



Article

Application of a Hybrid Explainable ML–MCDM Approach for the Performance Optimisation of Self-Compacting Concrete Containing Crumb Rubber and Calcium Carbide Residue

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Abstract

The combined incorporation of crumb rubber (CR) and calcium carbide residue (CCR) in self-compacting concrete (SCC) induces competing and nonlinear effects on its fresh and hardened properties, making the simultaneous optimisation of workability, strength, durability, and stability challenging. CR reduces density and enhances deformability and flow stability but adversely affects strength, whereas CCR improves particle packing, cohesiveness, and early-age strength up to an optimal replacement level. To systematically address these trade-offs, this study proposes an integrated multi-criteria decision-making (MCDM)–explainable machine learning–global optimisation framework for sustainable SCC mix design. A composite performance score encompassing fresh, mechanical, durability, and thermal indicators is constructed using a weighted MCDM scheme and learned through surrogate machine-learning models. Three learners—glmnet, ranger, and xgboost—are tuned using v-fold cross-validation, with xgboost demonstrating the highest predictive fidelity. Given the limited experimental dataset, bootstrap out-of-bag validation is employed to ensure methodological robustness. Model-agnostic interpretability, including permutation importance, SHAP analysis, and partial-dependence plots, provides physical transparency and reveals that CR and CCR exert strong yet opposing influences on the composite response, with CCR partially compensating for CR-induced strength losses through enhanced cohesiveness. Differential Evolution (DEoptim) applied to the trained surrogate identifies optimal material proportions within a continuous design space, favouring mixes with 5–10% CCR and limited CR content. Among the evaluated mixes, 0% CR–5% CCR delivers the best overall performance, while 20% CR–5% CCR offers a balanced strength–ductility compromise. Overall, the proposed framework provides a transparent, interpretable, and scalable data-driven pathway for optimising SCC incorporating circular materials under competing performance requirements.



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1. Introduction

The United Nations (UN) is continuously advocating for the adoption of environmentally sustainable materials and practices in the production of green concrete and building constructions by 2050. This opens a wide gap for researchers to investigate the possible use of more sustainable materials from waste products, renewable materials, and by-products as a substitute for cement and aggregates in concrete [1]. With concrete being the most utilised construction and building material, and possibly the second most used material after water [2,3], it consumes huge amounts of natural materials, thereby negatively impacting the effort of achieving environmentally sustainable materials and protecting the environment [4]. For example, ordinary Portland cement is the predominant binder material for making concrete, mortar, and blocks. Its production alone leads to a high rate of emissions and global warming in the environment, where the cement industry alone accounts for almost 8% of the global CO₂ emissions [5–7]. Additionally, cement is the most expensive constituent material for making concrete and mortar, owing to its high energy demand during the production process which leads to substantial CO₂ and greenhouse gas emissions and the promotion of global warming [8]. These problems led researchers to find a sustainable solution through developing a cost-effective and environmentally and materially sustainable concrete with a lower intrinsic energy demand, produced using the abundant resources on the planet or using recycled products and by-products [8,9]. The utilisation of materials that have cementitious and pozzolanic properties from by-products and waste materials will significantly suppress the high demand of cement in the construction and building industries and possibly lower construction costs and consequently lessen the global CO₂ emissions contributed by cement factories [10,11]. These cementitious and pozzolanic materials are used as supplementary cementitious materials (SCMs), where they are used to partially substitute cement in concrete or are used as a total replacement for cement and produce concrete with zero cement as in geopolymer or alkali-activated binders [1,12–14].

The amount of cement content needed depends on the type of concrete; for example, roller-compacted concrete requires a lower amount of cement to achieve the desired properties compared to conventional concrete [15,16]. In contrast, self-compacting concrete needs a higher cement content to achieve a lower water-to-cement ratio and still be able to flow, making it less cost-effective and more environmentally sustainable than normal concrete [1,17,18]. SCC exhibits the consistency of high-performance concrete, having different behaviours in its fresh state compared to conventional concrete, which is measured by its fluidity through rheology. To achieve this behaviour in its fresh state, SCC is designed to have a high paste volume, meaning it consumes higher amounts of cement and other ingredients like aggregates and admixture [18,19]. Due to the high demand for cement in SCC, SCMs are often used as binder materials in SCC to partially substitute cement, or sometimes blended cement is used (cement mixed with SCMs during production) to reduce cost, make the SCC more environmentally friendly, and enhance its long-term durability performance [1,20,21].

Recent advancement in the construction industry and materials has led to the creation of SCC for a high-performance and sustainable concrete, where it was first developed in 1988 in Japan. Some attributes of SCC include the ability to flow under its own weight and fill congested reinforced concrete formworks and tiny gaps without the need for external vibration. This makes it suitable for use in building complex, geometrical, and irregular-shaped structures, bridges, tall buildings, and tunnels that use huge quantities of reinforcements and where the concrete must be pumped to high levels. Using SCC reduces the need for workmanship, shortens construction time, minimises machine use on-site, and reduces noise- and vibration-related injuries. The use of SCC also enhances the structural

integrity and quality of construction by eliminating honeycomb and voids through filling all congested and difficult-to-access-zones and superior surface finishing [5,22–25]. These exceptional properties of SCC are achieved using a large quantity of cement and fine materials (from fine aggregates) to achieve a high paste volume, adding a substantial dosage of water-reducing admixtures (superplasticizers) and viscosity-modifying admixtures. This gives it the filling ability, to be able to flow under its own weight; passing ability, to be able to pass and fill through congested reinforcements and narrow gaps; and lastly segregation resistance, to be stable and uniform throughout the construction process with segregating [22,26].

Sustainable SCC can be achieved by employing ecofriendly constituent materials. Materials from industrial and agricultural by-products or municipal and other wastes can be used as substitutes for natural materials for producing SCC. Using these ecofriendly materials as an alternative to conventional materials in SCC has several benefits which include the conservation of natural resources, promotion of waste management, cost optimisation and reduction, and protection of the environment from landfilling and other pollutants [17,27]. Different industrial by-products and agricultural wastes in the form of ash have been used as SCMs in SCC. These include fly ash [5,28], silica fume [28], slag [29,30], limestone powder [18,31], metakaolin [18], waste banana leaf ash [32], rice husk ash [33,34], bagasse ash [35,36], etc. Other SCMs like calcium carbide residue (CCR) have not been fully explored for use in SCC [37].

Although self-compacting concrete with crumb rubber (CR) coupled with calcium carbide residue (CCR) has been experimentally investigated in several works previously, including Ref. [37], the current work does not propose novelty related to the material apparatus. In fact, the main contribution of this research is the creation and demonstration of an integrated, transparent MCDM–explainable machine learning–global optimisation framework for SCC mix evaluation and synthesis. The CR–CCR SCC dataset is selected deliberately as a representative case showing how multi-objective experimental performance measures/metrics can be aggregated to reach a composite score, learned by surrogate models, processed through explainable AI tools, and optimised through a process called Differential Evolution. Such a workflow facilitates data-driven but ultimately practically interpretable decision support for SCC mix design where competing fresh, mechanical, durability, and thermal performance demands are present.

