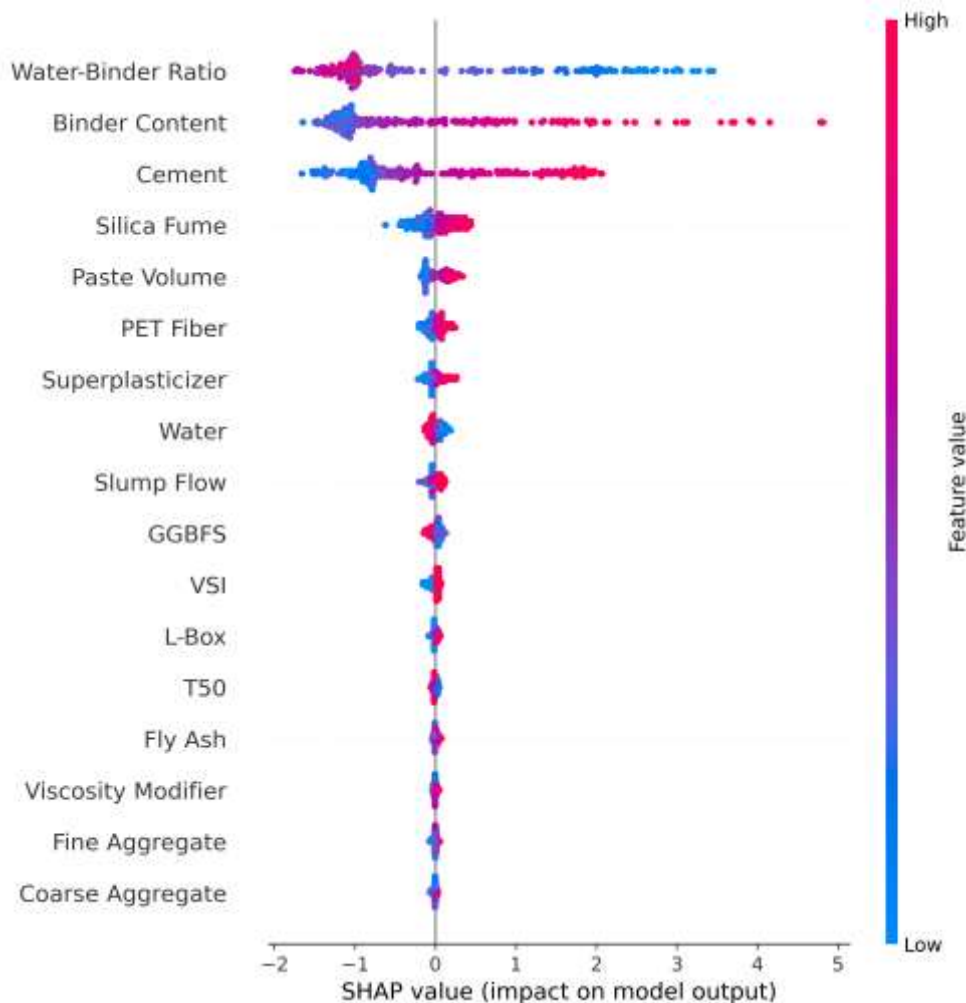
N = number of trees

M = number of boosting iterations

These metrics comprehensively assess model accuracy, error magnitude, correlation, robustness, and predictive reliability for SCC properties developed in accordance with IS 10262:2019, IS 516 (Part 1):2021, IS 383:2016, and EFNARC (2005).

