

# Divergent Hydration Kinetics: Type-Aware Artificial Intelligence Framework for Compressive Strength Prediction and Sustainability Evaluation in Concrete Composites

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## Abstract

Artificial Intelligence (AI) offers significant utility for compressive strength prediction for concrete. However, existing data-driven approaches assume homogeneous material behaviours without accounting for the compositional differences in conventional and sustainable concrete. This study examines the feasibility of developing ‘material-aware’ machine learning models that are capable of predicting compressive strength, without overlooking how intrinsic properties of sustainable or conventional concrete govern microstructural stability, and in turn, the compressive strength. Concrete datasets were preprocessed to identify parameters with statistically relevant correlation with compressive strength. Feature Engineering was employed to introduce a novel attribute ‘type’ for each concrete instance in the datasets, and the attributes corresponding to concrete sustainability were segregated to be modelled for sustainability evaluations.

Further analysis of the datasets revealed a pronounced anomalous behaviour between age and compressive strength. While age demonstrated a positive correlation with compressive strength in conventional concrete, a contrasting negative correlation was observed between age and compressive strength in sustainable concrete. This disparity revealed that both concrete types had divergent kinetic pathways during the hydration process; these differing behaviours were further explained by the presence of Supplementary Cementitious Materials (SCMs) and their distinct potential for Calcium Silicate Hydrate (C-S-H) gel generation. Under these conditions, Linear Regression (LR) and Random Forest (RF) models were trained and evaluated using  $R^2$ ,  $MAE$  and  $MSE$ . The results indicated that the majority of compressive strength correlations with concrete properties were non-linear, justifying Random Forest’s more robust and precise predictive capability. The RF model significantly outperformed the linear baseline model, achieving a near-perfect  $R^2$  of 0.993, compared to 0.831 for LR, confirming the non-linear nature of the predictor-target interactions in concrete. The research further translated the predictive results into user-friendly Graphical User Interfaces (GUIs) that allow compressive strength estimation and sustainability assessment.

Collectively, the findings of this research highlight the significance of incorporating material classification into AI-driven modelling of concrete properties and demonstrate how domain-informed machine learning can enhance both predictive accuracy and real-world usability. The study contributes a practical and scalable framework for integrating intelligent modelling into sustainable construction analysis and decision-making workflows, providing a meaningful resource for engineers and field experts.

**Keywords:** Compressive Strength; Sustainable Construction; Hydration Kinetics; Linear Regression; Concrete; Ferrock; Random Forest; Rice Husk Ash; Ferrock; Water to Cement Ratio; Artificial Intelligence; Cement Chemist Notation; Sustainability; Pozzolanic Materials; Supplementary Cementitious Materials; Superplasticisers; Coarse Aggregate; Fine Aggregate; Calcium Silicate Hydrate; Hyperparameters; Target Variables; Predictor Variables; Life Cycle Assessment

## Introduction

### The Continuous Growing World Population

The world population is slowly but steadily rising towards its projected peak. Each year, there is a reported natural increase of approximately 77 million people (Badii et al., 2017). Ultimately, the demand for construction and infrastructure continues to intensify. Governments and industries, especially from developing countries, have increased their efforts to cater the nation's augmenting need for construction and development. This, in turn, has brought attention to one of the most prevailing options to bolster the civil innovation and engineering sector: concrete. In recent years, the concrete industry has undergone substantial industrialisation and refinement. Existing concrete staples, such as Portland Cement, are now being replaced by emerging sustainable alternatives, such as Ferrock and Rice Husk Ash (RHA) based concrete. Ferrock, derived from Ferrous Rock, is a popular carbon-negative (carbon-absorbing) construction material. It is made from recycled steel dust, silica, and water. Rice Husk Ash (RHA) is a by-product of rice cultivation which is used in concrete formation. This is owing to its siliceous (silica-containing) nature and tremendous carbon sequestering ability. It is used in the sustainable concrete industry as a substitute for conventional concrete.

### The Use of Concrete

The standard concrete industries running today have been delivering consistent quality and coarse compositions, owing to their foundational remixing principles and deterministic ratios, such as the water-to-cement ratio. However, these concrete products tend to leave grave environmental impacts from the time of mineral extraction until the structure is standing. According to Uddin et al. (2023), 53 million tons of coal, while 1 million cubic feet per day (mcf) of gas was consumed by the cement sector of Pakistan. As a result, their atmospheric emissions have increased by 17% from 2015 to 2020. The production of cement itself annually could reach over 5 billion metric tons, with approximately about 4 billion tons of CO<sub>2</sub> (carbon dioxide) emissions. Conventional concrete, thus, is regarded as a non-environmentally friendly building material (Lomite & Kare, 2009).

### The Use of Sustainable Alternatives

On the other hand, the study and investigation of the use of sustainable alternatives to basic construction staples, primarily concrete and steel, remain unexplored to a large extent. Despite great environmental benefits and production potential, expert discussion led by Kavathia (2024) on Research Gate suggested that less than 15% of the construction projects worldwide involve the use of eco-friendly building materials. This is because the choice of a building material is dependent on its innate properties. These

properties determine the suitability of that material for use in a given engineering application. One of these properties is called Compressive Strength (CS).

Compressive Strength, measured in MPa or kPa, is defined as the maximum measured resistance to axial loading of a concrete specimen until it changes its shape or breaks. It is the ratio of the maximum load or force that is applied to the initial cross-sectional area of the specimen. However, calculating an experimental value for compressive strength for a certain material requires accountability for a range of different factors. These include the sample's age, testing standards, material variability and the substance's brittleness.

Given the established protocol of conducting 28-day tests on standard concrete, ensuring accurate and efficient prediction of compressive strengths for emerging sustainable alternatives through experimental procedures is both inefficient and expensive (Terlumun, 2024). The Hydration Kinetic Profile, for instance, represents the experimentally determined data that explains the rate at which concrete hardens after chemically reacting with water. Characterising this reaction's pathway for every concrete sample is a time-consuming and demanding procedure, which curbs the experimental throughput in determining correlated compressive strength. Thus, industries across the world are shifting their focus towards the use of Artificial Intelligence to estimate the strength of building materials, substantially reducing the labour, equipment and their associated costs.

### **Significance of the Paper**

This paper is significant to engineers, researchers, and policy-makers who are focused on sustainable construction. It uses AI and ML models to predict the compressive strength and sustainability of complex concrete structures, making it a cost-effective and efficient prediction system. By modeling the non-linear interactions of concrete properties and its strength, the study aids manufacturers and contractors in optimising sustainable mixes, while informing policy decisions aimed at reducing the environmental impact of construction. In addition, the study explores the anomalous trend in age and compressive strength in two separate compositions of concrete.

### **Aims and Goals of the Paper**

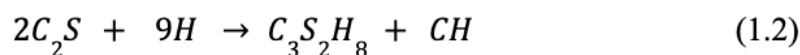
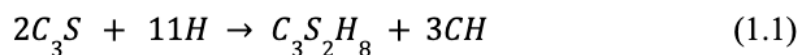
This study explores the varying rates of concrete hardening and the use of AI and Machine Learning models to predict the compressive strength for an assortment of concrete compositions. In this context, Artificial intelligence refers to data-driven techniques that learn patterns from experimental data to predict compressive strength. This is achieved by modeling complex relationships between mix design and microstructural properties in sustainable and conventional concrete. While not the primary goal, the study also investigates potential ways to determine a quantitative measure of sustainability for sustainable concrete samples. The findings of this study are expected to be meaningful to civil and environmental engineers, stakeholders in the sustainable construction industry, and policymakers who wish to use data-driven predictive modeling of compressive strengths. Ultimately, the paper aims to support the wider adoption of sustainable construction materials.