CCR has been adopted as a chemical activator for geopolymer and other cementless concretes like UHPC owing to its high Ca(OH)_2 and some traces of CaCO_3 [38,39]. CCR is obtained as a by-product during the production of acetylene gas, mostly for welding purposes. Calcium carbide undergoes hydrolysis to produce acetylene gas, and the by-product of the carbide is termed CCR. CCR is utilised for different purposes including fermentation, bottle molds greasing, odor neutralisation, and preparing organic chemicals and metal fabrications [40]. Bawab, et al. [40] in their extensive review reported that about 21 million tons of calcium carbide were utilised for acetylene gas production in 2020 alone, with this amount expected to reach 27 million tons by 2026. Global CCR generation exceeds 24 million tons because for each ton of calcium carbide consumed, about 0.41 tons of acetylene gas and 1.15 tons of CCR are generated [40,41]. Due to its high alkalinity with $\text{pH} > 12$, disposing of the CCR into landfills pollutes and causes severe risks to the environment, where leaching can easily occur and contaminate the soil and groundwater/water system [40–42]. The content of Ca(OH)_2 in CCR can be up to 85%, although other compounds like SiO_2 , CaCO_3 , Al_2O_3 , and Fe_2O_3 can be found in CCR [42,43]. The Ca(OH)_2 in CCR if left in open air or under the sun long term can react with CO_2 to form CaCO_3 [44]. The high content of Ca(OH)_2 in CCR can react with natural pozzolanic materials containing high silica and alumina and lead to the formation

of cementitious products through pozzolanic reactions [45,46]. CCR has been utilised in several studies either as a partial substitute to cement in concrete or a binder material in geopolymer and cementless concrete. Wang, et al. [47] developed a cementless UHPC utilising CCR as the activator and silica fume and slag as the precursors. They achieved excellent mechanical properties similar or even higher than those of conventional UHPC. Their developed UHPC achieved compressive and flexural strengths of 132.5 MPa and 19.3 MPa, respectively. In a similar study, Peng, et al. [38] achieved a compressive strength ranging from 120 to 175 MPa, by using CCR as the activator, with silica fume and slag as precursors in cementless UHPC, though they added 2% steel fiber. Bawab, et al. [48] partially substituted 0–20% cement with CCR and 0–40% with volcanic ash (VA) in mortar. They reported enhancement in compressive strength and UPV using a combination of 5% CCR and 10–20% VA; they achieved highest strength with the blends 5% CR and 20% VA. Through microstructural analysis, they observed a depletion of $\text{Ca}(\text{OH})_2$ and increase in C-S-H and C-A-S-H. Bawab, et al. [43] substituted 0%, 5%, 10%, and 20% cement with CCR in concrete. They reported an improvement in compressive strength and a reduction in the volume of permeable voids with replacement of 5% cement with CCR. Additionally, the CO_2 uptake of the concrete also improved with substitution of up to 10% CCR addition.

One of the major environmental challenges faced by many government agencies which need to be addressed through research is the recycling and management of scrap/waste tires. Annually more than 1 billion waste tires are generated globally and more than half of them end up disposed of in landfills [49–51]. Landfilling with waste tires causes serious threats to the environment, human health, and the ecosystem at large due to their difficulty degrading [52]. Other methods of recycling, which include pyrolysis, combustion, or refining, are also not environmentally sustainable as they create other problems like air and land pollution [50,53]. Therefore, one of the most sustainable approaches to waste tire management is to reduce it to a small size by grinding and removing the steel and thread and then utilising the rubber particles named crumb rubber (CR) as an aggregate in concrete. The rubber particles can be made in different sizes to replace either fine or coarse aggregate to produce rubberised concrete [50,54,55]. CR has been reported to enhance many properties of cementitious composites, especially concrete. CR reduces the brittleness of concrete, making it more flexible by improving its toughness and energy absorption capacity [50,56,57]. CR has also been reported to improve the impact resistance and fatigue performance of concrete [58–60]. CR is also used as a lightweight aggregate owing to its lower specific gravity to produce lightweight concrete for overall load reduction in structures [61,62]. On the contrary, many findings have shown that CR decreases concrete's mechanical properties, especially compressive strength, and durability. This reduction is linked to the hydrophobicity of CR causing the entrapment of air and weak bonding in the interfacial transition zone between the rubber particles and the cement matrix; the inferior stiffness of the CR compared to natural aggregates causing substantial expansion in comparison to the cement paste under low stress, resulting in crack formation within the rubber surface; and poor chemical adhesion between rubber CR particles and the cement matrix due to the smooth surface and other electrons present in the CR [52,54,55]. To address these drawbacks of CR in concrete, several techniques have been developed by different researchers to mitigate these effects, one of which uses SCMs such as silica fume, fly ash, graphene nanoplatelets, and nano silica [63–66]. CCR has also been used as an SCM to partially mitigate the negative effect of CR on the properties of concrete [67,68].

The research aims to combine the effects of crumb rubber (CR) and calcium carbide residue (CCR) in self-compacting concrete (SCC), which offers sustainability benefits but also presents certain challenges. Due to its lower specific gravity, CR makes concrete lightweight and more deformable but drastically affects its compressive strength, water

absorption, and durability performance. However, CCR provides strength gains and improves cohesion. It is a challenge to optimise the combined effect of these materials to develop an enhanced performance of the SCC mix. Hence, to address this gap, this study evaluated the performance of CR-CCR SCC concrete through experimentation. Furthermore, it employs an analytical technique with a novel approach, utilising a hybrid MCDM-ML method to select the optimised mix. The machine-learning models capture the complex interactions between the materials used (variables). In this research, tools such as SHAP, VIP, and partial dependence plots are used to explain which mix components have the most significant influence on performance. Finally, Differential Evolution (DEoptim) is applied to identify the best mix proportions under practical engineering constraints. This integrated MCDM-ML-optimization pipeline provides a clear, scalable, and data-efficient method for designing sustainable SCC, especially in situations where experimental data are limited.

2. Materials and Methods

2.1. Materials

In this study, Type I cement was utilised which conformed to the requirements of BS EN 196-6 [69], having a specific gravity of 3.15 and properties as summarised in Table 1. The raw calcium carbide residue (CCR) was collected during acetylene generation from calcium carbide (CaC_2) at industrial welding stations in Kano, Nigeria. The CCR underwent a series of processes, which included air-drying, oven-drying, grinding, and sieving. The CCR was air-dried for 96 h and then oven-dried at $110 \pm 5^\circ\text{C}$ for 24 h. After it cooled, the CCR was ground with the aid of a powerful electric grinder and then sieved through a $45\ \mu\text{m}$ sieve; the CCR particles that passed through the sieve were used in this research. After conducting X-ray fluorescence (XRF) analysis, the chemical composition of the CCR was determined as presented in Table 1. The materials used and the process were reported in previous studies by Uche, et al. [37]. The aggregates (fine and coarse) and crumb rubber (CR) utilised in this study were all well graded and fall in the Zone II category based on BS 882 [70] classification. The CR has a water absorption and specific gravity value of 0.62% and 1.13, respectively. The fine aggregate also exhibits a water absorption, specific gravity, and fineness modulus of 1.3%, 2.6, and 2.88, respectively. With regard to the coarse aggregate, it was crushed granite with a nominal maximum particle size of 19 mm. Additionally, it has a water absorption, density, and specific gravity of 1.44%, $1542\ \text{kg/m}^3$, and 2.69, respectively [68]. To achieve self-compacting ability, a high-range water-reducing admixture was added, where a Complast 60 Superplasticizer was utilised in the dosage of 1.3–9.8 mL/kg of binder materials based on the recommendation of the manufacturer [71].

Table 1. Properties of binder materials.