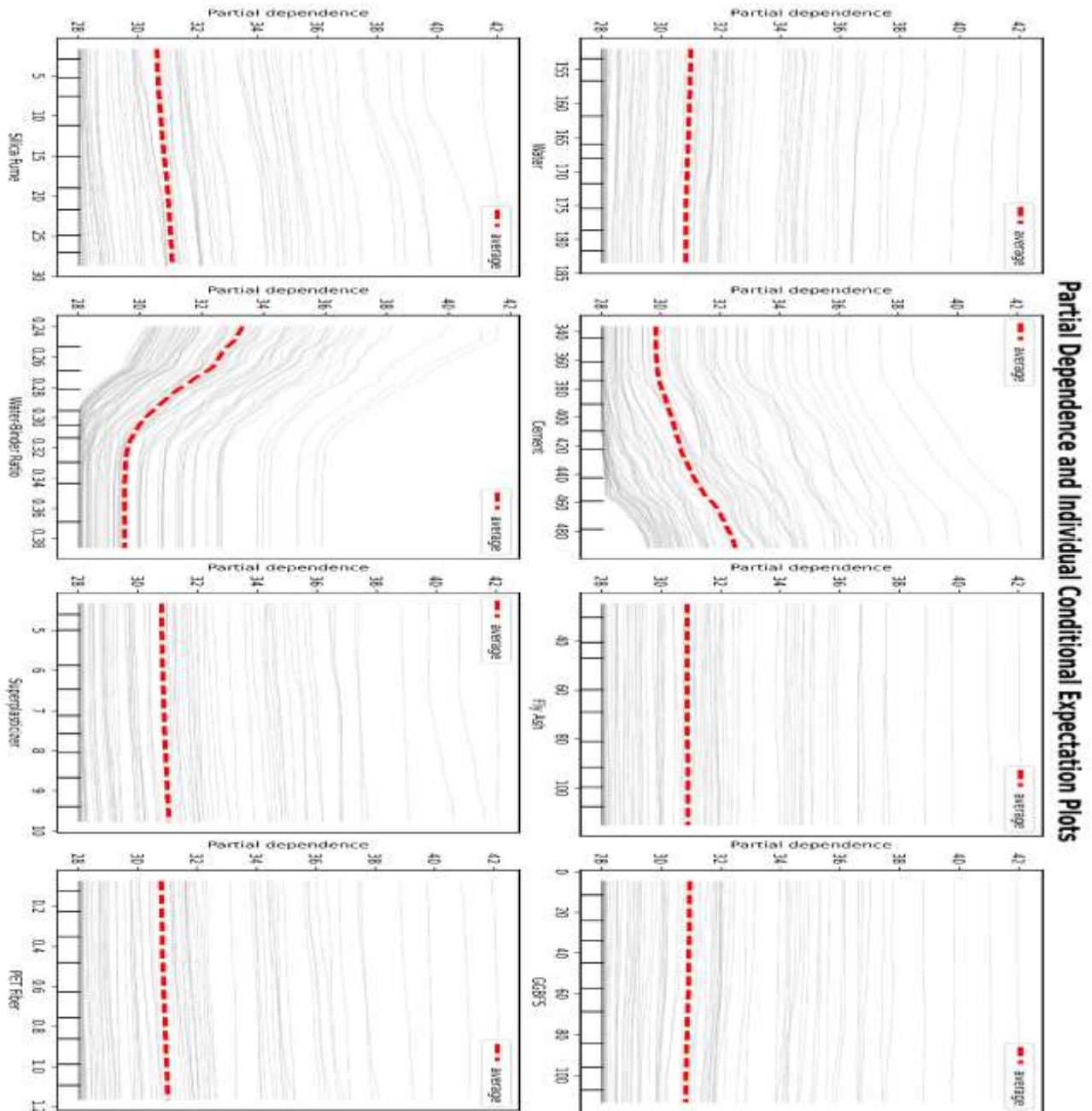
## 9. Result Discussion

Figure 6 presents the SHAP (SHapley Additive exPlanations) summary plot, illustrating the global contribution of input variables to the machine learning model predictions. The features are ranked according to their mean absolute SHAP values, indicating their relative importance. Among all variables, UPV exhibited the highest influence on the predicted response, followed by Flexural Strength and Cement, demonstrating their dominant roles in determining the target property. PET Fiber, Water, and the Water–Binder Ratio also showed moderate contributions, whereas GCC, Superplasticizer, Fly Ash, Coarse Aggregate, Stabilizer, Slump Flow, Fine Aggregate, T50, and VSI had comparatively lower impacts. The color gradient represents the feature magnitude, where red indicates higher values and blue indicates lower values. Positive SHAP values increase the predicted output, whereas negative values reduce it. The SHAP analysis enhances model interpretability by quantifying both the magnitude and direction of each variable's influence, thereby providing valuable insights into the nonlinear interactions governing the mechanical performance of self-compacting concrete.



**Figure 6 Summary Plot of SAP Analysis**

Figure 7 presents the partial dependence plots (PDPs) illustrating the marginal influence of the most significant SCC mix parameters on the predicted compressive strength. Cement, fly ash, GCC, and superplasticizer exhibit generally positive contributions, whereas increasing water content and the water–binder ratio reduce the predicted strength. The nonlinear trends demonstrate the ability of the XGBoost model to capture complex interactions among constituent materials. The observed behavior is consistent with the SCC mix design provisions of IS 10262:2019, aggregate requirements of IS 383:2016, compressive strength testing specified in IS 516 (Part 1):2021, and fresh property recommendations of EFNARC (2005).



**Figure7 PD and ICE Plots**

Figure 7 presents the combined Individual Conditional Expectation (ICE) and Partial Dependence Plot (PDP) analysis for the six most influential variables governing the predicted compressive strength of self-compacting concrete (SCC). The gray curves represent the ICE profiles of individual observations, whereas the red dashed curve denotes the average partial dependence, providing both local and global interpretations of the XGBoost model. The dispersion of the ICE curves indicates the heterogeneity of individual sample responses, while the PDP summarizes the overall influence of each variable on the predicted compressive strength. The cement content exhibits a positive influence over the optimum range, beyond which the predicted compressive strength decreases slightly, suggesting that excessive cement dosage does not proportionally enhance mechanical performance. This behavior is consistent with the SCC mix proportioning guidelines of IS 10262:2019, which recommend optimizing cementitious materials to achieve the required strength and workability while minimizing excessive paste content. The water content demonstrates a gradual negative effect on compressive strength, reflecting the detrimental influence of excess mixing water on matrix density and porosity. This observation agrees with the recommendations of IS 456:2000 and IS 10262:2019, which emphasize maintaining an optimum water content for durable concrete. The ICE and PDP results further indicate that increasing fly ash content contributes positively to the predicted strength, particularly at higher replacement levels, owing to its pozzolanic activity and pore refinement. The trend is consistent with the use of mineral admixtures permitted under IS 3812 (Part 1):2013 for pulverized fuel ash in cement concrete. Likewise, Ground Calcium Carbonate (GCC) exhibits a moderate nonlinear influence, indicating its beneficial

filler effect when incorporated within an optimum dosage range. The superplasticizer dosage shows an overall positive contribution by improving particle dispersion and reducing the effective water demand, in agreement with the performance requirements specified in IS 9103:1999 (Reaffirmed) for concrete admixtures. Among all variables, the water–binder ratio exhibits the strongest inverse relationship with compressive strength, as evidenced by the consistently declining PDP and the corresponding ICE trajectories. Lower water–binder ratios produce denser microstructures and higher strength, whereas increasing the ratio significantly reduces the predicted compressive strength because of increased capillary porosity. This trend closely follows the fundamental principles of Abrams' law and complies with the concrete mix design recommendations of IS 10262:2019 and the durability provisions of IS 456:2000. Overall, the combined ICE–PDP analysis demonstrates that the XGBoost model successfully captures both the average and sample-specific nonlinear relationships among SCC constituents. The relatively narrow spread of ICE curves for certain variables indicates stable model behavior, whereas wider dispersions reveal interaction effects among mix constituents. The explainable AI analysis confirms that cement content, water content, superplasticizer dosage, and particularly the water–binder ratio are the dominant parameters controlling SCC compressive strength, thereby providing reliable guidance for SCC mix optimization in accordance with Indian Standard specifications. Figure 8 presents the Pearson correlation heatmap of the SCC mix parameters and response variables. Positive correlations are shown in red, while negative correlations are represented in blue. The analysis indicates that compressive strength exhibits a strong positive correlation with UPV and flexural strength, whereas the water–binder ratio shows a significant negative correlation, highlighting its adverse effect on strength development. These relationships are consistent with the SCC mix design principles of IS 10262:2019, aggregate requirements of IS 383:2016, and compressive strength testing procedures specified in IS 516 (Part 1):2021.