## Literature Review

### Conventional Concrete

According to the International Journal of Mechanical and Civil Engineering (2024), more than ten billion tons of concrete are produced annually, making it one of the most widely used building materials today. Due to its unmatched durability and ubiquity, concrete is a strong, affordable and low maintenance material. One common way to understand the strength of concrete is to analyse its compressive strength and the factors influencing it. Compressive strength, as defined in the introduction, is the ability of a material to resist load pressure.

Given concrete's prevalence in the construction of roads, overhead bridges and even skyscrapers, compressive strength is used to gauge the feasibility of a sample of concrete for civil use. This characteristic changes in concrete throughout its lifetime because of a certain chemical reaction involving the cement mixture used. Portland cement, the most commonly used cement mixture, contains rich amounts of Tricalcium Silicate ( $C_3S$ ) and Dicalcium Silicate ( $C_2S$ ). A study by Snellings et al., (2012) has highlighted that these two compounds undergo a primary hydration reaction (1) to produce a glue-like gel structure called Calcium Silicate Hydrate ( $C_3S_2H_8$ ). The primary hydration reaction expressed in Cement Chemist Notation (CCN), where C = CaO, S = SiO<sub>2</sub>, H = H<sub>2</sub>O, is:

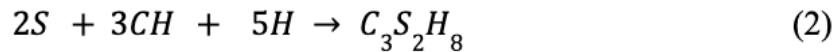


This C-S-H gel is what gives concrete its hardness and strength. It forms as tiny amorphous particles inside concrete which bind aggregates in concrete together. This ultimately fills any pores in the structure and increases the concrete's density. It further adds to concrete's strength by distributing incoming load evenly, reducing the likelihood of microcracks that could weaken the overall structure. As the reaction proceeds throughout concrete's lifetime, the strength of conventional concrete typically increases with age. The by-product of this reaction, Calcium Hydroxide ( $Ca(OH)_2$ ), is an alkaline solid that generally plays a negligible role in the early compressive strength of conventional concrete. However, it is instrumental in sustainable concrete models where it participates in spontaneous secondary hydration reactions, producing the C-S-H binding gel. Therefore, while predicting compressive strength under standard curing conditions is possible via empirical testing methods, such as the 28-day concrete tests, it is relatively complex to do so for sustainable concrete.

### Sustainable Concrete: Materials, Strength and Durability

In recent times, sustainable concrete has been a widely discussed topic. Sustainable concrete is an environmentally friendly alternative to conventional concrete. It is formed through partial replacement of Portland cement with Supplementary Cementitious Materials (SCMs), including Palm Oil Fuel Ash

(POFA), Rice Husk Ash (RHA) and calcined clay. These Supplementary Cementitious Materials (SCMs) are regarded as highly pozzolanic materials; they contain Silicon Dioxide ( $S$ ) which can react with Calcium Hydroxide ( $CH$ ) in the presence of water ( $H$ ) to constitute C-S-H gel. This reaction (2), referred to as the secondary hydration reaction is expressed in Cement Chemistry Notation (CCN) as:



Therefore, the strength development in sustainable concrete is largely done through secondary hydration reactions, unlike the primary hydration reaction dominant in conventional concrete. These SCMs are the reason why sustainable concrete is now sought as an alternative to conventional concrete which has been in use for the past few centuries. Mosaberpanah (2020) has discussed the potential of Rice Husk Ash (RHA). He called it a very effective pozzolanic material that is a suitable replacement for cement.

However, it is interesting to note that the initial strength of sustainable concrete materials was found to have an inverse correlation with age of the sample. Analysis of dataset for sustainable concrete shows that for an age of less than 365 days, the compressive strength tends to follow a negative correlation with the age of the sample. This is because the secondary hydration reaction is a very slow process. In the initial stages of concrete's structural development, the microstructures begin bearing external pressure and load which increase its porosity and tendency to bear microcracks. Whilst the repairing glue (C-S-H) is not being produced at a rate equivalent or greater than the rate of microstructural degradation, the compressive strength gradually falls. Thus, divergent hydration kinetics in both sustainable and conventional concrete impact how concrete composites redistribute incoming force and sustain pressure.

Despite the slower early-age strength development, the incorporation of SCMs enhances the density of sustainable concrete in the longer term, reducing permeability and increasing resistance to chemical attacks. These properties still make sustainable concrete a viable alternative to conventional concrete, standing at the intersection of trade-off between physical strength and environmental friendliness.

### Factors Affecting Compressive Strength

Compressive strength of materials, whether sustainable or not, is contingent on a plethora of factors. These factors determine the chemical composition of structures, which ultimately determines the way structures interact with the atmosphere and world around them. Age of the sample is one of the most prominent factors that affects compressive strength. As discussed earlier, the age of concrete tends to behave differently for sustainable and conventional concrete. The correlation of age is positive with compressive strength for conventional concrete, reflecting the continuous strengthening of microstructures and filling of porous amorphous Calcium Silicate Hydrate (C-S-H).

On the contrary, the age of concrete, for the initial stage of concrete's lifetime, has a negative correlation with compressive strength for sustainable concrete, reflecting the relatively slower production of C-S-H gel. It is worth noting that sustainable concrete in this case is a homogenous classification of a broad range

of concrete varieties composed of different SCMs. Therefore, after an initial stage of approximately 365 days, the effect of sample's age on compressive strength changes based on the composition of a sustainable concrete model.

Hence, composition is the next crucial factor involved. The most important constituent of modern-day conventional concrete is Portland cement. The cement content is an integral factor affecting compressive strength. Higher cement proportions increase the binder volume and contribute to denser concrete, leading to higher early-age strength. In sustainable concrete, partial replacement of cement with SCMs can reduce early strength, highlighting the importance of considering cement quantity alongside other compositional factors. For example, Hassan et. al. (2025) observed that increasing the cement content from 350 kg/m<sup>3</sup> to 450 kg/m<sup>3</sup> increased the compressive strength of normal weight and lightweight concrete mixes by over 20 %.

Similarly, the choice of Supplementary Cementitious Materials (SCMs) also dictates the initial strength of sustainable concrete. In a study by Liu et al. (2018), the median particle size ( $D_{50}$ ) of SCMs was found to directly influence its pozzolanic activity, thus impacting the quantity of hydration products. For example, refining  $D_{50}$  (from ~26.4  $\mu\text{m}$  to ~1.5  $\mu\text{m}$ ) can increase compressive strength (from ~38 MPa to ~55 MPa), despite SCM incorporation generally being associated with reduced early-age strength.

Additionally, compressive strength relies largely on the aggregate composition of concrete. Aggregates are defined as the granular materials that provide structural filling in concrete. They constitute the majority of concrete volume and are classified into two broad categories: coarse aggregate and fine aggregate. Coarse aggregate are the larger particles within the aggregate that are the primary foundations for load-bearing. These generally include gravel or crushed stones that are greater than 4.75 mm in diameter. Increasing the content of coarse aggregate, particularly angular-shaped particles that support interlocking, increases the compressive strength of concrete. Conversely, fine aggregates are smaller particles that are used to fill voids between coarse aggregate particles. They enhance packing density and reduce the overall porosity, bolstering concrete microstructure.

