

INVESTIGATIVE STUDY OF NANOCEMENT AS A PARTIAL REPLACEMENT FOR CEMENT IN CONSTRUCTION USING MACHINE LEARNING MODELS



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ABSTRACT

The research paper addressed the application of nanotechnology in construction. The study showed that local materials like silica sand, and waste such as slag, fly ash, etc., at the nanoscale could improve the technical strength of concrete and other cement-based products. These nanoparticles also have carbon neutrals that help to reduce greenhouse gas emissions. Nanocement, which refers to the cement derived from nanoparticles, formed the basis of this study. The research paper employed machine learning algorithms to determine the compressive strength of concrete made from nanoparticles. The machine learning algorithms used in this paper were K-Nearest Neighbour, Random Forest Regressor, CatBoost Regressor, and XGBoost Regressor. The study used Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and the Coefficient of Determination (R squared) to evaluate the models. The best-performing model was deployed using FastAPI for interactive usage, and the link to the app is in the body of the paper. In addition, this research paper explained the need for Portland cement to be replaced with cement containing nano silica and micro silica (nanocement). The effect of nano silica and micro silica on the early-age compressive strength of concrete was thoroughly evaluated and compared. It was concluded that the partial replacement of cement with nanoparticles significantly increased the compressive strength of concrete, and hence, nano cement should be embraced.

Keywords: Nano silica, Micro silica, Compressive strength

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INTRODUCTION

GENERAL BACKGROUND

Construction, which is the design, planning, and erection of infrastructures like buildings, roads, bridges, airports, and so on, is not new science or technology. Over time, there have been several concepts that have optimised processes in the construction industry. Similarly, nanotechnology is neither a new science nor technology. It involves the breaking down of materials from larger scales to nanoscopic scales of about 1–100 nanometres to increase the proportion of atoms on the surface. Nanoparticles have an enlarged surface area concerning their volume, and as a result, they are highly reactive and possess improved properties (Hossain, 2015).

Over the last decades, several studies have investigated the performance of different concrete mixtures to improve their mechanical strength and durability while developing more sustainable concrete with reduced cement content. Among the studies are those that incorporate nanotechnology developments. Nanotechnology is an emerging field of research that has come to the limelight in the last few years. Its potential impact in several scientific and technological areas, including construction, has made nanotechnology a hot cake in research. Understanding the cement hydration process and chemical reactions at the nanoscience level allows for partial replacement of Ordinary Portland Cement (OPC) with nano-sized materials (*Helena Monteiro et al., 2022*).

About 4.3 billion tons of cement are generated globally each year, which is accompanied by increased demand (Alyasri et al, 2017). The major component of building materials is cement, which serves as a binder, and is a vital construction material. It is a principal constituent of most structural elements that make up most modern infrastructure, such as buildings, bridges, roads, dams, etc. (Britannica, 2022). Nanoparticles increase the compressive strength and the durability of concrete through a series of processes that involve stimulation of the hydration reaction and filling the micro pores in the cement paste structure. (Parva Chhantyal, 2020).

Interestingly, replacing Portland cement with nanocement is a proven way to alleviate the environmental impact associated with concrete production. Sadeghi-Nik *et al* (2017) investigated the reduction of the environmental impact of cement by replacing 1, 2, and 3 percentage weight of cement in cement mortar with nano-montmorillonite and nano-Titanium

(nano-MT) particles. Cement with nano-MT particles had better microstructure and lower greenhouse gas emissions.

In an attempt to reduce the cost associated with carrying out tests to determine the compressive strength of concrete, the emergence of machine learning has helped to give room for saving costs. Machines can now be trained to perform tasks at the human intelligence level. This application of machine learning is of enormous benefit in the construction industry and should be well engaged.

PROBLEM STATEMENT

Sustainable development is the leading civilization idea, alongside nanotechnology, a new wave in the technology space significantly affecting society, are brought together in this research paper. The construction industry uses 42% of all generated power and emits 35% of all greenhouse gases. The concrete industries use about 20 billion tons of aggregates, 1.5 billion tons of cement, and 800 million tons of water per year. That is a lot of matter, and implementing the principles of sustainable development in construction is essential (*Czarnecki, L., 2013*).