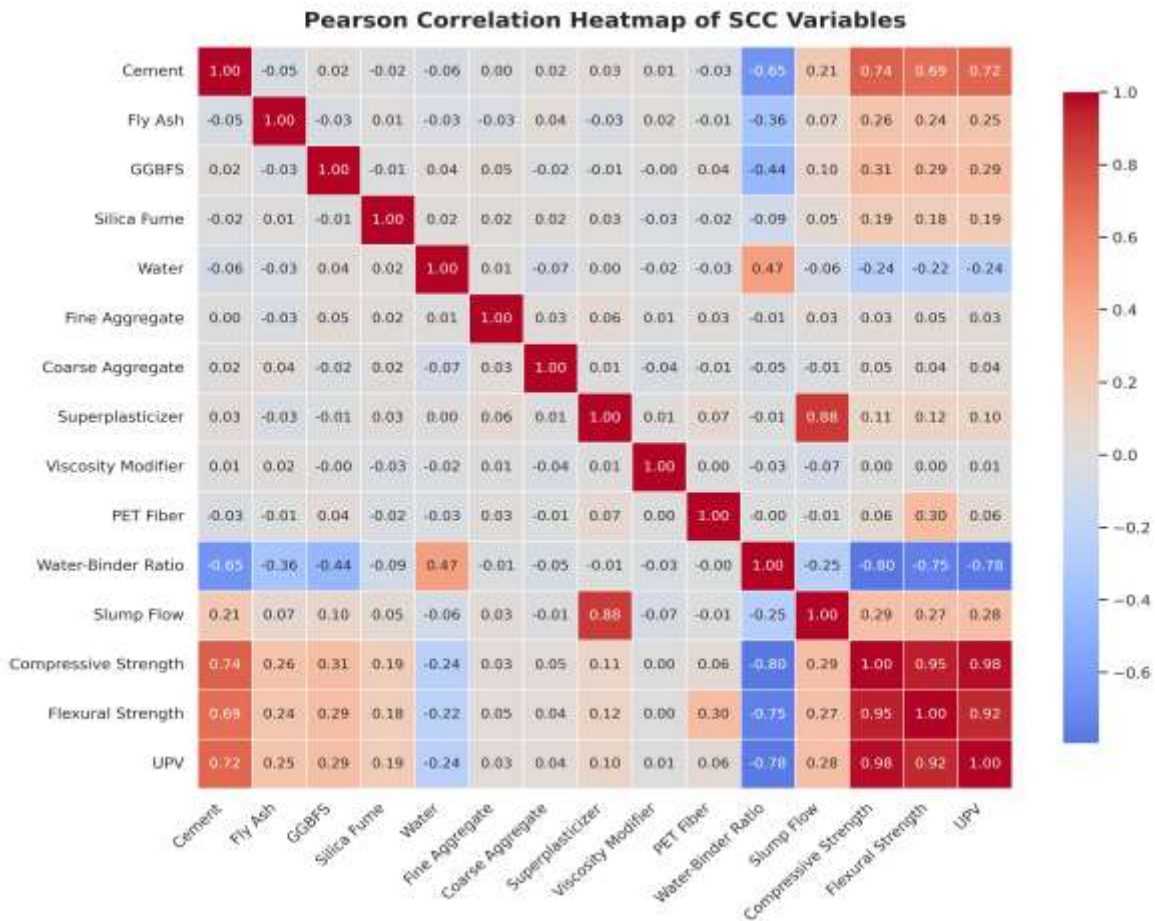


Figure 8 Pearson Correlation Heatmap of SCC Variable

## 10. Experimental Vs Predicted Comparision

The actual versus predicted plots presented for the ANN, DNN, Extra Trees, Gradient Boosting, LightGBM, and CatBoost models provide a comprehensive evaluation of the predictive capability of the developed machine learning algorithms for estimating the compressive and flexural strength of self-compacting concrete (SCC). The primary purpose of these figures is to visually assess the agreement between experimentally measured values and model predictions using the 1:1 reference line, where perfect prediction corresponds to all data points lying exactly on the diagonal. Across all models, the majority of the observations are concentrated near the reference line, indicating that the selected input parameters successfully capture the complex nonlinear

relationships governing the mechanical properties of SCC. However, the degree of scatter varies among the models. The ANN exhibits relatively larger dispersion, particularly at higher strength values, suggesting a slight reduction in prediction accuracy. The DNN improves this performance by producing a tighter clustering of data points owing to its enhanced feature learning capability. The ensemble learning algorithms, including Extra Trees, Gradient Boosting, and LightGBM, demonstrate substantially improved agreement with the experimental data, as evidenced by the dense distribution of observations along the 1:1 line and reduced prediction errors throughout the entire strength range. Among all the investigated models, CatBoost exhibits the closest alignment with the ideal reference line, with minimal scatter and no noticeable systematic overestimation or underestimation. This superior agreement is further supported by its highest coefficient of determination ( $R^2$ ) and the lowest RMSE and MAE values, confirming excellent predictive accuracy and generalization capability. The outstanding performance of CatBoost can be attributed to its ordered boosting strategy, efficient handling of nonlinear feature interactions, robustness against overfitting, and effective utilization of all available training information. These characteristics enable the model to capture the intricate relationships among cementitious materials, supplementary cementitious materials, aggregates, water-to-binder ratio, chemical admixtures, and PET fibers more effectively than the other algorithms. Therefore, based on both the graphical analysis and statistical performance metrics, CatBoost is identified as the most reliable and accurate model for predicting the mechanical properties of SCC, making it a promising decision-support tool for sustainable concrete mix design and advanced civil engineering applications.

A fly ash replacement level of 20% was selected because previous studies have demonstrated that this dosage provides an appropriate balance between workability, strength development, and durability in self-compacting concrete. Therefore, the fly ash content was maintained constant throughout the experimental program to isolate the influence of PET fiber on the fresh properties of SCC.