Another factor that influences compressive strength is the choice of superplasticizer. Superplasticizers are chemical compounds that increase fluidity of the concrete mixture without the need to increase the water-to-cement ratio. This allows less porosity and high usability of concrete mix. Xun et al. (2020) pinpointed how functional polycarboxylic acid superplasticizers influenced cement hydration and microstructure in unique fashions, owing to steric hindrances from their side chain structures. While these material and compositional factors largely determine compressive strength, predictive modeling using artificial intelligence allows us to analyse complex interactions between these factors and quantify strength outcomes, even when trends differ between conventional and sustainable concrete.

### **AI and Machine Learning in Concrete Strength Prediction**

Concrete is an intricate composition of various materials. Multiple variables interact with one another to dictate the behaviour and performance of concrete. To understand the wide range of concrete behaviours, researchers have employed the use of Artificial Intelligence (AI) in mapping trends and correlations

between certain material properties and mixture compositions. AI, as elucidated in the introduction, is an evolving technology that leverages the ability of systems to learn using preprocessed and cleaned data. Multiple studies conducted by Altunci (2024) and Albostami (2024) indicated that AI models, such as Artificial Neural Networks (ANNs), Random Forest (RF), Gradient Boosting Regression (GBR) and Support Vector Regression (SVR), are influential ways to model and predict conventional concrete properties, including compressive strength. These models typically receive water-to-cement ratio (w/c), coarse aggregate, fine aggregate, sample age and superplasticiser content as inputs and use supervised learning algorithms to predict compressive strength, with performance evaluated through mean squared error (MSE) or mean absolute error (MAE).

Even though AI models can model compressive strength of conventional concrete made primarily from Portland cement, most Machine Learning models are unable to account for the differing properties and behaviors of sustainable concrete. This limitation highlights a void in the existing literature, discounting the characteristic properties of various SCMs that constitute different models of sustainable concrete.

### **Research Gaps and Motivation**

Despite the latest advancements in AI, many models tend to overlook the distinct properties that SCMs bring. A common oversight made in most models is the generalization of sustainable and conventional concrete under a homogenous umbrella, without acknowledging the differences introduced by certain SCMs and aggregates and their quantities. As a result, a plethora of concrete properties are misrepresented, yielding a false prediction for compressive strength.

Additionally, several studies tend to generalise the role of factors across conventional and sustainable concrete. For instance, Bhuyan & Hakimi (2024) employ age, cement content, SCMs, and other mix variables in ML prediction models without distinguishing material types or divergent age against strength trends between conventional and alternative concrete. A plausible cause for this may be the lack of availability of datasets and generalisation of sustainable concrete characteristics. Motivated by these limitations, this study aims to develop AI models that explicitly consider material type, enabling more accurate predictions of compressive strength for both conventional and sustainable concrete.

### **Methodology**

#### **Data Sources and Data Selection**

As part of the research methodology, experimentally determined datasets with varying mixes and compositions for concrete were used. The study recognised and explored two extensive datasets as the primary sources of data. Each of them included data points with properties that were tested through laboratory concrete specimens. These included cement ( $\text{kg/m}^3$ ), blast furnace slag ( $\text{kg/m}^3$ ), fly ash ( $\text{kg/m}^3$ ), water ( $\text{kg/m}^3$ ), superplasticiser ( $\text{kg/m}^3$ ), coarse aggregate ( $\text{kg/m}^3$ ), fine aggregate ( $\text{kg/m}^3$ ) and age (days). The purpose was to analyse and find correlations between different factors and composing substances against the target variable, compressive strength of concrete samples. The first dataset used was a spreadsheet of various concrete mixes, with their aggregate compositions, age and water content. The

dataset, made available in 1998, was accessed through the University of California Irvine's Machine Learning Repository. The dataset contained over 1000 instances, referencing 8 attributes for each concrete sample.

The second dataset was a collection of sustainable and low impact concrete formulations. It was acquired online on Kaggle. Last updated in 2024, this dataset included over 1000 instances. Each instance incorporated standard mix parameters, which were similar to the ones that were used in conventional concrete dataset, along with some additional attributes. These attributes included embodied CO<sub>2</sub> (kg/m<sup>3</sup>), energy consumption (MJ/kg) and resource consumption (MJ/kg). They highlighted the environmental friendliness of each specimen. Therefore, these additional attributes make the dataset structurally richer and resourceful for gauging sustainability of concrete samples.

Both the datasets share a common physical basis of linking mix designs to compressive strength. There are several other attributes which are common for both datasets, such as sample age, coarse aggregate and fine aggregate, allowing meaningful comparisons and easier correlation mapping. However, it has been observed that there are certain attributes which are specific to a single dataset. For instance, embodied CO<sub>2</sub> and energy consumption attributes were unique to the sustainable concrete dataset, while blast furnace slag and fly ash attributes were specific to the conventional concrete dataset. These differences in the datasets reflect the intricacy of materials' design paradigms, which dictates how certain characteristics can influence compressive strength. As a result, it was crucial to identify these differences so that they could be accounted for in the data pre-processing.

All the conclusions and deductions derived in this study were based primarily on the two aforementioned datasets. No interpolated or synthetic instances were generated, and only real experimentally determined values were used in the training, testing and validating stages of the AI models.

## Data Preprocessing and Feature Engineering

The initial cleaning of raw data was essential before any further operations could be executed. Both datasets were subject to fundamental data cleaning and quality assessment. The data were screened to identify any missing, null or erroneous values to ensure maximum accuracy and validity. Both sets of data reported no missing or inconsistent entries that could distort the outcomes of this study. Furthermore, each instance was scrutinised to verify that unrealistic values, such as negative numbers for water content or zeroes for sample age, were not present. These steps ensured that any anomalous behaviour could be ruled out prior to development of the AI model. Thus, complete, numerically valid and structurally reliable datasets were studied.

Before further analysis and design could be executed, the datasets had to be combined to form an extensive data resource for training, testing and validation purposes. To achieve this without compromising on the accuracy, the data was not merged indiscriminately at the feature level. Although both datasets contained several core material and physical parameters, there were certain parameters that were specific to the type of concrete. Thus, rather than merging the datasets without distinction, feature names and units were standardised where the variable represented an overlapping feature, such as cement content or coarse

aggregate content. On the contrary, dataset-specific features were not synthesized or used interchangeably between the two datasets, maintaining authenticity and mitigating the risk of feature misrepresentation.

Feature inclusion was an imperative step in the preprocessing phase. The choice to include a certain parameter in the AI based predictive model did not rely solely on the availability of data. It was based on the logical and physical significance in determining the target variable. Concrete age and mixture compositions, such as the cement content, water content and fly ash percentage, are deterministic factors which are available for each concrete specimen that impacts the C-S-H gel formation and hydration processes, thereby indirectly affecting the compressive strength. It is important to note that not all available attributes had a meaningful correlation with the target variable. For instance, the energy consumed in preparing a sustainable concrete mix did not largely influence its compressive strength. Instead of misrepresenting data by including such attributes into the mathematical model, embodied CO<sub>2</sub>, energy consumption and resource consumption were disregarded in compressive strength prediction. The inclusion of these non-causal variables would introduce statistical noise and reduce the interpretability of the model from an engineering standpoint. However, they were alternatively used to design a supplementary sustainability predictor, ensuring no sections of data were unutilised.

Conventional and sustainable concrete differ on the basis of their compositions and the underlying processes and design philosophies that define how they behave. It is likely that conventional concrete's compressive strength diverges significantly from that of sustainable concrete even with the same compositions. As shared in the literature review section, the use of different Supplementary Cementitious Materials (SCMs) causes the expected compressive strength of conventional concrete to deviate from the benchmark. Thus, it is unreasonable to make predictions and judge concrete's strength only on the basis of its composition, without accounting for the categorical nature of concrete.