Cement is produced through a process involving the use of raw materials treated and reacted at extreme conditions like high temperatures. When raw materials are heated at high temperatures for solid-state reactions to take place, this is called pyroprocessing processes. The processes utilise fuel sources such as coal, fuel oil, natural gas, tires, hazardous wastes, petroleum coke, and anything combustible (Singh, G. B., & Subramaniam, K. V, 2019). Some cement manufacturing plants use the organic waste generated in other industries (e.g., the rubber processing industry.) As such, the cement industry contributes to a significant extent of anthropogenic carbon dioxide emissions, which is in the range of 5–7% of total human-influenced carbon dioxide emissions. It is a serious global environmental problem since an increase in carbon dioxide in the atmosphere leads to an increased rate of global warming. In addition to CO₂, dust is another polluting substance emitted into the air by the cement industry. There are also some other pollutants like carbon monoxide (CO), nitrogen oxides (NO_x), sulphur oxides (SO_xs), polychlorinated dibenzo-*p*-dioxins, etc. All of the abovementioned have severe health-hazardous substances, and some are hilariously odorous (*S. P. Dunuweera et al., 2018*).

Nanocement improves the technical quality of Portland cement, reduces the cost of production due to the use of mineral additives, it reduces the fuel cost and emission of NO_x , SO_2 , and CO_2 per tonne of cement. The strength of concrete is a principal structural requirement that determines the capacity of the concrete to support the load without breaking and maintain the structure's stability and integrity. Over the years, the development of nanotechnology has presented different materials that can enhance the mechanical performance of concrete. The development ratio solely depends on the type and percentage of the nanomaterial used. The use of machine learning models that can estimate the compressive strength of concrete made with nanomaterials is yet to be widely embraced. Hence, this is another vital area this study seeks to address

AIM AND OBJECTIVES OF THE PROJECT

The application of nanotechnology has proven to be an immense success in the life sciences. It is still a relatively new concept in the engineering and construction technology space with great potential for more sustainable and eco-friendly construction. It enhances the qualities of Ordinary Portland Cement (OPC) using nanomaterials that are by-products of industrial processes and effluents such as slag.

Machine Learning is an emerging field with applications even in optimising construction practices. Machine learning (ML) is a discipline of artificial intelligence (AI) that trains machines with the ability to automatically learn from data and past experiences while identifying patterns to make predictions with minimal human intervention.

In this project, machine learning models were used to predict the compressive strengths of concrete using nanoparticles as additives. Using data from past experiments, we cleaned, wrangled, and analysed the data. Afterwards, we carried out feature engineering before using four models to predict the strength of concrete with new variables.

The aim and objectives of this project include:

1. The incorporation of machine learning models to predict the compressive strength of concrete using nanoparticles like nano silica and micro silica as additives.
2. The production of concrete that has improved strength, durability, and other mechanical properties.

3. Re-using industrial wastes as nanoparticles in producing concrete to help reduce the volume of industrial effluents discharged into rivers and oceans.
4. The elimination of construction wastes produced in the course of performing concrete tests. With the introduction of computer models in determining the compressive strength of concrete, there will be a decrease in materials and equipment used in determining the strength of concrete.

LIMITATIONS OF THE CONCEPT

Nanomaterials can be derived in small quantities in daily life through processes like combustion. Fires represent complicated reactions and can produce pigments, cement, and fumed silica. Because of the recent development of nanotechnology, the health and safety effects of exposure to nanomaterials and what levels of exposure may be acceptable are subjects of ongoing research. Nanoparticles, which are principal components of nanocement, can be produced on large scales by industrial chemical reactions. Hence, most of the previously done research employing nanotechnology has been small-scale. The small-scaled research has been due to the unavailability of nanomaterials on a large scale, not limited to the following reasons: (Pendharker et al., 2016)

Price competition

The primary reason for the vast inaccessibility of nanomaterials is the high cost. Nanomaterials and nanoproducts are significantly more expensive than non-nano alternatives due to the technology involved in producing them.

Technical performance

The strict technical performance of nanoproducts is another limiting factor for large-scale nanoproduct introduction. The technical performance should be thoroughly proven to meet standards for that material.