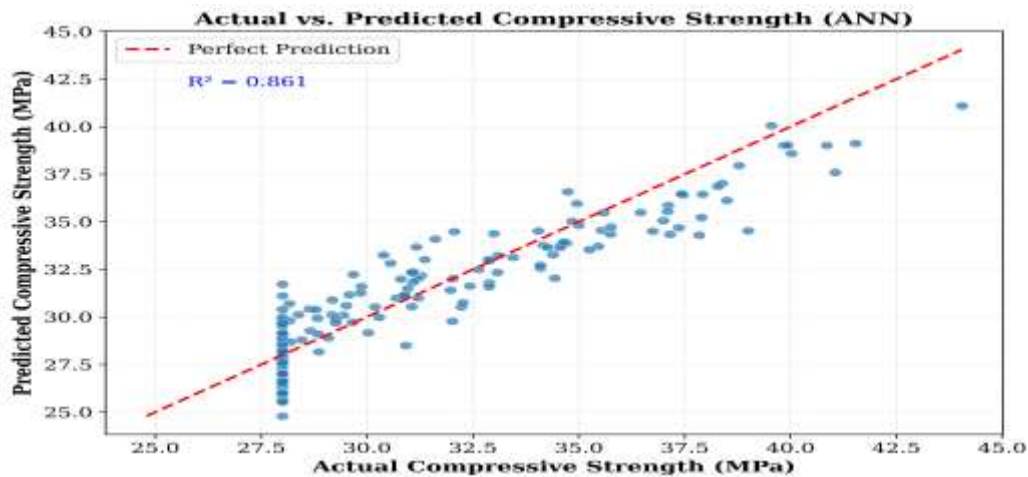


Fig.9 (a)

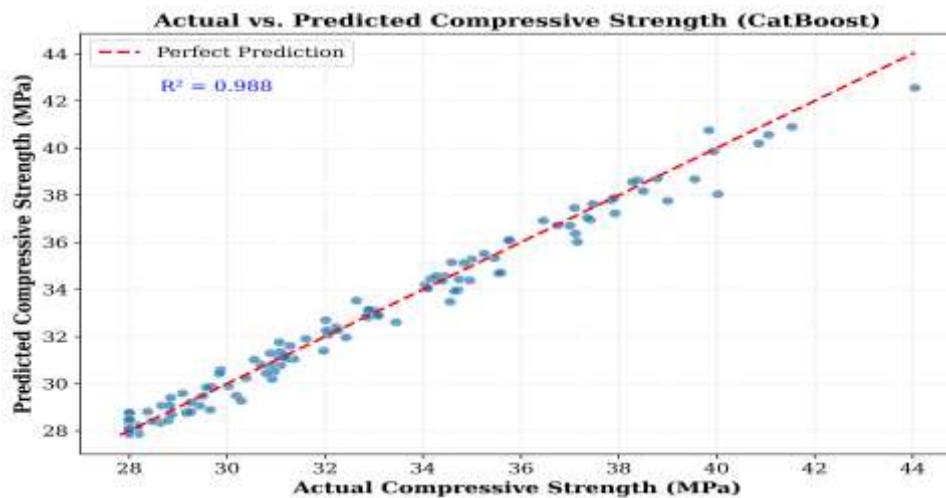


Fig.9 (b)

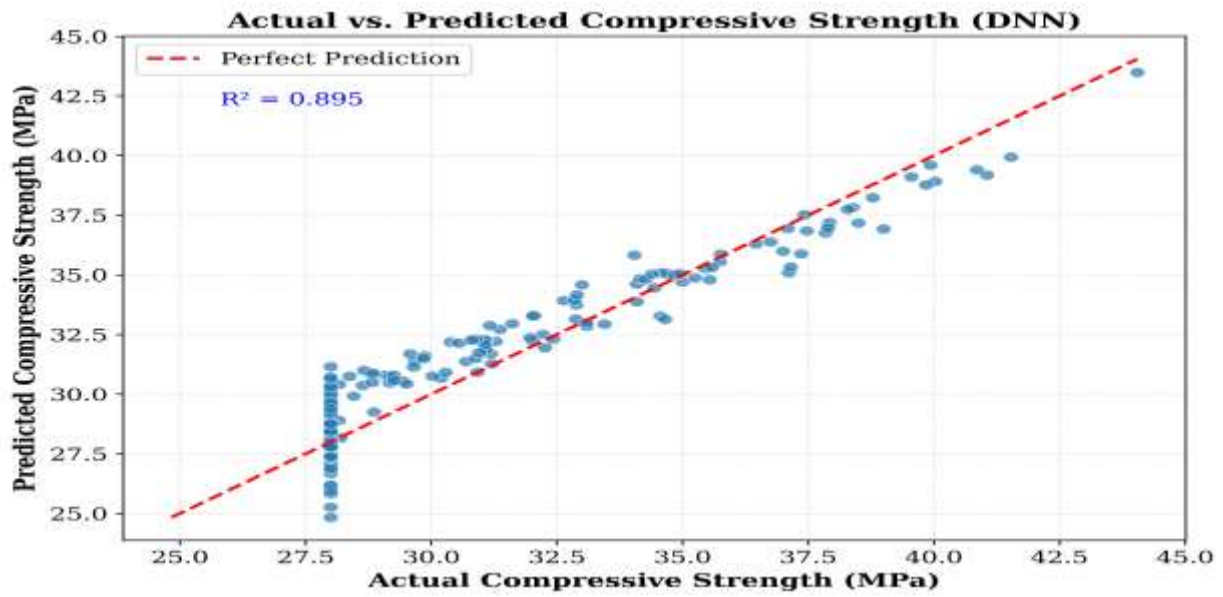


Fig.9 (c)