To mitigate this limitation, a new 'type' attribute was introduced for the AI predictive model to segregate concrete into sustainable and conventional categories. This ensures that intrinsic behavioural properties of sustainable concrete are not employed in predicting compressive strength for a conventional concrete model and vice versa. This approach can avoid any misleading generalisations and preserves engineering realism. This is necessary for real-world analysis and predictive modelling of compressive strength, by using a data-driven AI Model.

Defining target and predictor variables is a crucial step in Machine Learning. The target variable is the primary outcome or label that a supervised machine learning model is trained to predict or classify based on input data. On the contrary, the predictor variables are inputs, factors or independent variables that are manipulated to measure their influence on the target variable. Following data cleaning and feature aligned and construction, compressive strength was labelled as the target variable, while the other variables were labelled as predictor variables and were conserved in their original units. The entirety of the dataset was split in a 70:30 ratio, allowing 70% of the data to be used for model training and the remaining 30% for model testing and validation. This ensured adequate data was available for model training and pattern recognition, leaving unbiased and independent data instances for fair evaluation and performance testing.

## Model Selection and Development

The choice of model was contingent on two key factors: interpretability and predictive capability. It is instrumental that AI models function on mathematical formulae that align with the requirements of the task. This is without compromising the coherence and model robustness in the context of its use. To achieve this, a Linear Regression (LR) model was chosen as the baseline model. It was employed to gauge the quality of predictions, if utmost linearity in material behaviour is assumed. While this approach aided interpretability, real life material compositions do not follow complete linear projections. Subsequently, to address the limitation of Linear Regression to model non-linear relations, a Random Forest (RF) model was used and tested for the same purpose. This allowed a multi-faceted approach to the prediction capabilities of the two AI models, whilst offering potential for comparative analysis of the two AI models - LR and RF.

Linear Regression (LR) algorithm was first considered for the development of the AI predictive model. This is because the Linear Regression (LR) algorithm identifies parameters and establishes linear relationships between the predictor and target variables. It achieves this by summing the weighted inputs for each composition and an intercept term. The mathematical formula for Linear Regression (3) used in this calculation is:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n + \varepsilon \quad (3)$$

Where  $Y$  represents the predicted compressive strength,  $x_n$  are the input features (such as: age, cement content, water content and SCM proportions),  $\beta_n$  are the regression coefficients,  $\beta_0$  is the intercept and  $\varepsilon$  is the error term. Each coefficient is a quantifiable representation of the influence for that corresponding variable in the determination of compressive strength. Although less efficient, a Linear Regression model provides a suitable and physically intuitive baseline.

However, the assumption of a perfectly linear and oversimplified relation proved inadequate upon testing the model. To overcome this, a Random Forest (RF) Model was employed that could model the non-linear dependencies by using an ensemble of decision trees. Each tree recursively partitions the feature space which is based on threshold values that minimise prediction error. It could accommodate heterogeneous features, while simultaneously leveraging the type-aware dataset structure effectively. The final prediction is obtained by averaging the predictions made by each tree. The mathematical formula for RF Model (4) used in determining the final prediction is:

$$\hat{y} = \frac{1}{N} \sum_{i=1}^N \hat{y}_i \quad (4)$$

where  $\hat{y}$  is the prediction from the  $i^{th}$  decision tree and  $N$  is the total number of trees in the forest. This ensemble averaging reduces variance and mitigates overfitting, making RF particularly suitable for heterogeneous datasets involving both conventional and sustainable concrete. In addition, RF makes use

of certain configuration settings that are defined before training to control the model's structure, growth and complexity. These settings are referred to as 'hyperparameters'. In the case of our study, these include the number of trees, maximum depth of trees and the number of features considered for splitting.

Both models were trained by using the same sets of data. Thus, ensuring unbiased and fair analysis. The dataset was divided as per the previously stated 70:30 training:testing split. This allowed the testing data to be reserved only for fair validation purposes. For the RF model, key hyperparameters were set in order to achieve an equilibrium between the tradeoff of model complexity and prediction competence. No data leakage was permitted between training and testing phases, preserving the integrity of the evaluation process and ensuring that model predictions reflected genuine generalisation to unseen data.

After the data had been processed and the models had been developed, they were evaluated on the basis of certain metrics which allowed transparent comparison between LR and RF models. This included the coefficient of determination ( $R^2$ ) which measures the proportion of variance in compressive strength explained by the model. It is one of the most direct evaluation metrics to gauge efficiency and accuracy, and is defined as:

$$R^2 = 1 - \frac{\Sigma (y_i - \hat{y}_i)^2}{\Sigma (y_i - \bar{y})^2} \quad (5)$$

where  $y_i$  are observed values,  $\hat{y}_i$  are predicted values, and  $\bar{y}$  is the mean of observed values. Alternatively, Mean Absolute Error (MAE) is another evaluation metric that quantifies the average magnitude of prediction errors. It is given by (6):

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (6)$$

Additionally, Mean Squared Error (MSE) provides higher sensitivity to outliers and penalises larger errors more strongly, the extent to which could be judged with the summation of squares of the errors. The equation for MSE (7) is given by:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (7)$$

The combined use of these metrics ensures a comprehensive evaluation of both accuracy and robustness. Therefore, enabling meaningful comparison between linear and non-linear modeling approaches.

## Analysis of Age-Dependent Behaviour and Anomaly Identification

As discussed in the literature review, the age of a concrete sample is one of the key determinants for compressive strength. It governs the production of C-S-H gel and internal hydration processes. This in turn influences concrete's microstructural stability: more C-S-H gel means stronger internal binding. While conventional concrete typically exhibits predictable early-age strength gain, sustainable concrete may incorporate supplementary cementitious materials that can alter hydration rates and delay strength development. Consequently, assuming constant strength patterns against age of different types of concrete samples was physically inconsistent and oversimplified fundamentally distinct mechanisms and properties. To address this, the correlation between sample age and compressive strength was studied at a greater depth before model designing. This ensured that material-specific behavior was considered rather than generalising properties.

Furthermore, to examine age-dependent behaviour, compressive strength trends were analysed by grouping specimens according to concrete type and age. Concrete strength was observed across specific intervals of age, where the sustainable and conventional concrete datasets were treated independently to identify behaviours which were intrinsic to that particular type.

It is important to note that during age-based trend inspection, an anomaly was observed. The inspection reported an anomalous behaviour in the correlation of sample's hydration timeline and compressive strength for sustainable concrete. This was particularly during the early-age strength latency stage for sustainable concrete samples. As explained in the literature review, SCM driven processes in sustainable concrete may disrupt conventional strength gaining mechanisms and, unlike conventional concrete, a negative correlation between age and strength was observed.

Ultimately, the Linear Regression model became statistically inadequate for predicting compressive strength, given the non-linear interactions between compressive strength and the factors determining it. Consequently, the significance of accounting for these divergent hydration kinetics led to the choice of Random Forest Model. This ensured that the non-monotonic trends were accurately captured, which would otherwise have been overlooked.

## Development of Practical Prediction and Sustainability Evaluator

Following the comparative analysis of the LR and RF models, a final concrete strength predictor was developed using the RF model. The predictor is an intuitive Graphical User Interface (GUI) which calculates and predicts a value of compressive strength based on various inputs. The interface first asks the user for the type of concrete (that includes sustainable or conventional). This leverages the categorical 'type' feature which was curated for the case of this research to allow only material-specific parameters to be requested and utilised in strength prediction.