Awareness within the sector

Awareness (or the lack thereof) is another vital element hampering the introduction of nano products in construction works. Without awareness, there cannot be room to apply or explore a concept

RELEVANCE OF THE IDEA

The emergence of nanotechnology ushered in various areas of science and engineering where processes take place at the nanometre scales to improve the design, production, and maintenance of devices, systems, and materials. There has been enormous research to apply nanotechnology in construction. One of the ways is by introducing materials such as microsilica, nanosilica, fly ash, slags, and other additives in cement production. The addition of fly ash, slags, and other waste in nanocement, has proven to be an effective way to encourage the sustainability of materials. These additives improve mechanical properties and other physical properties of cement-based end products like concrete.

The possibility of these additives enhancing the properties of cement-based products is because of the nanoscale nature of the particles that birthed the term “nanocement.” The production of nanocement start by introducing a tonne of ground Portland cement to many materials containing silica sand or sand. Polymeric modifiers like sodium naphthalene in its dried state containing silica sand additives and some percentage of polymeric modifiers ranging from 0.6% to 2.0% are then added. Afterwards, mineral supplements in nuggets form (~diameter 300mm), gypsum and moisture content (~ 0.3% to 6.0% gypsum rock) are introduced (Sada et al., 2014). The outcome of this process yields two tonnes of nanocement, implying that the cost of consumed fuel per tonne of cement has reduced, given that there is no need for additional grinding and energy.

Unarguably, one of the most common construction elements is concrete which is a composite material containing a binder medium within which aggregate particles are embedded. And because cement is a key element in concrete, this is why the study focused on using nanocement to improve the quality of concrete. Nanocement improve both the physical and chemical properties of concrete. Nanomaterials are materials possessing, at minimum, one external dimension measuring 1-100nm (Jeevanandam J et al, 2018). Conventional cement-based concrete has inadequacies like low tensile strength and increased alkalinity due to the reaction of cement with water during hydration. As the concrete dries out, calcium hydroxide remains in the pores

Furthermore, the research paper employed Machine Learning to predict the compressive strength of concrete made from nanoparticles to eliminate the need of carrying out compressive tests every time, thereby saving cost and time. The introduction of machine learning helps to eliminate the need for repetitive tasks that can be done by teaching a machine learning model

what to do by training it with data from performed quality experimental data. Consequently, it will give results at the rate of human intelligence.

RELEVANCE IN ADDRESSING SUSTAINABLE DEVELOPMENT GOALS



A large amount of pollution emanates from the production process of various construction materials. The high-temperature process in the production process of cement accounts for about 8% of the world's human-influenced carbon dioxide emissions (Mitch Jacoby). Based on these concerns, this study seeks to adopt the application of nanotechnology to solve some of the global problems faced. Replacing cement with nanocement reduces the carbon contents of cement and other cementitious construction materials (Sada et al., 2014).

Because the earth's crust is a central raw material in cement production, for every 1 ton of cement produced, approximately 700kg – 800kg of carbon dioxide gas (CO₂) is released. Carbon Dioxide is a principal element of greenhouse gas causing global warming and environmental pollution. In a way to reduce global warming and environmental pollution, in line with SDG 13 (taking actions to combat climate change and its impact), nanocement, which essentially contains nanoparticles that are carbon neutral, is replaced with cement in construction. (Jo, B. W., et al., 2014).

Arum Chattopadhyay, a renowned member of the Faculty of Chemistry at the Center for Nanotechnology, Indian Institute of Technology, said that nanomaterials could help to mitigate pollution because they act as effective catalysts and are mostly recyclable. Nowadays, nanomaterials have become highly cost-effective for commercialization and better to replace present-day traditional materials to promote sustainability, in line with SDG 11, which encourages making cities and human settlements inclusive, safe, resilient, and sustainable.

To further explain the impact of this idea in line with SDG 11, the use of nanotechnology in the production of nanocement helps to transform local materials like silica sand and waste such as slag, fly ash, etc., into environmentally friendly materials. Rather than constituting some nuisance to the environment, they help to improve the technical strength of reinforced concrete in human settlements.