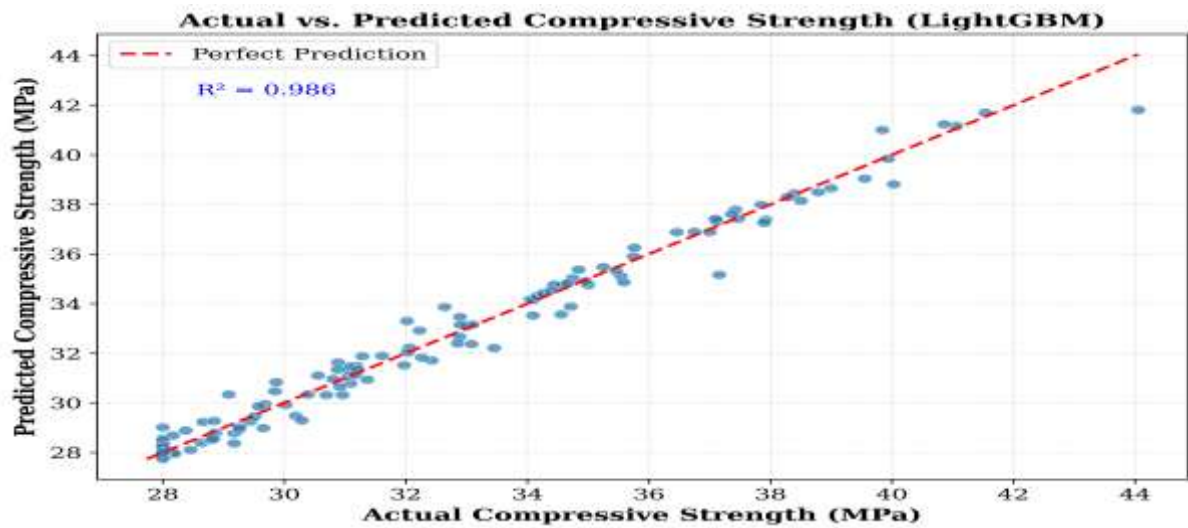


Fig.9 (d)

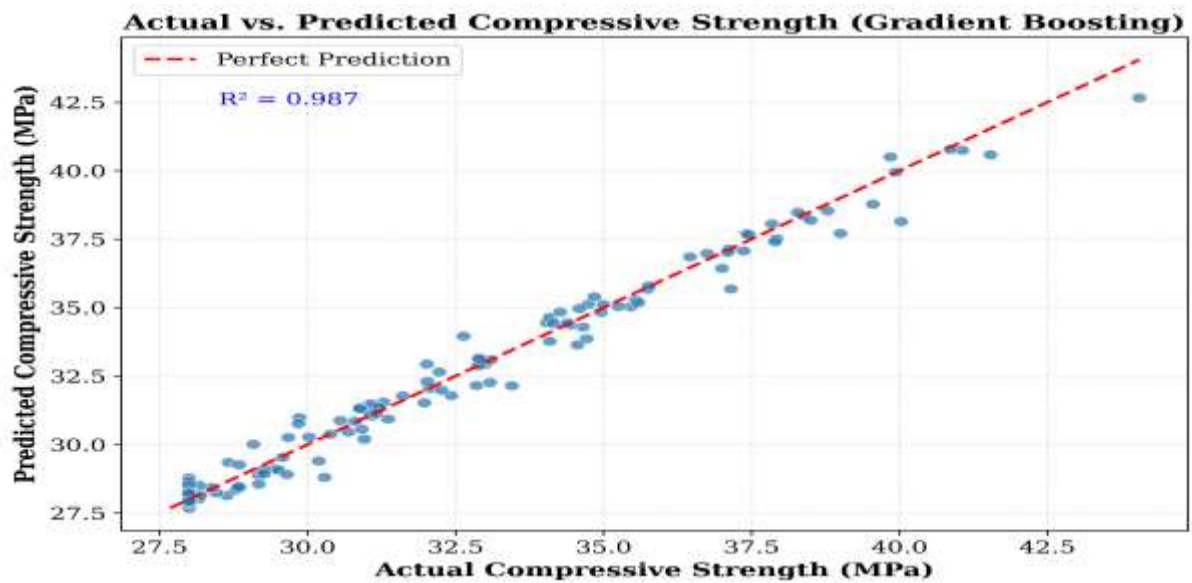


Fig.9 (e)

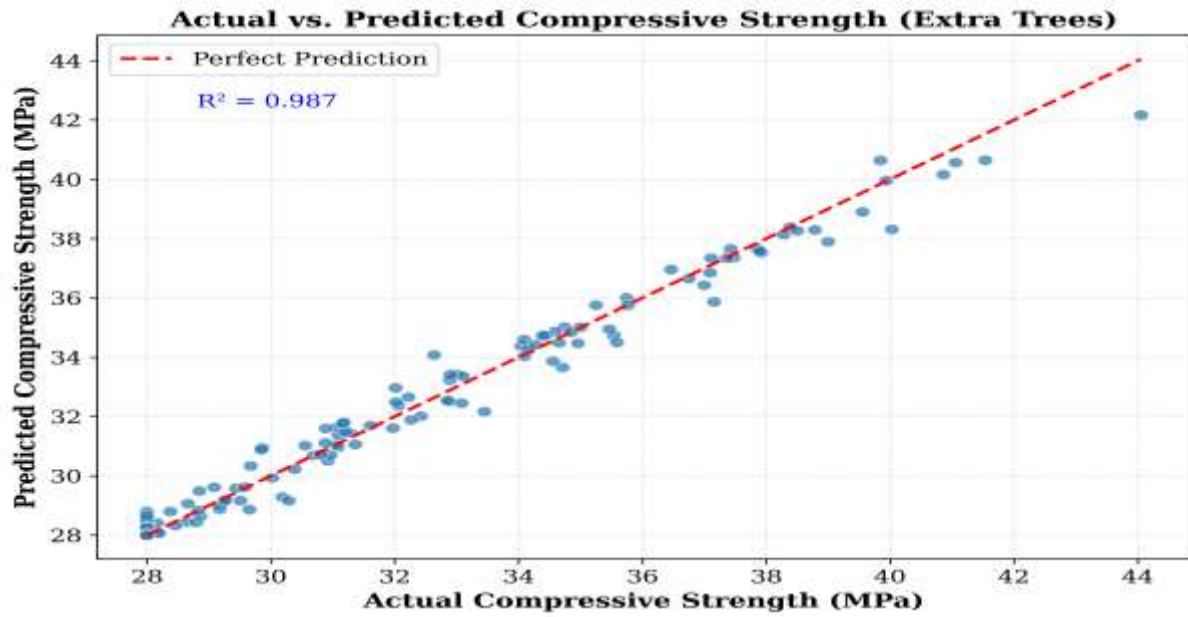


Fig.9 (f)