The interface upon selection of sustainable or conventional concrete dynamically adjusts the requested input variables to reflect only the relevant material attributes which were associated with that concrete category. These input variables were kept harmonious to the attributes available in the dataset, ensuring

all units were kept consistent. The entirety of the UI works using interactive slider-based widgets. Besides the only binary input (that is the Type of Concrete), each input variable allows the user to choose from a continuous range of values. This enables the interface to bridge the theoretical and analytical understanding of compressive strength with real world applications of strength modelling.

In addition to the primary aim of this research to compare AI efficiency and propose a ‘material-specific’ predictor for concrete compressive strength, a sustainability evaluator was also designed for sustainable concrete samples. As referenced earlier, the dataset for sustainable concrete contained three additional attributes: embodied CO<sub>2</sub>, energy consumption and resource consumption. These attributes did not play a substantial role in influencing the compressive strength of sustainable concrete and exhibited negligible statistical correlation.

Rather than incorporating these factors into the Compressive Strength predicting UI, a separate framework was developed for sustainable concrete samples that employed these three factors in order to quantify the environmental impact of that concrete sample. The framework presents the sustainability score through an interactive spectrum meter, providing added resourcefulness for civil and environmental engineers.

## Findings and Discussion

### Dataset Behaviour and Correlation Insights

The two datasets were run through a correlation analysis, where the predictor variables and their behaviour with the target variable were studied prior to the model development. Figure 1 and Figure 2 illustrate the Pearson Correlation Heatmaps for conventional concrete compositions and sustainable concrete compositions respectively, highlighting distinct behaviours and variations.

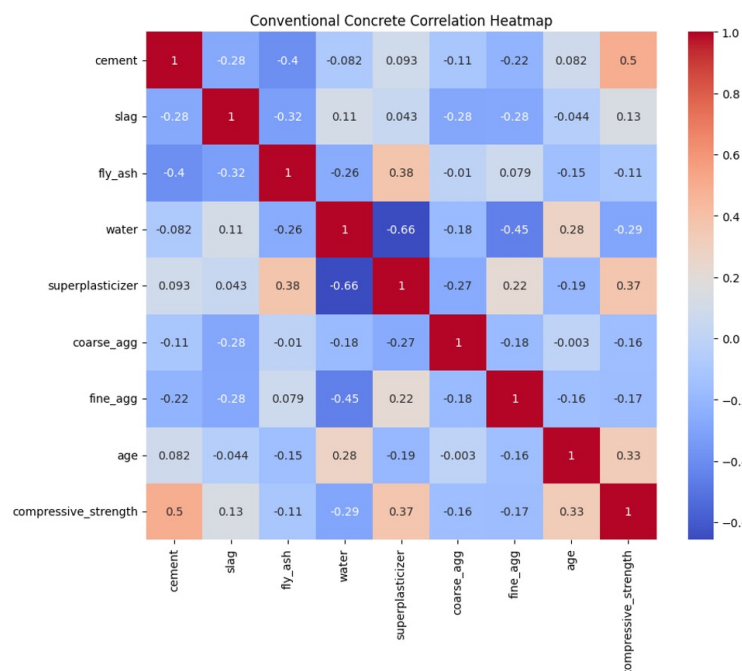


Figure 1. Pearson Correlation Heatmap for Conventional Concrete

The figure illustrates a positive correlation between compressive strength for conventional concrete for certain factors including age, superplasticiser, blast furnace slag and cement. Negative correlations with compressive strength are observed with fine aggregate, coarse aggregate, water content and fly ash.

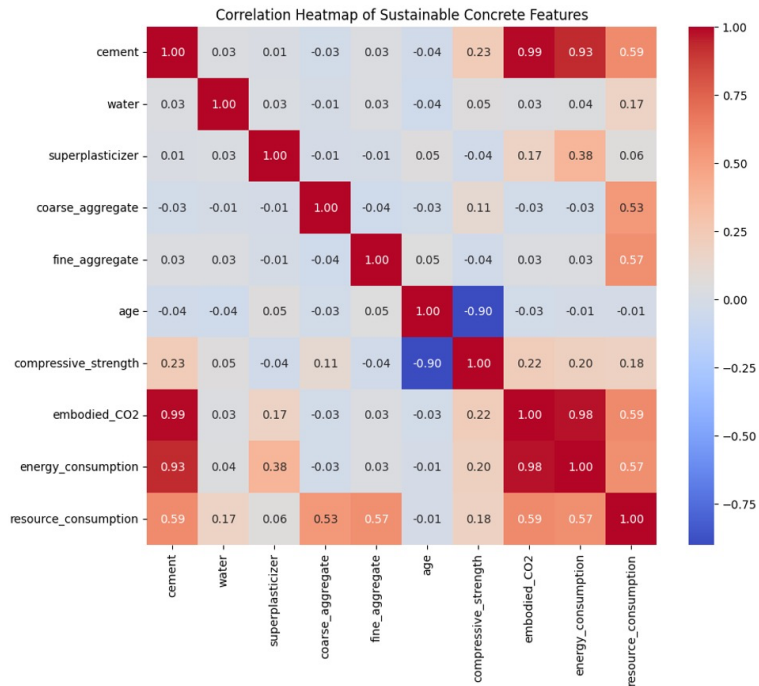


Figure 2. Pearson Correlation Heatmap for Sustainable Concrete

The figure indicates a positive correlation between compressive strength for sustainable concrete for certain factors including coarse aggregate and cement content. Negative correlations with compressive strength are observed with age, fine aggregate and superplasticizer.

The heatmaps demonstrate that compressive strength in conventional concrete and sustainable concrete can largely follow similar correlations. For example, some predictor variables common to both, such as cement content, water content and fine aggregate, had the same trend across both sustainable and conventional concrete. On the contrary, certain features were found to have non-uniform behaviour across sustainable and conventional concrete. These include the superplasticiser dosage, coarse aggregate and the age of concrete sample. The contrast in strength trends in sustainable and conventional concrete make it evident that the compressive strength cannot be linearly modelled.

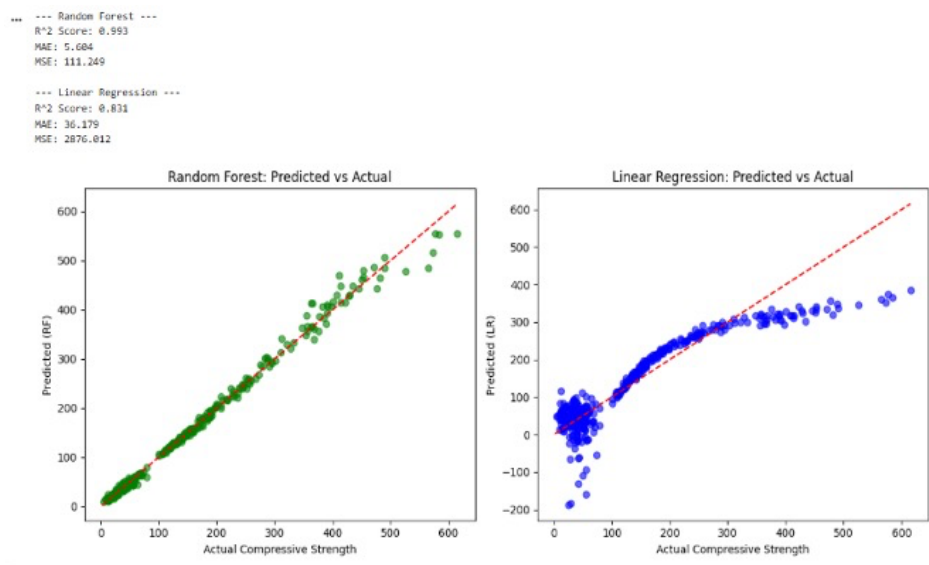
The variation of age with compressive strength was a significant observation of the study. This is because the analysis revealed the contrasting correlation of age with conventional and sustainable concrete, consistent with the mechanisms discussed in the literature review. Age demonstrated the strongest positive association within the conventional concrete dataset, thus reflecting progressive hydration and strength gain over time. Similarly, cement content yielded a consistently positive trend with both conventional and sustainable concrete compressive strengths. However, superplasticiser and aggregate contents exhibited contrasting behaviours in the case of sustainable and conventional concrete.