Chemical Compounds	Cement	Calcium Carbide Residue
CaO	74.03	96.46
Al_2O_3	3.01	0.04
SiO_2	12.00	1.1
SO_3	2.07	0.29
MgO	1.3	-
K_2O	1.28	0.45
Na_2O	0.19	0.01
LOI	1.02	1.02
Specific Gravity	3.15	2.22

2.2. Mix Design and Proportioning

The mixes utilised in this study were adopted from the existing literature by Uche, et al. [37], where they employed response surface methodology (RSM) techniques to proportion SCC mixes containing crumb rubber (CR) and calcium carbide residue (CCR) as the variables. The control SCC was designed using several trials by varying the amount of superplasticizer and the water-to-binder ratio, and the rheological requirements of the SCC based on the EFNARC [72] guidelines were assessed. The final SCC mix was obtained using a Superplasticizer dosage of 7.8 kg/m³ and a water-to-binder ratio of 0.37, meeting the requirements of EFNARC [72] for SCC. The CR partially substituted fine aggregate at dosages of 0%, 10%, and 20% by volume replacement. CCR was also used as a partial substitute for cement at 0%, 5%, and 10% by volume. A total of nine mixes including the control SCC (with 0% CR and 0% CCR) were used for the hybrid MCDM–machine learning–optimisation framework for deriving optimal mix designs under data-limited conditions (refer Table 2). These mixes were produced in the laboratory and tested for fresh, mechanical, and durability properties. Additionally, the SCC was tested for elevated-temperature resistance, subjected to 400 °C, and its weight and strength reductions measured. Finally, the density and thermal conductivity were measured, all of which were reported by Uche, et al. [37].

Table 2. Mix proportions [37].

Mix No	Variables (%)		Constituent Materials for 1 kg/m ³ (kg/m ³)							
	CR	CCR	Cement	CCR	Fine Agg	CR	Coarse Agg	Water	SP	W/B
1	0	0	520	0	880	0	850	192.4	7.80	0.37
2	0	10	468	36.65	880	0	850	192.4	7.59	0.38
3	10	5	494	18.32	792	38.25	850	192.4	7.68	0.38
4	10	10	468	36.65	792	38.25	850	192.4	7.59	0.38
5	20	10	468	36.65	704	76.49	850	192.4	7.59	0.38
6	20	5	494	18.32	704	76.49	850	192.4	7.68	0.38
7	10	0	520	0	792	38.25	850	192.4	7.80	0.37
8	20	0	520	0	704	76.49	850	192.4	7.80	0.37
9	0	5	494	18.32	880	0.00	850	192.4	7.68	0.38

2.3. Samples Preparation and Test Methods

The sampling, batching, and mixing of the SCC was carried out in accordance with the specifications of BS 1881-125 [73] as reported by Uche, et al. [37]. The SCC was mixed in the laboratory using a rotating pan mixer until a homogeneous concrete mix was achieved. After mixing, the fresh SCC was tested for the required fresh property performance before being cast in the designated concrete molds and kept for 24 h until the concrete hardened. After hardening, the concrete specimens were removed from their molds and cured in water at normal temperature and humidity until the required date of testing was reached.

The fresh properties of the SCC were measured as reported by Uche, et al. [37]. The slump flow of the fresh SCC was measured after mixing in accordance with the standard specifications of [74] using a standard slump cone. The passing ability of the fresh SCC was measured using the J-Ring test in accordance with the BS EN 12350-12 [75] specifications. The segregation resistance of the fresh SCC was measured using the methods outlined in BS EN 12350-11 [76].

The testing methods in this study were reported in previous studies by Uche, et al. [37], where the density of the hardened concrete was evaluated by adopting the experimental methods explained in BS EN 12390-7 [77], using 100 mm concrete cube samples after curing for 28 days. The compressive strength of the hardened concrete was tested in accordance with the BS EN 12390-3 [78] requirements after the hardened 100 mm concrete cubic specimens were cured for 28 days in water. For the split tensile strength, cylinder-shaped concrete specimens with a 100 mm diameter and 200 mm height were subjected to normal water curing for a 28-day period. The tensile strength was then measured in accordance with the BS EN 12390-6 [79] specifications. The flexural strength was determined in accordance with BS EN 12390-5 [80], in which concrete beams measuring 100 mm × 100 mm × 500 mm were prepared and cured for 28 days before testing. The methodology outlined in ASTM C642 [81] was followed to determine the water absorption of the SCC, using 100 mm cubic samples, after 28 days of water curing. The resistance of the SCC to salt and acid attack was measured by employing the methods in ASTM C642 [81]. Cubic specimens with 100 mm dimensions were cured in normal water for 28 days before testing. The samples were then air-dried and weighed until a constant weight was achieved; this weight was recorded as the initial weight M_i . For the acid salt attacks, the dried SCC samples were soaked in H_2SO_4 and $MgSO_4$, respectively, for 28 days. After 28 days, the soaked samples were removed from the solutions and air-dried; the weight after soaking was recorded as M_f . The weight reduction due to acid and salt attacks was computed using Equation (1). For the effect of high temperature on the SCC, 100 mm cubic samples were cured for 28 days in water. After 28 days of curing, the samples were air-dried until a constant weight was obtained; the weight was recorded as M_i . The dried samples were then subjected to an elevated temperature of 400 °C. Heat was applied at a constant rate of 10 °C/min until the maximum temperature of 400 °C was reached in an electric furnace, and the samples were allowed to heat for 2 h. After heating, the furnace was switched off and kept closed until the samples cooled completely to avoid heat stroke. After cooling, the samples were weighed and the value recorded as M_f . The weight reduction due to the temperature effect was calculated using Equation (1). The residual compressive strength of the heated samples was measured using the EN 12390-3 [21] procedures with a 2000 kN universal testing machine. The thermal conductivity of the SCC was measured in accordance with BS EN 12667 [82] using the hot-guarded-plate method.

$$Weight\ Reduction(\%) = \frac{M_i - M_f}{M_i} \times 100 \quad (1)$$

In Equation (1), M_i designates the initial weight in kg, while M_f denotes the final weight after soaking or heating in kg.

2.4. Data Source and Pre-Processing

This study utilised a dataset of nine laboratory-tested concrete mixes containing the physical, mechanical, and mix-design attributes of concrete specimens. The target was a composite performance score constructed as a weighted aggregation of the slump, compressive strength, density, workability, and water-absorbing performance indices. All predictor variables representing the mix proportions (cement, fine aggregates, coarse aggregates, and superplasticizer) were converted to a consistent unit of kg/m³. No missing values were present in the dataset. All continuous predictors were standardised to facilitate model convergence, comparable scale influence, and meaningful partial dependence analysis. Performance metrics were automatically detected using a regex-based parser, which classified each metric as maximise or minimise and extracted any user-specified weighting. Owing

to the small sample size, no conventional train–test split was used for inferential evaluation as such splits produce unstable and non-representative estimates.