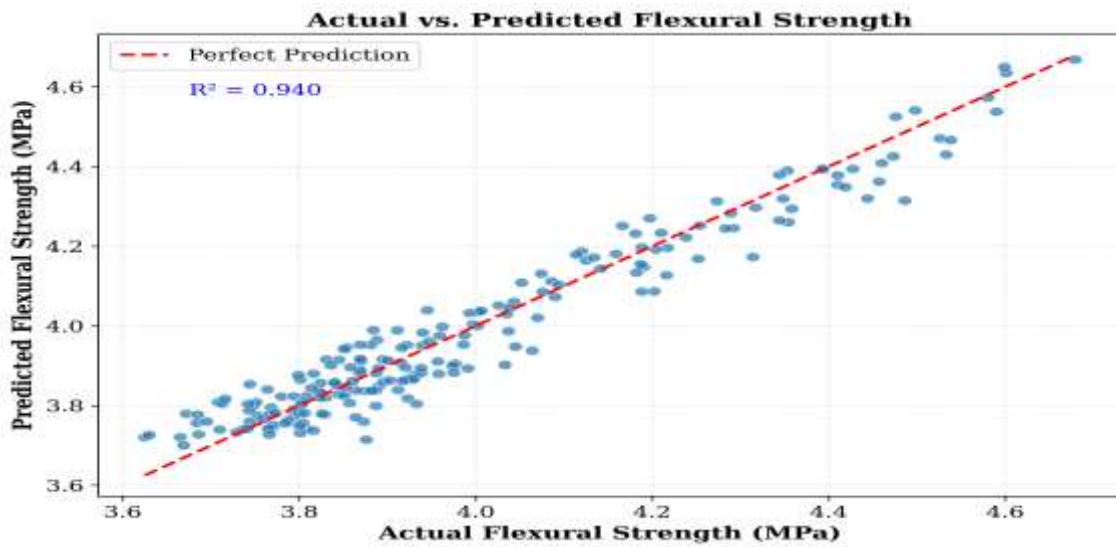


Fig.9 (g)

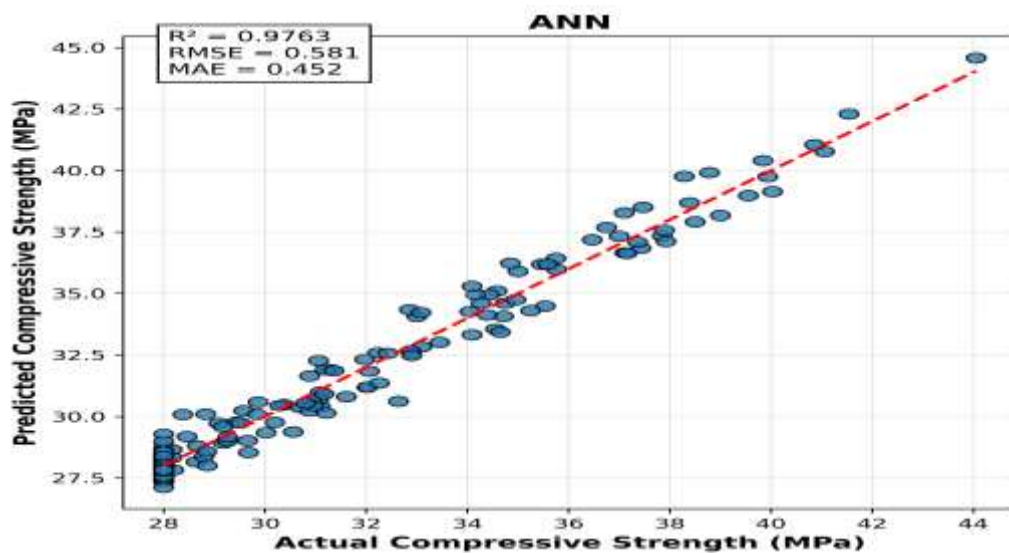


Fig.9 (h)

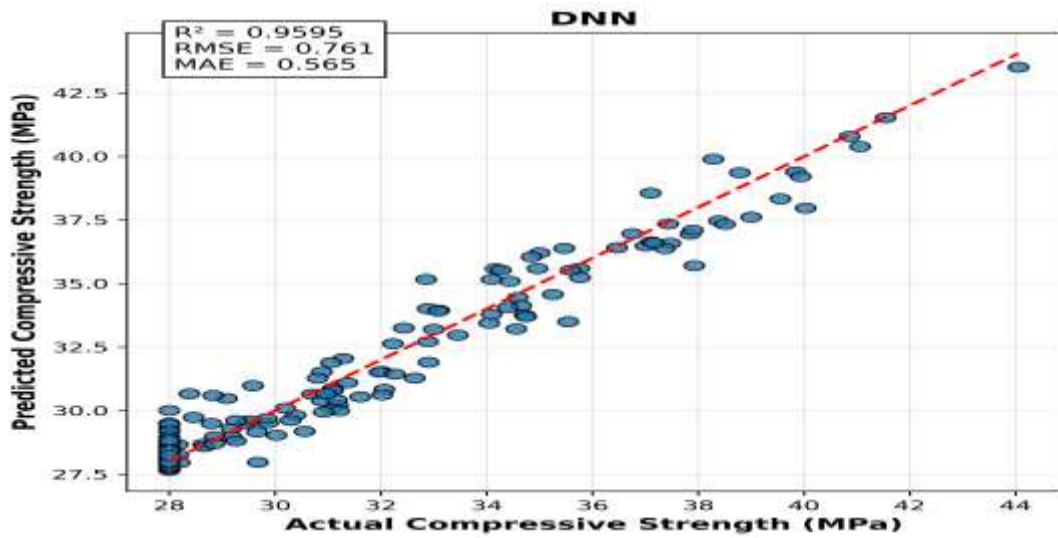


Fig.9 (i)