Therefore, the variation in how the material property correlates with the compressive strength of concrete provides the rationale for a categorical evaluation of compressive strength for sustainable and conventional concrete. This made it evident to avoid the generalisation of concrete by assuming homogeneity in concrete behaviour against the factors affecting compressive strength. A notable divergence was observed in the correlation of sample age and compressive strength. While age remained a strong determinant of strength in conventional mixtures (a positive correlation of 0.33), its influence appeared less consistent in sustainable concrete (a pronounced negative correlation of -0.90), potentially reflecting the delayed hydration behaviour that was associated with supplementary cementitious materials. Additionally, certain parameters, such as cement content had varying degrees of influence on strength in the case of conventional and sustainable concrete. Consequently, a ‘type’ attribute was deemed critical to leverage type-specific attributes and material philosophies in making accurate predictions.

### Model Performance and Predictive Accuracy

As discussed previously, data preprocessing and analysis highlighted the importance of not relying solely on linear modelling of compressive strength against the predictor variables. For the sake of a comparative analysis and real-world demonstration on how linearity was insufficient in defining and predicting compressive strengths, LR model was used as a baseline statistical model and RF was used as a non-linear ensemble model.

After training the models under the same conditions, the models were subjected to evaluation. Both the models were evaluated using  $R^2$ ,  $MAE$  and  $MSE$ , the results of which are shown below (Figure 3). While the Linear Regression model delivered a moderately fit  $R^2$  value of 0.831, the Random Forest Model outperformed Linear Regression model, with a near-perfect  $R^2$  value of 0.993. Similarly, RF demonstrated smaller values for  $MAE$  and  $MSE$ , signalling its aptness in compressive strength modelling without assuming linearity. The use of numerous decision trees with known depths via RF emerged to have a clear performance advantage over the linear baseline model (LR).

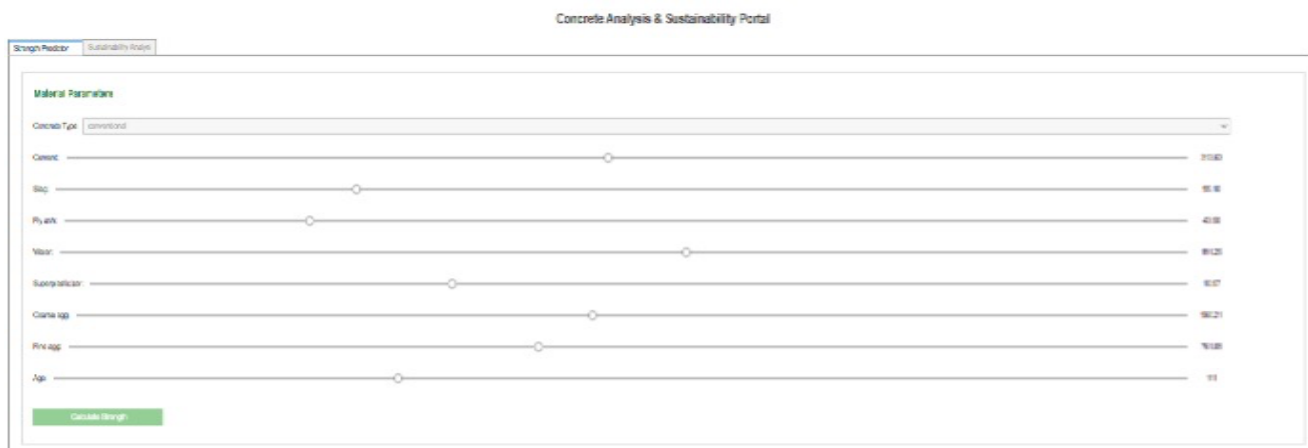


**Figure 3. Predicted vs Actual Compressive Strength Regression Plots and evaluation metric values for LR and RF models**

Additionally, the predictive accuracy of both the models was plotted as a regression plot. Visual inspection of model capabilities demonstrated that RF predictions were closely aligned to the ideal prediction line, also referred to as the identity line (line  $y = x$ ). This indicated consistent performance of RF across both low and high strength ranges. However, LR predictions illustrated significant deviations from the ideal prediction line, particularly in high strength regions. The scatterplots confirmed that compressive strength prediction is inherently non-linear. Consequently, RF was confirmed as the more robust architecture for compressive strength prediction.

### Engineering Interpretation

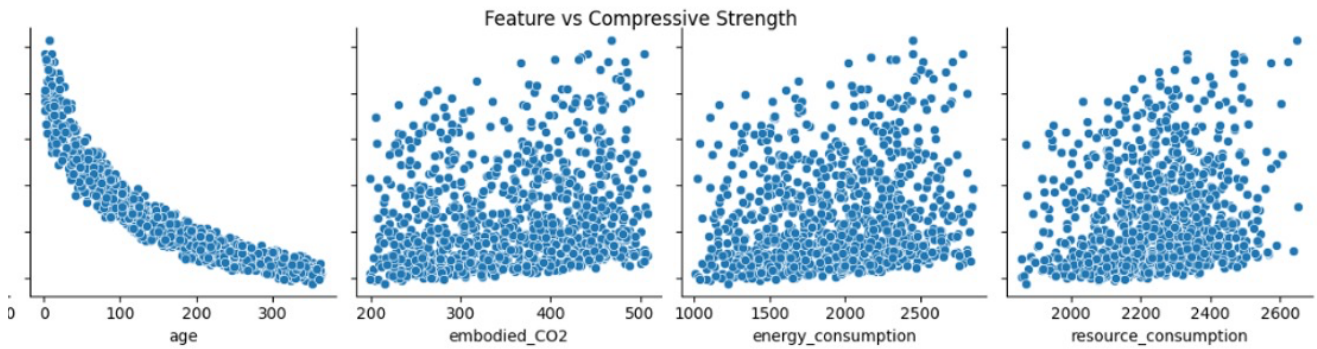
After the comparative analysis of AI models, RF was chosen as the final model for building an interactive interface that models the theoretical understanding of concrete and its compositional behaviour to real-world applications. A compressive strength prediction dashboard was created that could take inputs for the predictor variables and calculate a value for compressive strength, taking into account the concrete type and its associated determining factors. The interface (Figure 4) can enable engineers and field experts to determine compressive strength for an assortment of concrete compositions, allowing them to plan material choices for infrastructural and development projects. This can significantly reduce testing time, providing a cost-effective, efficient and robust alternative to long and labour-intensive laboratory testing procedures.



**Figure 4. RF based Compressive Strength Predicting Interface**

The interface is a material-aware system, requiring concrete material type-specific target variables to predict strength of concrete. It allows the user to input from a continuous range of values for the input parameters, aiding practical application.