2.5. Composite Score Construction (MCDM Layer)

To unify the assessment and optimisation of SCC mixes in heterogeneous characteristics, a composite performance score was developed with the utilisation of MCDM methodology. Specified criteria were fresh characteristics (passing ability, slump flow, and segregation resistance), mechanical properties (compressive, flexural, splitting tensile, and residual compressive), durability considerations (water absorption and sulphate-induced mass loss), and thermal conductivity. Workability and strength-related performance indicators were treated as benefit metrics and maximised, while durability loss measures and thermal conductivity were treated as cost metrics and minimised. Each criterion was normalised to a [0, 1] scale by applying min–max scaling before aggregation, and inverse scaling was used with respect to the minimisation objectives. In order to prevent subjective bias (as this study is exploratory and the amount of tested data was small), equivalent weights were granted to all criteria. The composite score for all the mixes was calculated as a weighted sum of the normalised criteria. A transparent composite scoring method was used that allows multi-objective integration without requiring manual rescaling.

$$\text{Composite Score} = \sum_{j=1}^n w_j * m_j$$

2.6. Model Training and Selection

Three model classes were evaluated: (i) Elastic Net (glmnet), (ii) Random Forest (ranger), and (iii) Gradient Boosting (xgboost).

Given the limited dataset size ($n = 9$), a conventional train–test split was deemed statistically unreliable and potentially misleading. Instead, model evaluation was performed using bootstrap resampling with out-of-bag (OOB) validation, which provides a more appropriate assessment of predictive behaviour and uncertainty for small-sample problems. Multiple surrogate models were trained within this bootstrap framework, and performance was assessed using distributions of error metrics rather than single point estimates. This approach avoids the over-interpretation of artificially high goodness-of-fit values that can arise from resubstitution or fragile hold-out splits in very small datasets. Model calibration and predictive consistency were visualised using a bootstrap OOB predicted-versus-observed composite score plot (Figure 1), which illustrates both central tendency and uncertainty structure without implying strong generalisation claims beyond the experimental domain.

2.7. Model Evaluation

The predicted and observed composite scores for the sequestered test set were compared using scatter diagnostics. Perfect calibration corresponds to points lying on a 45° line. Because a statistically meaningful test set cannot be extracted from a 9-sample dataset, all inferential performance estimates relied solely on bootstrap cross-validation.

2.8. Model Explainability

Model-agnostic explainability techniques, including permutation feature importance, SHAP values, and partial dependence plots (PDPs), were employed to interpret the surrogate model behaviour from complementary perspectives.

Permutation importance quantifies the impact of each variable on the predictive error and is sensitive to interaction effects and correlated inputs. SHAP values measure the average marginal contribution of each variable to the model output, while PDPs illustrate the main-effect shape of individual variables when averaged over all others.

In the present study, the superplasticizer consistently exhibits a strong, monotonic influence on the composite score in both SHAP and PDP analyses, reflecting its dominant role in SCC rheology and cohesiveness. In contrast, CR and CCR display comparatively flat PDP trends within the explored range, indicating that their influence is primarily interaction-driven rather than univariate. This behaviour is physically consistent with SCC systems, where CR adversely affects density and strength while CCR acts as a packing and cohesiveness modifier only within a limited replacement range.

2.9. Continuous CR–CCR Optimisation

For physical interpretability and practical relevance, optimisation was directly formulated over continuous material contents rather than discrete shares of experimental mixes. Differential Evolution was performed on the trained surrogate model to find the optimal combination of CR and CCR within the experimentally observed domain, with the other constituents maintained at representative values. The optimisation surface indicates a relatively weak sensitivity of the composite score to CCR in a moderate range and a consistently negative effect of increasing CR content. The optimum solution yields negligible CR content and moderate CCR replacement, resulting in a predicted composite score close to 0.51. This optimisation result is verified by experimental findings and explainability diagnostics and, therefore, enhances the physical credibility of the proposed decision-support framework.

2.10. Overfitting Mitigation

To minimise the risk of overfitting, model complexity was intentionally limited via conservative hyperparameter selection (i.e., limited tree depth, regularisation, and learning rate control). Hyperparameters were chosen based on bootstrap resampling performance rather than maximising in-sample fit. Furthermore, explainability diagnostics provided qualitative safeguards to ensure that learned relationships were physically meaningful. Flat or weak partial dependence trends for some variables were interpreted as interaction-driven effects rather than artefacts of overfitting.

3. Results

3.1. Experimental Results

The experimental results in this study were reported in our previous research [37], which is summarised here in order to explain the analysis carried out in this work. Table 3 presents a summary of the fresh and mechanical properties of the SCC mixes containing different dosages of crumb rubber (CR), while Table 4 presents the results for their durability and thermal properties. The incorporation of CR and CCR as a single variable or a combination of the two affects the fresh properties of the SCC. The slump flow for most of the mixes was within the range specified by EFNARC [72] for SCC (550–700 mm), except for the mixes containing more than 10% CR as substitute to fine aggregate which exhibited lower slump flow values between 550 and 560 mm, such as in Mix 4, Mix 5, and Mix 8. This lower slump flow in the mixes can be linked to the irregular and hydrophobic nature of the CR particles, which increases the internal friction in the SCC mix and depletes the flow capacity [37]. The passing ability of the SCC also followed a similar trend, with Mix 8 (20% CR, 0% CCR) falling slightly below the recommended J-ring ratio threshold of 0.80 (0.77), whereas mixes incorporating 5% CCR, even with up to 20% CR (Mix 6: 0.84), maintained acceptable deformability through congested reinforcement. However, segregation resistance deteriorated markedly across all modified mixes (12.1–13.8% vs. 5.4% for control), indicating that CCR's ultra-fine particles and CR's buoyancy jointly increased susceptibility to phase separation unless mitigated by viscosity-modifying admixtures.

Table 3. Results of fresh and mechanical properties of SCC.

Mix	CR (%)	CCR (%)	Passing Ability	Slump Flow (mm)	Segregation Resistance (%)	Density (kg/m ³)	Compressive Strength (MPa)	Flexural Strength (MPa)	Split Tensile Strength (MPa)
1	0	0	0.86	680	5.4	2176.07	45.4	5.37	3.8
2	0	10	0.88	723	13.6	2161.44	41.5	3.01	3.32
3	10	5	0.86	750	13.8	2117.55	39.5	3.2	3.32
4	10	10	0.8	560	12.5	2110.23	39	4.31	3.29
5	20	10	0.8	557	12.6	2059.19	39	4.31	3.29
6	20	5	0.84	723	13.5	2066.5	40.1	3.11	3.66
7	10	0	0.84	723	13.5	2124.85	40.1	3.11	3.66
8	20	0	0.77	550	12.1	2073.79	37	4	3.09
9	0	5	0.93	785	7.1	2168.76	44.7	3.15	3.07

Table 4. Results of durability and thermal properties of SCC.

Mix	CR (%)	CCR (%)	Weight Reduction in H ₂ SO ₄ (%)	Weight Reduction in MgSO ₄ (%)	Water Absorption (%)	Residual Compressive Strength at 400 °C (MPa)	Weight Reduction at 400 °C (%)	Thermal Conductivity (W/mK)
1	0	0	7.78	1.89	1.74	33.8	3.89	1.13
2	0	10	10.17	2.78	1.78	34.1	3.11	1.04
3	10	5	4.24	1.14	2.35	30.4	4.1	0.94
4	10	10	4.12	0.99	2.5	29.5	4.61	0.89
5	20	10	5.45	1.5	2.15	27	5.39	0.77
6	20	5	6	2.2	2.19	27.6	5.38	0.79
7	10	0	6.58	2.04	2.37	31	4	0.98
8	20	0	10.4	2.91	2.83	28	5.35	0.82
9	0	5	9.49	2.16	1.76	34	3.75	1.09