ECONOMIC VIABILITY

With the introduction of the concept of nanocement, the addition of nanoparticles improves the technical properties of cement-based construction products. Nanoparticles also reduce cement prime cost, specific fuel consumption, and emissions of NO_x, SO₂, and CO₂ gases, in the production of Portland cement. (Bickbau, M. Y, 2016).

Some advantages of using nanocement are:

- The use of nanocement makes it possible that local materials like silica sand, and waste such as slag, fly ash, etc. can be beneficial to a noble cause. These waste materials - slag and fly ash, rather than constituting some nuisance to the environment, are used to improve the technical strength of concrete and other cement-based products.
- The nanoscale nature of nanoparticles results in increased fineness of cement, concretes made from nanocement develop tremendously high strength, and have high resistance to water, chlorides, sulphates, and acids. In turn, the nanoscale nature helps to increase the lifespan of complex construction members like columns, beams, slabs, concrete frames, etc. The increased lifespan is a result of how nanocement improves the impermeability of concrete
- The use of nanocement in construction can make room for an allowance for reduction of reinforcement ratio by about 30 to 50%, as a result of the incredibly strong concrete from nanocement (Alyasri, S. A. H et al., 2017).
- Addition of nanocement can tremendously increase the compressive strength of concrete to as high as 60-70MPa within 24 hours and can achieve up to 70% of what could be achieved in 28 days using Portland cement in 72 hours. Consequently, it helps to accelerate form release time and considerably reduce overall project completion time (Alyasri, S. A. H et al., 2017).

LITERATURE REVIEW

Concrete is a highly valued and highly researched construction material whose importance cannot be undervalued. It accounts for 60% of construction material in a project (Aytekin & Mardani-Aghabaglou, 2022). The make-up of concrete comprises different composition and design variables. Al-Jamimi et al., (2022) employed a data-driven machine learning approach to predict the compressive strength of concrete. Computational intelligence techniques and non-linear models like the Support Vector Machines (SVM), genetic algorithm (GA), and the hybridised models of the duo (SVM-GA) to predict the relative strength of concrete using a set of independent properties and variables. The variables include the quantity of the Ordinary Portland Cement (OPC), water-cement ratio, cement content, silica fume (SF), and curing time among others. The variables were optimised to get the best value for the compressive strength. The model gave an R2 score of 0.99, and a root mean square error (RMSE) of 0.002.

The nanotechnology industry is a fast-evolving sector with an application in the fields of physics, chemistry, and biology. Owing to its recorded successes in the physical sciences, the need to replicate the revolutionary developments in the construction and engineering sectors is necessary. In the research done by Patil & Pendharkar (2016) to study the effect of nanomaterials as possible replacements on the Physical Properties of Concrete. Nano-particles such as Nano-Alumina, Nano Titania & Zinc Oxide, and Nano Silica were studied extensively. The roles of these particles in the optimization of the physical properties of cement were evaluated. Nano Alumina can help increase the mechanical properties of cement without an improvement in its compressive strength. In the same vein, Nano Titania in concrete improves its self-cleaning or photocatalytic properties, although it activates the killing of relevant microorganisms. Nano silica is less costly and improves concrete's compressive strength. The high cost of nano-products compared with its non-nano alternatives has limited its application in construction.

Nanotechnology is one of the most active research areas that covers several disciplines, including civil engineering and construction materials. It has the potential to enable construction and building materials to replicate the features of natural systems improved until perfection for aeons. As stated earlier, nanotechnology has been in vogue in microbiology, medicine, and other life sciences, but its interest in civil and construction materials is just growing. Firoozi & Raihan Taha (2014) explained the numerous applications of nanotechnology, its benefits, and the limitations to its glorious future. The applications cut

across the preparations of nano-cement, nano-composites, nano-coatings for concrete, nano-steel, nano-glass, nano-particles for fire protection, and so on. More research is ongoing to determine the impact of nano-products on the environment. Also, the novelty of the technology has caused the cost of procurement of nano-products to be relatively high. The equipment used for nano-scale investigation includes Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD), Photon Correlation Spectroscopy (PCS), and Nanoindentation.