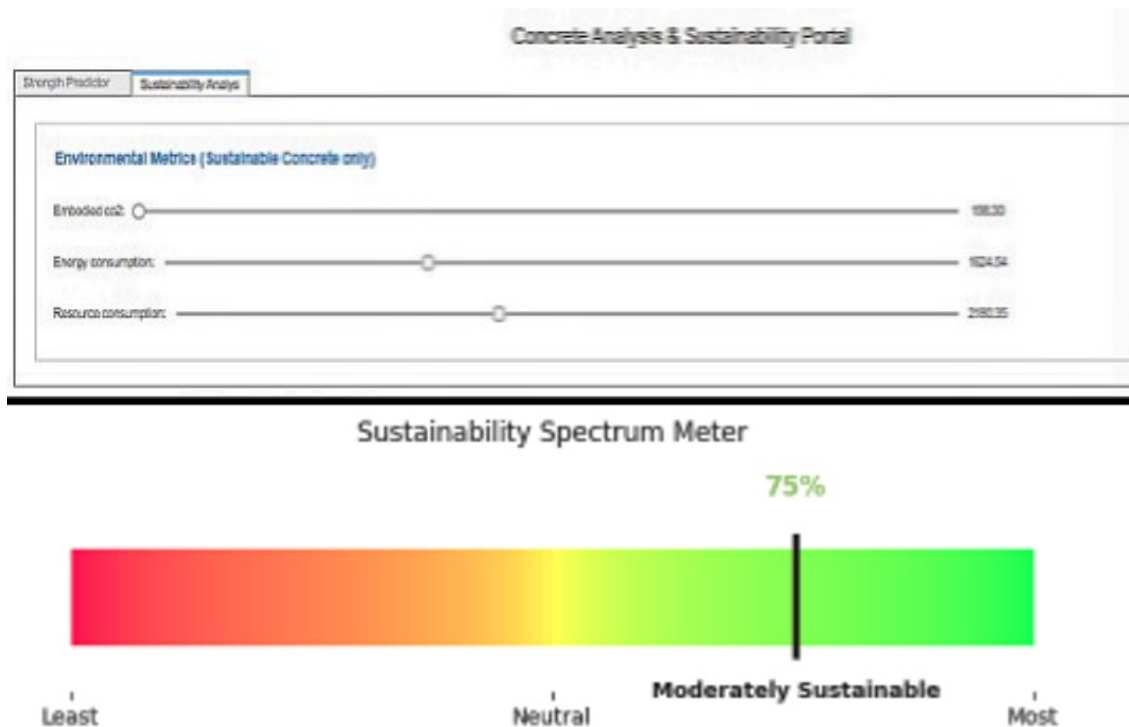
In addition to the strength predictor, a sustainability spectrum meter was created using the three non-causal attributes in the sustainable concrete dataset: embodied CO<sub>2</sub>, energy consumption and resource consumption. The trend analyses in Figure 5 demonstrate the correlations between compressive strength and age, embodied CO<sub>2</sub>, energy consumption and resource consumption.



**Figure 5. Correlations between Compressive Strength of Sustainable Concrete and sample age, embodied CO<sub>2</sub>, energy consumption and resource consumption.**

A downward trend for age variation confirms a negative correlation between sample age and compressive strength. Meanwhile, graphs for embodied CO<sub>2</sub>, energy consumption and resource consumption exhibit no correlation.

Extending beyond the primary scope of strength prediction, this supplementary tool (Figure 6) harnessed the additional attributed data available for sustainable concrete into an interface that provides visual analytics for concrete’s sustainability. It uses a spectrum meter to rank concrete specimens based on environmental impact thresholds, transforming machine learning outputs into user-friendly decision-support tools suitable for practical engineering.



**Figures 6 and 7. Sustainability Analysis Interface for Sustainable Concrete samples.**

This interface only evaluates sustainability for sustainable concrete specimens by allowing users to input values for embodied CO<sub>2</sub>, energy consumption and resource consumption.

## Limitations of the Study

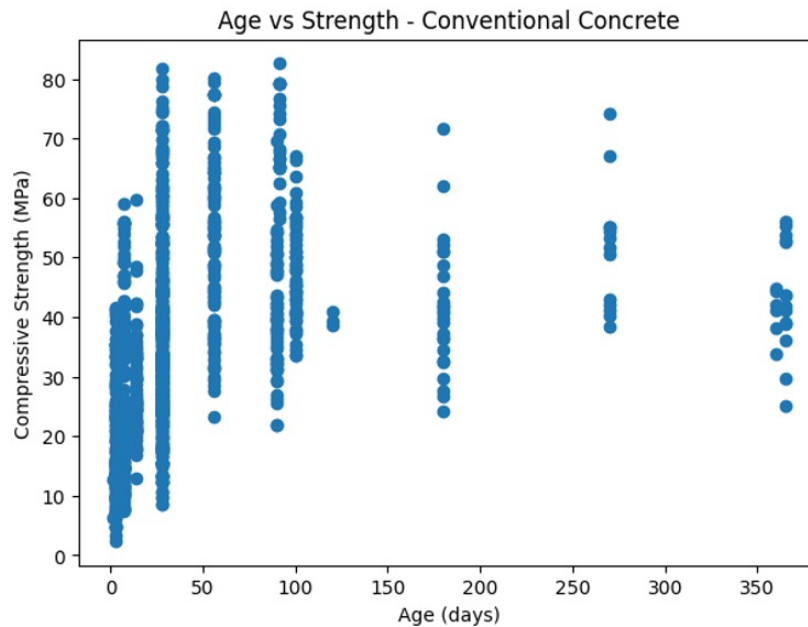
The predictive models developed in this study were trained using two datasets. Each of them contained over 1000 instances for sustainable and conventional concrete. The efficiency of model training is contingent on the volume and diversity in training data. AI and ML models that are trained with more facts and data tend to perform better when giving predictive outcomes. Therefore, while the datasets used are well-established and widely used in concrete research, real-world concrete mixtures vary depending on regional material availability, construction practices and environmental conditions. These variations are not reflected with high-fidelity representation in experimentally determined datasets. This, in turn, emphasizes the need for more extensive and vast datasets that aim to reduce the chances of error. However, despite these considerations, the datasets used provide a sufficient and reliable benchmark for model training and meaningful comparative analysis of the models.

In addition to the compressive strength prediction, a sustainability evaluation tool was developed to incorporate embodied CO<sub>2</sub>, energy consumption and resource consumption. This was done to determine an arbitrary degree of sustainability for the sustainable concrete sample. While these three parameters are pivotal in determining concrete's environmental impact, real-world sustainability assessments are contingent on a multitude of factors. These include transportation factors, life-cycle analysis, curing age and recycled concrete aggregate. The dataset used to train the sustainability analysis model was only limited to the three aforementioned parameters. As a result, it was unable to factor the remaining determinants into sustainability prediction. Furthermore, concrete mixes were broadly categorised into two families: sustainable and conventional concrete. In reality, concrete does not exist in discrete levels of sustainability, rather it is a continuous spectrum of varying environmental behaviours. Adjusting mix compositions can harmonically influence the mechanical properties of concrete, including its compressive strength. Therefore, while the classification of concrete into two categories is an important research and methodological step ahead from previous generalisations, there is scope for further classifications - based on microstructural properties and concrete compositions.

The study employed two different AI models for the purpose of predicting compressive strength and environmental friendliness of concrete specimens. The selected models - LR and RF - exhibited strong predictive accuracy, with RF significantly outperforming LR. While alternative AI models with greater architectural complexity could be explored, such investigations were beyond the scope of the present study, which focused on establishing a robust, interpretable comparison between linear and ensemble methods. Similarly, the interfaces developed require the user to input values for the target variables. This feature is indeed beneficial in early design and engineering applications for real-world projects. However, the interface may produce erroneous results when dealing with large batch-to-batch inconsistencies and on-site sample-to-sample variations in concrete.