The results of the hardened density of the SCC decreased increasingly with CR addition, giving the CR an advantage for use in lightweight SCC. The reduction in density with CR is ascribed to the lower bulk density of CR in comparison to the fine aggregate it replaced. Similar results could be observed when cement was partially substituted with CCR only (see Mix 9, where it has lower density than the control). This reduction is also due to the lower density of the CCR in comparison to cement, since replacement was carried out by the volume method. The SCC mix with the highest CR and CCR mix, i.e., Mix 5 (20% CR, 10% CCR), exhibits the lowest density, making it the most lightweight among the SCC mixes. The compressive strength of the SCC mixes decreases with the addition of either CR or CCR individually, for instance, comparing the strength of the control mix (45.4 MPa) with that of Mix 8 (20% CR/0% CCR) at 37 MPa and Mix 2 (0% CR/10% CCR). The reduction in compressive strength with the incorporation of CR was due to the weak interfacial transition zone formed by CR in the cement matrix, which led to premature failure and consequently reduced strength, while the reduction due to CCR's effect is linked to its limited pozzolanic activity ($\text{SiO}_2 + \text{Al}_2\text{O}_3 < 1.2\%$). Notably, synergistic combinations, particularly Mix 6 (20% CR/5% CCR) and Mix 7 (10% CR/0% CCR), achieved similar compressive strength (40.1 MPa) and split tensile strengths (3.66 MPa), surpassing the performance expected from simple additive effects and suggesting that CCR's micro-filler action partially densifies the matrix around rubber particles. Flexural strength exhibited a nonlinear response, peaking at 4.31 MPa for Mixes 4 and 5 (10–20% CR + 10% CCR) despite their lower compressive strength, indicating enhanced post-cracking ductility, wherein CR acts as a micro-reinforcement bridging cracks under bending loads.

Table 4 summarises the durability and thermal behavior of SCC mixes incorporating varying proportions of crumb rubber (CR) and calcium carbide residue (CCR), revealing the complex and often contrasting effects of the two waste materials. Regarding chemical durability, weight loss after 28-day immersion in H_2SO_4 and MgSO_4 generally increases with the addition of CCR when used alone, demonstrated by Mix 2 (0% CR, 10% CCR) showing the highest acid-induced mass loss (10.17%) and relatively high sulfate loss (2.78%) compared to the control (7.78% and 1.89%, respectively). This deterioration correlates with CCR's low pozzolanic activity, which compromises matrix densification and increases vulnerability to aggressive ion penetration and expansive reactions (e.g., ettringite formation in sulfate environments). Conversely, CR incorporation, especially at 10%, appears to mitigate acid and sulfate attack when paired with CCR, as Mix 3 (10% CR, 5% CCR) and Mix 4 (10% CR, 10% CCR) exhibit the lowest weight reductions in both H_2SO_4 (4.24% and 4.12%) and MgSO_4 (1.14% and 0.99%). This counterintuitive improvement may stem from CR's hydrophobic nature and its ability to block capillary pathways, thereby reducing permeability; concurrently, it increases overall water absorption (2.35–2.50% vs. 1.74% in control), suggesting that CR's pore-blocking effect is selective, impeding aggressive ion ingress but not capillary water uptake. At 20% CR, however, chemical resistance deteriorates again (e.g., Mix 8: 10.40% in H_2SO_4), likely due to excessive microcracking around rubber particles and weakened interfacial transition zones, which overwhelm any barrier effect.

Water absorption consistently increases with CR dosage, attributable to CR's low specific gravity, higher intrinsic porosity, and poor bonding with the cement matrix, which creates interconnected voids. Notably, CCR alone (Mixes 2 and 9) has a minimal impact on absorption (1.76–1.78%), reinforcing its role as a micro-filler improving packing density—yet this benefit is neutralised or reversed when combined with CR, as seen in Mix 4 (2.50%), indicating that CR's dominant pore-forming effect overshadows CCR's filling potential.

Thermal performance at 400 °C also reflects the competing roles of CR and CCR. Residual compressive strength declines progressively with CR content, from 33.8 MPa (control) to 27.0 MPa (Mix 5: 20% CR, 10% CCR), reflecting CR's organic nature and poor thermal stability; rubber decomposes and volatilises (>300 °C), generating internal voids and microcracks that weaken the matrix. Interestingly, CCR alone (Mixes 2 and 9) enhances residual strength (34.0–34.1 MPa), likely due to its high lime content acting as a thermal stabiliser and promoting sintering or recombination of decomposition products. However, when CR and CCR are combined, this beneficial effect diminishes or reverses (e.g., Mix 4: 29.5 MPa), suggesting antagonistic interactions: CCR's carbonate decomposition ($\text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2$ above ~600 °C, though minor decomposition may initiate at 400 °C) may coincide with rubber pyrolysis, amplifying internal pressure and damage. Weight loss at 400 °C follows a similar pattern: CCR alone reduces mass loss (3.11% in Mix 2 vs. 3.89% control), whereas CR monotonically increases it (up to 5.39% in Mix 5). Combined CR–CCR mixes exhibit the highest thermal mass losses (Mix 4: 4.61%; Mix 5: 5.39%), reinforcing the hypothesis of concurrent decomposition pathways. Finally, thermal conductivity decreases systematically with both CR and CCR, reaching a minimum of 0.77 W/m·K in Mix 5, the lowest among all mixes, demonstrating their synergistic contribution to thermal insulation, a desirable attribute for energy-efficient building envelopes. This reduction is primarily driven by CR's entrapped air pockets and low intrinsic conductivity, with CCR further refining the pore structure.

3.2. Modelling and Simulation

3.2.1. Predictive Performance on the Test Set

A standard train–test split was not adopted, as it would create unstable and non-representative performance estimates for small datasets ($n = 9$). Model evaluation, however, was performed using bootstrap resampling and out-of-bag (OOB) predictions, which provide an unbiased estimate of generalisation performance under small-sample conditions. Bootstrap OOB predicted versus observed composite scores for all resamples are presented in Figure 1. A large number of predictions lie near the 1:1 reference line, confirming that surrogate model calibration has been performed. Predicted outputs are restricted within a narrow range (~ 0.48 – 0.53), whereas the observed composite scores are dispersed over a wider band (~ 0.44 – 0.64), reflecting conscious regularisation that precludes extreme extrapolations in flexible learners, such as gradient-boosted trees. Model performance was summarised on the basis of bootstrap OOB distributions instead of producing a single deterministic R^2 value. The mean OOB-predicted composite score of a representative design point was 0.4976 (Table 5), indicating the stability of the learned response surface. This conservative predicted behaviour reflects regularised ensemble models built on sparse experimental data and shuns over-confident claims of a perfect fit.

Table 5. Test set performance metrics.

Item	Description	Value
Mean OOB-predicted composite score	Bootstrap out-of-bag prediction (model stability indicator)	0.498
Optimised composite score	Maximum predicted value on continuous CR–CCR surface	0.509
Optimal CR content	Continuous optimisation result	$\approx 0 \text{ kg/m}^3$
Optimal CCR content	Continuous optimisation result	$\approx 36.6 \text{ kg/m}^3$

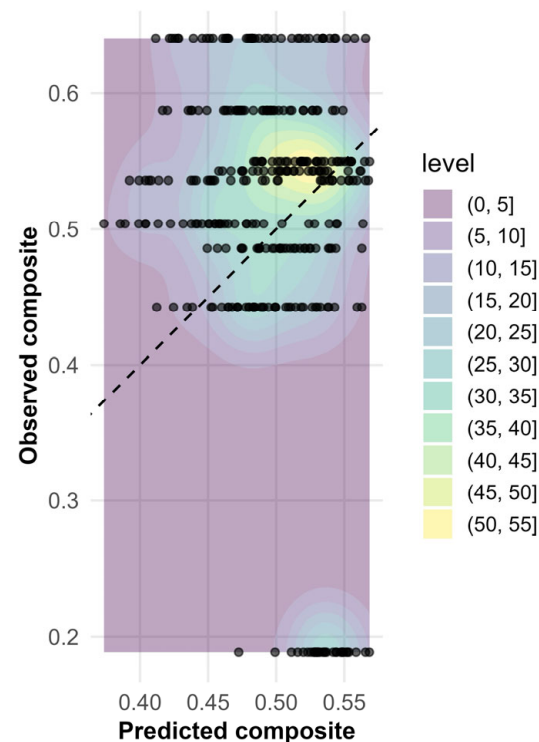


Figure 1. Predicted vs. observed composite score (test set).