Pendharker et al. (2016) stated the following nanomaterials and how they improve the qualities of concrete:

- Nano alumina can help to increase the mechanical properties of cement. It increases the early strength of concrete at seven days.
- Nano Titania: Due to its excellent ultraviolet resistant qualities, it was observed in early research to give concrete self-cleaning and disinfecting properties. A limitation was the initiation of the killing of bacteria in the concrete.
- Nano Silica: The addition of micro silica fumes in voids decreases alkalinity. Silica fumes fill the pores of the concrete, preventing the pores from being filled with water or air, alongside preventing chemical reactions in the concrete.

One of the researchers that have worked on nanomaterials in concrete, Nasution et al., concluded in one of his papers that nanosilica is capable of improving the performance of concrete, and it helps to resist sulphate attack.

RESEARCH METHODOLOGY

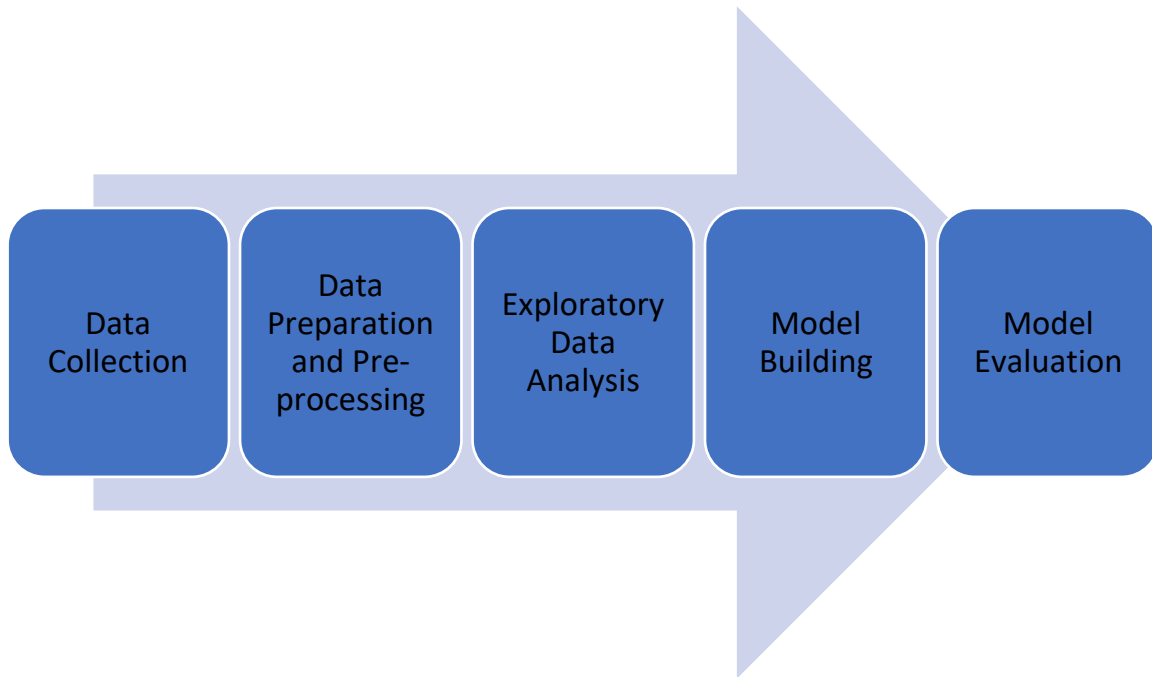


FIGURE 1: Chart denoting the procedures of the project

Materials

In total, 205 experimental data were gathered from a publication by Rahimzadeh et al., (2022)¹. The credibility of the journal and the quality of experimental procedures were the unbending criteria used for deciding to work with the dataset. It comprises dependent variables - water-cement ratio, curing time, percentage of nano-material additives (nanosilica (NS) and microsilica (MS)), and the dependent variable - the compressive strength.

These dependent variables are of great importance to accurately determine the value of compressive strength to a degree of precision. The water-cement ratio is the ratio of the volume of water quantity to cement in a concrete mixture. It ranges from 0.4 to 0.84 with a median of 0.5. Curing time is the duration of time before the cube tests were measured. It began from 3 to 28 days, with a median of 14 days.