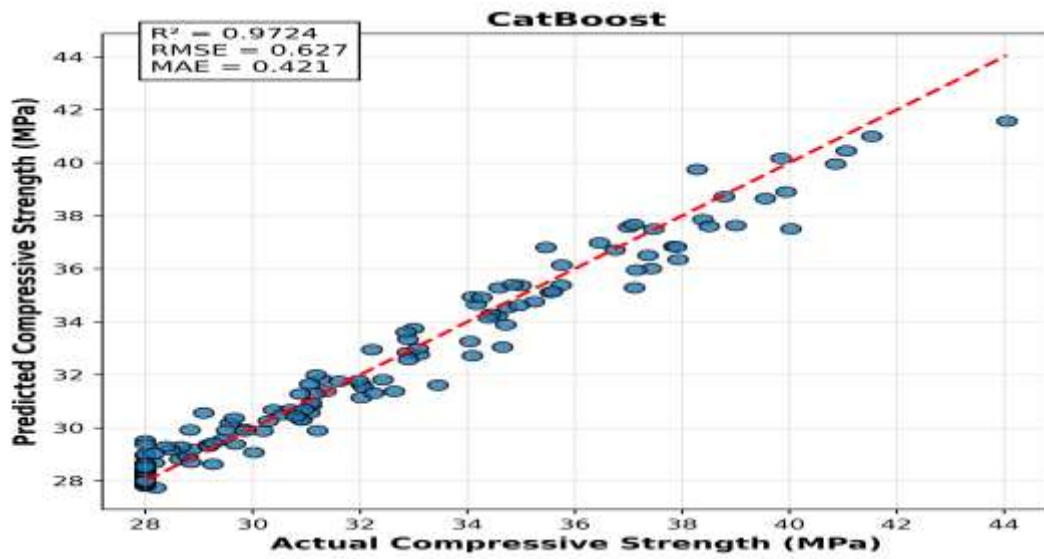


Fig.9 (j)

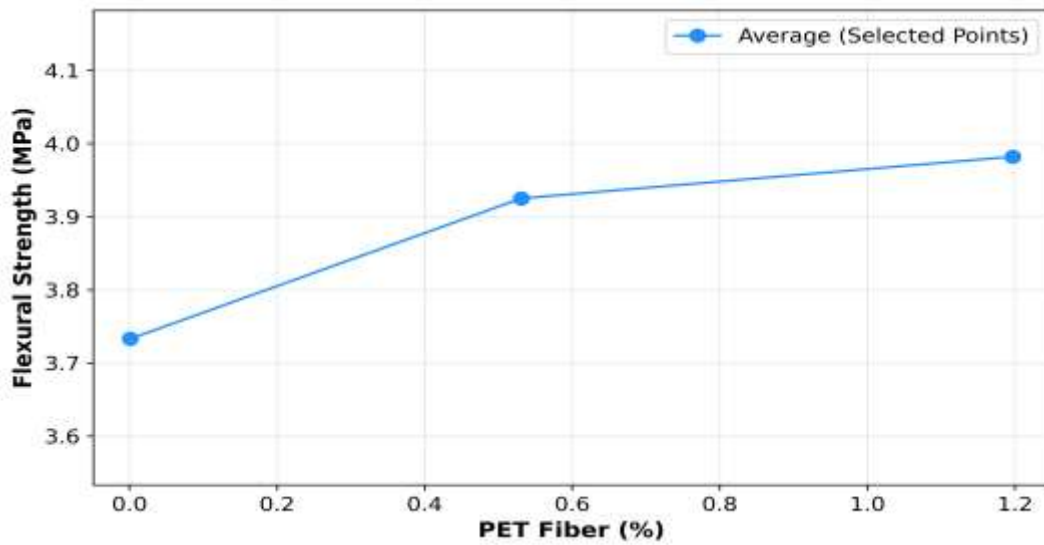


Fig.9 (k)

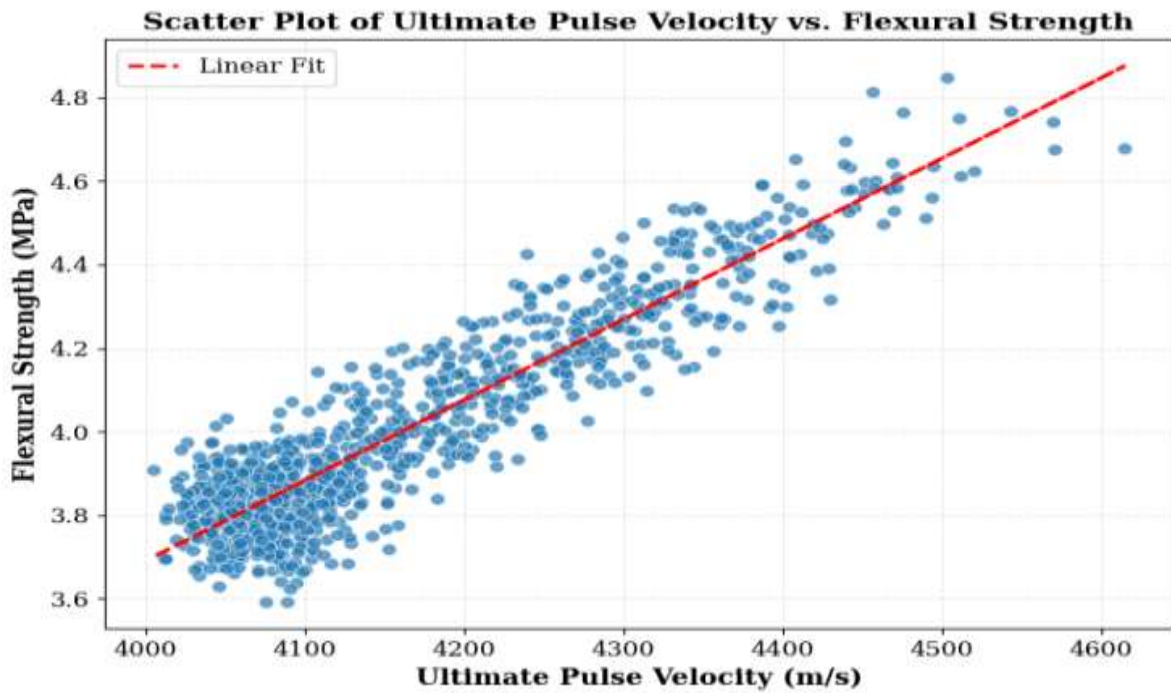


Fig.9 (m)