One inconsistency within the conventional concrete dataset was observed when correlations between compressive strength were mapped against the different predictor variables. Figure 7 demonstrates one such variation between compressive strength and age. The data clusters illustrate that the dataset contains instances from discrete days. This can be observed through the quantization in vertical lines containing

plot points. The conventional dataset lacks continuous temporal resolution, as data points were recorded at discrete intervals rather than across a continuous curing timeline. As a result, the dataset is not representative of a continuous range of days, risking the distribution and unbiased representation of data. Despite this limitation, the dataset remains statistically viable for robust compressive strength prediction.



**Figure 8. Correlation between Compressive Strength and Age for Conventional Concrete**

The discrete lines of plot points signify that the data in the Conventional Concrete dataset has been recorded for discrete days and not a continuous range of days similar to how it’s done for sustainable concrete (see Figures 6 and 7)

**Conclusion**

**Summary of Findings and Evidence**

This research identified that hydration kinetics in concrete are dependent on the mix composition; different concrete types exhibit different rates of hydration, nullifying the assumption of homogeneity in concrete behaviour. While the chemical reaction between cementitious binders in concrete and water is instrumental in determining compressive strength, the intricacy of traditional experimental procedures limits the potential study across a wide range of concrete samples. Consequently, this research explored and demonstrated how compressive strength for concrete can be modelled and predicted using Artificial Intelligence and Machine Learning algorithms, saving time, expenses and labour. Two structured datasets were used providing sufficient instances for sustainable and conventional concrete. Following pre-processing of datasets, it was determined that compressive strength varied differently with the same factors for sustainable and differently for conventional concrete. These variations in concrete behaviour led to the development of the ‘type’ concept.

A type feature was introduced to classify concrete into two broad categorisations: sustainable and conventional concrete. Exploratory analysis of type-specific concrete behaviours revealed that some factors affecting conventional concrete strength were different from the ones affecting sustainable concrete strength. Additionally, an anomaly was detected in the correlations of concrete age with compressive strength for sustainable and conventional concrete. Due to increased C-S-H gel production via primary and secondary hydration processes with age, compressive strength in conventional concrete demonstrated a positive trend with age. On the contrary, a negative trend was observed for age and compressive strength in sustainable concrete. This divergence is a consequence of the delayed hydration processes and pozzolanic activity due to complex chemical interactions of Cementitious Materials (SCMs). Thus, ‘material type-specific’ strength prediction was targeted, which required an efficient AI model. For this purpose, Linear Regression (LR) and Random Forest (RF) models were evaluated using a 70:30 train-test split to ensure reasonable training and unbiased validation.

Analysis of the datasets and compressive strength predictions confirmed that assuming homogeneity in concrete behaviour without accounting for the intrinsic properties introduced by SCMs leads to inaccurate results. The interaction of most factors, such as cement content, blast furnace slag and superplasticizer content with compressive strength is not always linear, thereby requiring an ensemble and efficient machine learning algorithm. Comparative analysis of Linear Regression (LR) and Random Forest (RF) reveals compromised predictive performance by LR ( $R^2 = 0.831$ ), in comparison to RF ( $R^2 = 0.993$ ). Collectively, the findings confirm that non-linear aptness and generalisation free AI/ML models were needed for accurate prediction of compressive strength in concrete.

### **Practical and Methodological Contributions**

Bridging the academic modelling and theory with the practical engineering implementation was a crucial step. The research mapped the analytical findings and conceptual backgrounds to formulate a framework that reflected the characteristics which were required for accurate compressive strength prediction. For this purpose, the Random Forest model was selected as the optimal choice, providing both improved efficiency and ability to handle non-linear relationships. A ‘type-aware’ modeling approach was adopted, ensuring misleading correlations could be avoided. Furthermore, some additional attributes available in the dataset for sustainable concrete were segregated during the development of an RF based compressive strength predictor. Figure 5 has underlined no direct correlation between compressive strength and the three environmental factors: embodied CO<sub>2</sub>, energy consumption and resource consumption. Thus, they were instead utilised to develop a supplementary tool that allows engineers and environmental authorities to understand the environmental performance of their concrete sample through an interactive spectrum meter.

Ultimately, the key practical contributions of the research were the Compressive Strength Predictor User Interface (Figure 4) and the Sustainability Analysis Meter (Figure 6). The two systems could enable engineers to perform type-specific strength predictions and sustainability evaluations for sustainable concrete samples, without deep understanding of Machine Learning or Artificial Intelligence. The compressive strength prediction interface allows inputs to type-specific variables, similar to the factors available in that concrete type’s dataset. This provides a user-friendly experience with less latency and

redundancy, providing mostly accurate predicted values for strength. Similarly, the sustainability analysis portal, while not the primary objective of the study, is a resourceful tool for environmental engineers and authorities in order to gauge the interaction of concrete with the environment. Combined with the AI Predictive models prepared, such as the compressive strength prediction interface and the sustainability analysis portal, the research signifies how artificial intelligence can contribute as decision aid during preliminary concrete choices and sustainable material planning.

### **Future Directions and Recommendations**

Further investigations and studies may build upon this framework by using a larger and more diverse repository of data. This would allow a larger variety of supplementary cementitious materials, concrete compositions and other factors to be accounted for when calculating predictive values for compressive strength. The current binary categorisation of concrete could also be transformed into granular concrete categories. Thus, further expanding microstructural behavioural understanding and more effective strength modelling. While intricate and complex, a multi-level classification of concrete will certainly increase the predictive robustness of the model and allow a myriad of varying compositions and conditions to be addressed.

The compressive strength prediction interface and the sustainability analysis portal may be further ameliorated to include real-time information that aids case-by-case compressive strength prediction. Existing construction and concrete industry leads could be reached out for utilising their resources and available concrete samples for testing and further analysis of AI modelled and experimentally determined compressive strength values. In addition, the systems can be made compatible for use in digital construction platforms, such as Autodesk BIM (Building Information Modeling) and Buildertrend.

With the introduction of new SCMs, for example, biomass ash and calcined clay, the augmentation of complexity in sustainable concrete highlights the need for effective and efficient analytical tools for further investigations. Predictive modelling approaches, similar to the ones presented in this research, may be devised to bolster the planning and design stages of infrastructure development and construction projects. Such data-driven frameworks will promote the adoption of AI and ML in the practical realm of engineering, fostering caution for sustainable and durable choices. This would propagate the idea of researching and investigating deeper into material behaviours with the advent of newer modifications and variations in SCMs.

In addition, the sustainability analysis portal could be extended to give a more dynamic outlook on the environmental compatibility of sustainable concrete samples by incorporating full Life Cycle Assessment (LCA). Compliant with the ISO 14040 framework, a Life Cycle Assessment would provide a framework for measuring the environmental impact of a product from the start till the end of its lifetime, facilitating decision-making (Zazala, 2024). While the current sustainability evaluation deploys only the embodied CO<sub>2</sub>, energy consumption and resource consumption, integrating the ISO approved LCA boundaries will enable a higher-fidelity determination of sample's sustainability through an all-encompassing analysis of its environmental impacts - including its transportation, raw material extraction and service life. Moreover, the current type aware AI model for prediction of compressive strength could be extended by leveraging

the use of more datasets in order to predict values for additional mechanical properties such as shear strength and modulus of elasticity. This would bring a newer breadth of practical usage to the system, providing a more holistic structural prediction resource and facilitating engineers and researchers to understand material's internal properties more comprehensively.

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