3.2.2. Global Feature Importance

Global permutation importance results are presented in Figure 2; each predictor was randomly permuted in order to evaluate its influence on the out-of-bag predictive error. We show that the superplasticizer dosage (SP, kg/m³) dominates the sample with a strong impact on predictive accuracy, which is the one whose perturbation results in the most significant loss of predictive accuracy. Crumb rubber (CR) and fine aggregate (FA) are the secondary ones, and cement (C) and calcium carbide residue (CCR) have a weak individual impact on the global model error. The relatively small absolute magnitudes of permutation importance across all variables suggest that the surrogate model has a smooth, low-variance structure, without any one predictor having highly disproportionate dominance. This behaviour is typical of SCC mix-design systems where performance is determined by a balanced compositional interaction, not unique marginal effects.

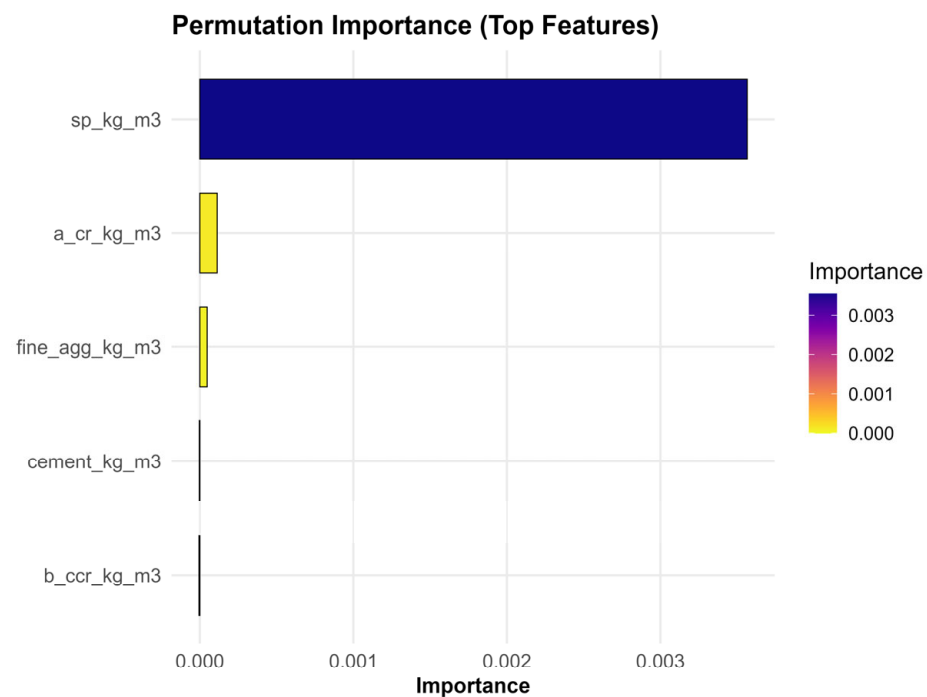


Figure 2. Permutation importance (top features).

3.2.3. SHAP-Based Marginal Influence

To complement global importance, the SHAP (SHapley Additive exPlanations) methodology was used to quantify the average marginal contribution of each variable across all samples. Figure 3 reports the mean absolute SHAP values. Contrary to permutation importance, superplasticizer (SP) overwhelmingly dominates the marginal contribution structure, with mean |SHAP| values an order of magnitude larger than those of other variables. CR, CCR, FA, and C contribute weak but consistent effects, indicating that their influence is largely conditional and interaction-driven rather than univariate. Such apparent divergence between permutation importance and SHAP rankings is expected: permutation importance reflects the impact on predictive error, while SHAP captures the average contribution to model output. Under correlated compositional variables (e.g., CR–FA and CCR–cement), these measures highlight different but complementary aspects of model behaviour.

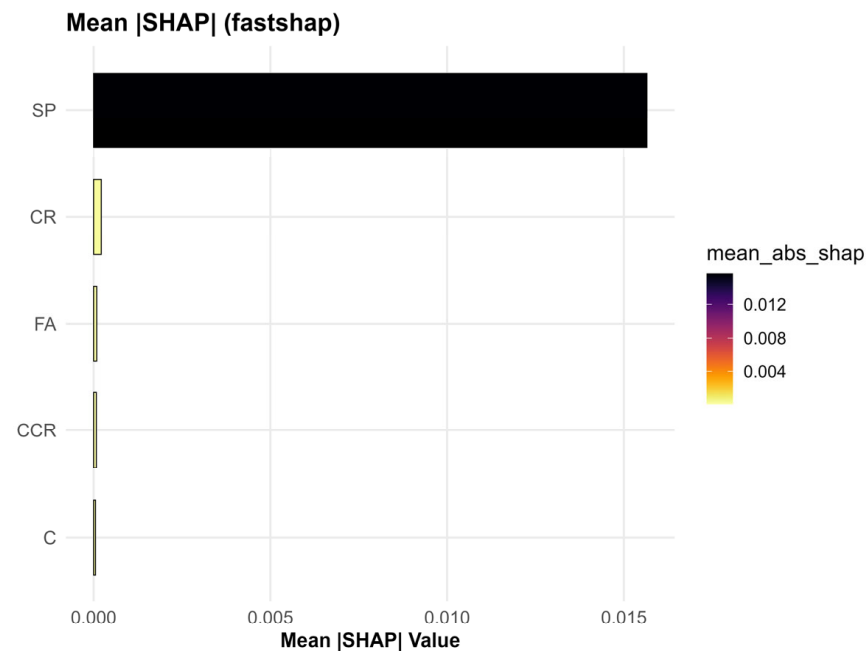


Figure 3. Mean absolute SHAP values.

3.2.4. Partial Dependence Trends

Partial dependence plots (Figures 4–8) were used to characterise the main-effect response shapes of individual predictors while averaging over the joint distribution of the remaining variables. A pronounced and monotonic decreasing trend is observed for superplasticizer dosage, indicating that excessive SP systematically lowers the predicted composite score. This behaviour aligns with SCC design principles, where over-dosage may reduce cohesiveness, increase segregation risk, and adversely affect mechanical performance. In contrast, CR, CCR, cement, and fine aggregate display near-horizontal partial dependence curves with narrow confidence bands. These flat profiles do not imply irrelevance; rather, they indicate that the model captures their effects primarily through interactions and proportional balance, which cannot be isolated as strong univariate nonlinearities in a small experimental dataset. Overall, the PDPs corroborate the SHAP findings and confirm that SP is the most sensitive control variable, while other constituents operate in stabilising or compensatory roles.