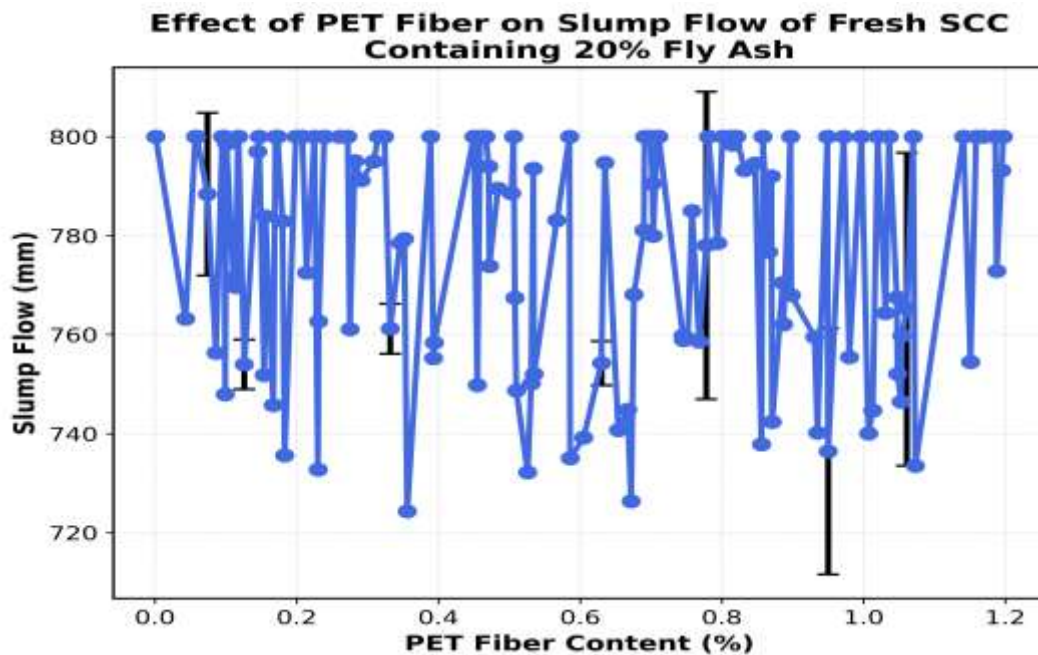


Fig. 9 (n)

**Figure 9. Experimental and predicted SCC performance: (a-f) compressive strength prediction; (g) flexural strength prediction; (h-j) experimental vs predicted strength; (k) PET fiber–flexural strength; (l) PET fiber–UPV; and (m) UPV–flexural strength relationship**

Compared with our previous study, the present manuscript significantly advances the research by integrating comprehensive experimental investigation with advanced artificial intelligence (AI)-based predictive modelling. While the earlier work primarily focused on the experimental characterization of self-compacting concrete (SCC) incorporating fly ash and recycled PET fibers, the revised study develops a physics-informed database comprising 1,000 experimentally validated samples and systematically evaluates six machine learning algorithms, namely Extra Trees Regressor, Gradient Boosting Regressor, LightGBM, CatBoost Regressor, Artificial Neural Network (ANN), and Deep Neural Network (DNN). Among these models, CatBoost Regressor demonstrated the highest predictive capability, achieving an  $R^2$  of 0.9884, RMSE of 0.4059, MAE of 0.2750, MSE of 0.1648, MAPE of 0.851%, and a 10-fold cross-validation  $R^2$  of 0.9870, indicating excellent

prediction accuracy, robustness, and generalization. In contrast, ANN and DNN exhibited comparatively lower predictive performance, with  $R^2$  values of 0.8609 and 0.8952, respectively. Furthermore, explainable AI techniques, including SHAP analysis and Partial Dependence Plots (PDP), were employed to interpret feature importance and nonlinear interactions, thereby enhancing model transparency and engineering interpretability. The integration of experimentally validated data with high-performance AI modelling provides a reliable, interpretable, and computationally efficient framework for intelligent SCC mix optimization, representing a substantial improvement in scientific novelty and practical applicability over the previous experimental-only study.

## 11. Conclusion

Combining Class F fly ash, ground calcium carbonate (GCC), and recycled PET bottle fibers, an environmentally friendly self-compacting concrete (SCC) was successfully created, proving that combining sustainable materials is feasible. According to EFNARC standards and pertinent Indian Standards, experimental investigations verified that all SCC combinations met the necessary fresh and hardened concrete performance parameters. To enable trustworthy machine learning model training and validation, a physics-informed database with 1,000 experimentally verified samples was created. Multiple statistical performance measures were used to assess the ability of six AI models (Extra Trees, Gradient Boosting, LightGBM, CatBoost, ANN, and DNN) to predict SCC features. With  $R^2 = 0.9884$ , RMSE = 0.4059, MAE = 0.2750, MSE = 0.1648, MAPE = 0.851%, and 10-fold CV  $R^2 = 0.9870$ , CatBoost Regressor demonstrated the strongest predictive performance. The proposed integrated experimental AI framework minimizes laboratory effort, improves prediction reliability, and provides an effective decision-support tool for intelligent SCC mix optimization. The findings contribute to sustainable concrete technology by combining recycled materials, experimental validation, and explainable AI, supporting the development of environmentally responsible and data-driven concrete design. The suggested integrated experimental AI framework reduces laboratory work, enhances prediction accuracy, and offers a useful tool for intelligent SCC mix optimization. By integrating recycled materials, experimental validation, and explainable AI, the findings advance sustainable concrete technology and aid in the creation of data-driven, ecologically conscious concrete design.

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