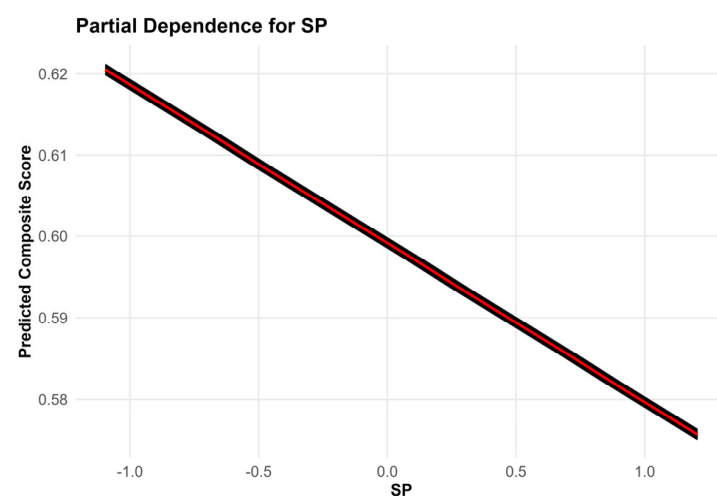


Figure 4. Partial dependence plot for superplasticizer (SP).

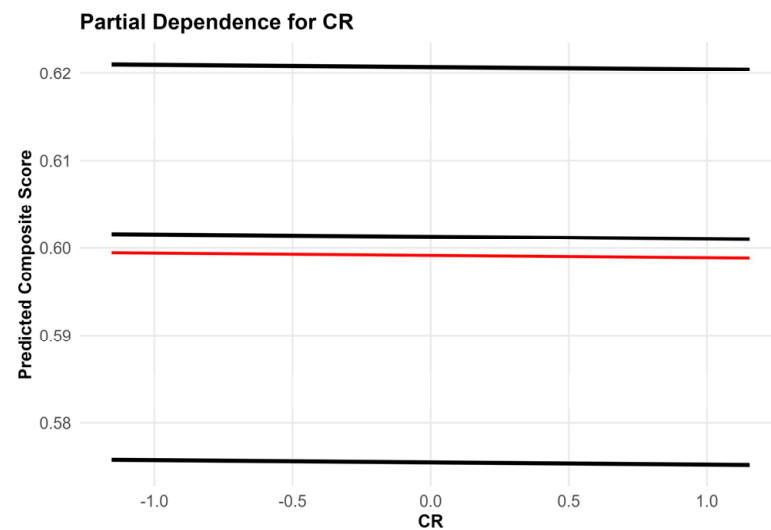


Figure 5. Partial dependence plot for CR.

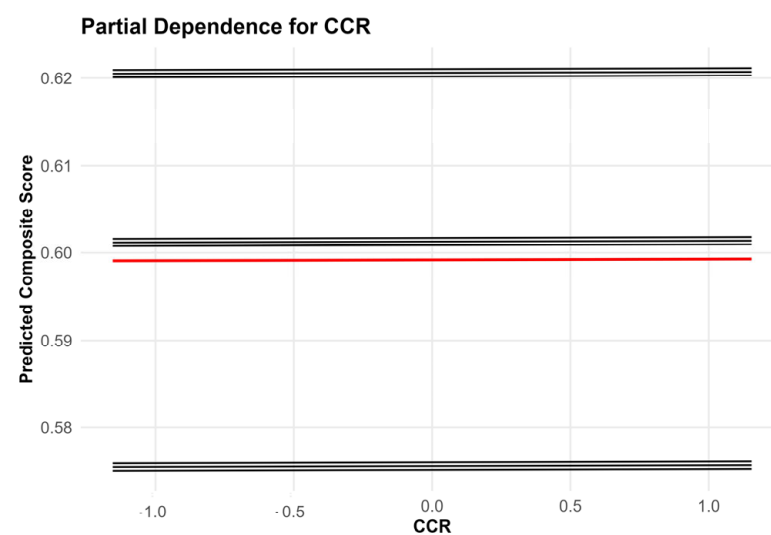


Figure 6. Partial dependence plot for CCR.

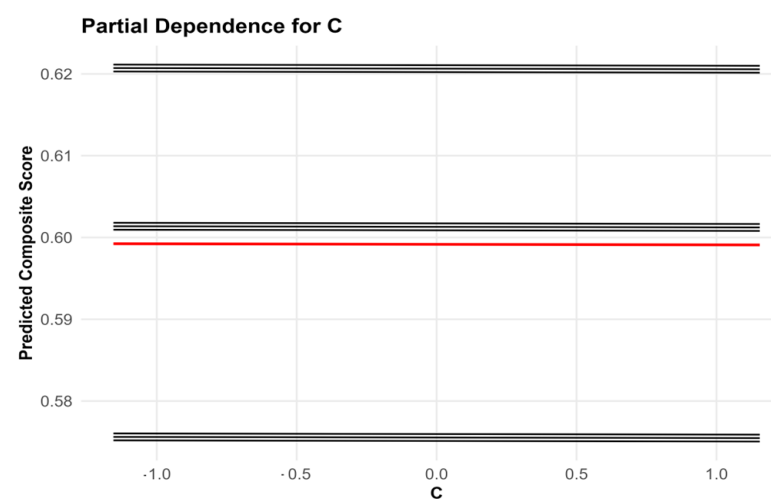


Figure 7. Partial dependence plot for C.

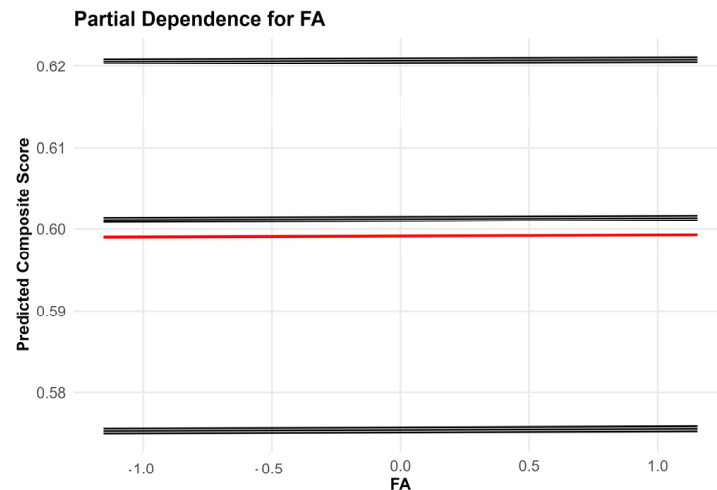


Figure 8. Partial dependence plot for FA.

3.2.5. Continuous Optimisation of CR–CCR Space

To address the physical constraints of the optimisation output, the previous discrete formulation of product mix shares as weighted combinations of experimental mixes was replaced with continuous optimisation of material proportions using the trained surrogate model. The predicted composite score surface for continuous ranges of crumb rubber (CR, kg/m³) and calcium carbide residue (CCR, kg/m³) is provided in Figure 9. Within the examined ranges, the composite performance index has a smooth, weakly sloping response surface, confirming limited sensitivity to independent variation in CR and CCR. As such, this observation is consistent with the model's interpretability results: both CR and CCR have secondary or interaction effects rather than being the main independent predictors of the composite score. Most importantly, there are no sharp local maxima in the optimised surface, thus implying the presence of broad, robust areas of suitable performance rather than one narrow, potentially mathematically fragile optimum. Practically speaking, such behaviour is desirable from the SCC mix-design point of view, as it maintains constructability and resilience to batching variability and allows for material substitution flexibility rather than the use of optimally well-designed proportions.

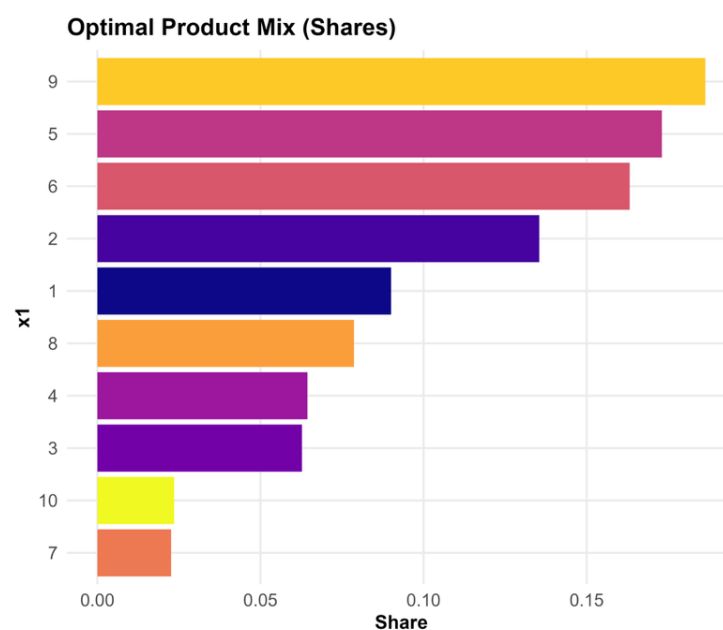


Figure 9. Optimal product mix (DEoptim).

3.2.6. Consistency Across Interpretation Methods

Triangulation across bootstrap validation, permutation importance, SHAP analysis, PDPs, and continuous optimisation reveals a coherent and internally consistent narrative. Superplasticizer emerges as the primary sensitivity driver across all interpretability layers, while CR, CCR, cement, and fine aggregate exert secondary, interaction-mediated effects. The smoothness of the prediction surface and the absence of abrupt nonlinearities confirm that the model is regularised and stable, despite the small dataset. The optimisation outcomes are therefore best interpreted as decision-support guidance, identifying favourable compositional regions rather than prescribing a unique deterministic mix.

3.3. Discussion

We combined multi-criteria decision making, machine-learning algorithms, and global optimisation into a unified modelling pipeline for SCC mixture evaluation in this study. While the experimental data is small, the framework provides strong consistency and the ability to interpret results through appropriate validation and explainability strategies.

In all interpretability diagnostics, superplasticizer dosage was the most powerful determinant of the composite performance index, confirming its centrality in regulating SCC rheology, as well as in regulating workability-sensitive responses. Conversely, crumb rubber (CR) and calcium carbide residue (CCR) had relatively little average marginal impact. The effect is better classified as conditional and interaction-based and mainly influences performance because of the coupling with other components rather than as a strong independent driver.

Partial dependence analysis indicated that cement and fine aggregate content exhibited almost flat univariate trends. This phenomenon cannot be interpreted as the absence of physical influence, but as the outcome of related compositional variables and limited independent variation in the experimental design. In these environments, PDPs largely represent average main effects, potentially concealing interaction-driven mechanisms and thus warranting additional interpretability tools like SHAP and permutation importance.

The optimisation results also lend support for a pragmatic, engineering-oriented interpretation. The continuous CR–CCR response surface shows no sharp local optima but rather wide regions of stable and acceptable performance. This is desirable for actual mix design, where robustness and constructability are put ahead of mathematical sharpness. The optimisation outputs here are thus not presented in such a way as to propose ultimate prescription. Instead, they serve as tips that can be applied to areas of design compatible with the learned performance landscape.

Overall, the principal contribution of this work lies in the methodological pipeline. This composite performance scoring, bootstrap-based validation, interpretable surrogate modelling, and evolutionary optimisation are complemented by a transparent, replicable, and flexible decision-support mechanism for data-driven SCC design and other sustainable material systems.

4. Experimental Variability and Limitations

The experimental results are reported as single representative values per mix and, in other words, full statistical dispersion (standard deviation or confidence intervals) is not available for all of the properties measured. Therefore, the overall score and any subsequent optimisation are subject to unquantified experimental uncertainty. With reference to over-interpretation, the modelling framework intentionally uses bootstrap validation, conservative regularisation, and smooth surrogate surfaces. Thus, the reported optima should be interpreted as indicative trends, rather than unequivocal prescriptions. Future work

incorporating replicated experiments and larger datasets will enable uncertainty-aware and reliability-based optimisation of SCC mixtures.

5. Conclusions

In this study, an integrated MCDM–machine learning–optimisation framework was developed that measures and informs the design of self-compacting concrete (SCC) using crumb rubber (CR) and calcium carbide residue (CCR). The framework thus offers a clear decision-support tool for multi-objective trade-offs in the sustainable design of SCCs by integrating experimental performance signals with surrogate modelling and evolutionary optimisation in combination.

The experimental results verified measurable reductions in fresh and hardened properties for incorporating CR. Slump flow reduced from about 785 mm (control mix) to 760–770 mm (higher content of CR), while compressive strength decreased from 44.7 MPa (0% CR, 5% CCR) to ~40 MPa (20% CR). Regarding the durability variables, greater water absorption and reduced resilience to hostile conditions were observed. In contrast, CCR addition at moderate concentrations (5–10%) had a protective effect, increasing residual compressive strength slightly at higher temperatures and decreasing water absorption, consistent with its contributions as a micro-filler and packer.

A composite performance index was constructed using a multi-criteria decision-making (MCDM) approach that incorporated strength, workability, durability, and thermal performance. This composite score was modelled using regularised linear (glmnet), ensemble (ranger), and gradient-boosted (xgboost) learners. Model verification was conducted using bootstrap out-of-bag rather than a traditional train–test split, commensurate with the minimal size of the dataset. The predictive capability is thus interpreted in a relative and exploratory sense and is more than likely treated as a stable measure of sensitivity test/optimisation (rather than a stringent assumption of generalisation).

The model interpretability analysis showed distinct differences between the dominant and secondary drivers of the composite score. Permutation power and SHAP analysis always indicate that the influence of the superplasticizer dosage is high, which implies its strong influence on SCC rheology and workability performance variables. In contrast, CR and CCR showed relatively weak average marginal effects, with partial dependence plots indicating almost flat trends across their investigated ranges. This means that CR and CCR are not active as independent variables but rather influence composite performance from their interactions with other constituents.

The optimisation stage was restructured from a discrete mix-weighting approach to a continuous optimisation of material proportions to guarantee physical realism. The created response surfaces of CR–CCR were smooth and slightly sloped, indicating relatively acceptable performance regions. This implies that, based on a very tight optima, SCC mixtures with CCR and low CR content can be created with effective robustness, accommodating batch variability and certain limitations in constructability.

Consequently, the proposed MCDM–ML–optimisation framework provides a reusable, interpretable, computationally efficient architecture for the design of AI-assisted materials. Instead of prescribing a single “optimal” mix, the framework generates actionable insights into performance sensitivities and realistic design regions that guide transparent, data-driven decision-making on sustainable SCC and other recycled or circular material systems.

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S.K.: Conceptualization, Methodology, Formal analysis, Investigation, Writing—review & editing. All authors have read and agreed to the published version of the manuscript.

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