The NS utilised in the mixing proportions had a particle diameter of less than 50 nm, a surface-to-volume ratio of between 50 and 200 m²/g, and a purity of more than 99 percent. These were all according to the examination of the gathered dataset from the literature. Between 0% and

¹ The dataset used can be accessed from https://bit.ly/dataset_for_the_research-paper

15% of NS was employed in paste mixes to replace the cement weight, with a median of 1.5 percent.

The MS utilised in the mix had a particle diameter of less than 50 nm, a surface-to-volume ratio of 10–20 m²/g, and a purity of greater than 99%. These were also according to the dataset derived from the literature. The minimum and maximum proportions of MS used in paste mixtures were between 0% and 40%, replacing the cement weight with a median of 5%.

The compressive strength is the only dependent variable in the dataset. It is measured in megapascals (MPa).

Methods

WHY MACHINE LEARNING?

Machine Learning is the practice of using algorithms to extract data, learn from it, and then forecast future trends. It allows machines to be trained with quality data to become more accurate in predicting outcomes. Instead of carrying out the compressive strength of concrete practically using financial resources and manpower, an innovative way of getting the same result was devised in the study.

TOOLS USED

Python programming language was used in building, then it was wrapped up using FastAPI and deployed on Heroku to be used by everyone. The link to the app is included in the later part of the result and implementation. Also, Pivot Tables using Google Sheets were used to make some visualisations to bring out insights from the data. This was in addition to the programmatic assessment done using Python (Jupyter Notebook as the Integrated Development Environment)

DATA PREPARATION AND PRE-PROCESSING

Outliers were observed in the curing time (days) column and the entire three rows where these occurred were dropped. This reduced the dataset from 205 observations to 202. Also, the headers were renamed for ease of programmatic assessment. The spaces between the column names were removed and replaced with underscores.

MODEL BUILDING

These datasets were properly analysed using different machine learning models for their prediction. Due to the quantitative values of the compressive strengths, a regression model was used against a classification model which is used for qualitative results. The regression models include:

1. K Nearest Neighbours (KNN) Regression.
2. Random Forest Regression.
3. CatBoost Regression.
4. XGBoost Regression.

K-Nearest Neighbours (KNN) Regression

KNN Regression is a Machine Learning model that does not involve using any assumptions about the characteristics of the samples. It works to get the value of prediction by approximating the association between features and the continuous values of the target by averaging the observations in the same *neighbourhood* (Srivastava, 2020). KNN is very prone to an outlier or anomalous variation of observations. This was the reason the features were standardised using Standard Scaler before training the model. Standard Scaler was employed to resize the distribution of the observations to make the mean of the features to be 0 and the standard deviation to be 1. That is, it reduces the mean to zero and scales the data to the unit variance.

Random forest Regression

It is a type of supervised learning algorithm that combines numerous base models to yield optimal predictive performance. The algorithm works by constructing a host of decision trees at training time, then it outputs the average of the prediction of individual trees. This model was employed in the study and performed incredibly well upon evaluation which will be discussed later in the study.

CatBoost Regression

This algorithm works on the concept of decision trees and gradient boosting. The central idea of boosting is to successfully combine several low-performing models to produce a very high predictive model. As gradient boosting helps to fit the decision tree successively, the new trees about to be will learn from the mistakes of previous ones and consequently, reduce error.

This process continues until the selected loss function is no longer minimised which is the reason for the Catboost high-quality model result.

XGBoost Regression

XGBoost Regression which means **eXtreme Gradient Boosting** works by minimising a regularised (L1 and L2) objective function. It then combines it with a convex loss function (established through the difference in the predicted values and target outputs) and a penalty term for regression tree functions. The training takes place repeatedly, accumulating new trees that determine the errors of prior trees, and afterward, they are combined with former trees to make the final prediction. The primary reason this algorithm is called gradient boosting is that it minimises loss using a gradient descent algorithm.

MODEL EVALUATION

Before arriving at the model to use for building the compressive strength prediction app, 8 models were used before bringing the number down to 4. The metrics for evaluation were Mean Absolute Error (MAE), Root Mean Squared Error, and R Squared (Coefficient of determination)

1. Mean Absolute Error (MAE)

MAE is the average magnitude of the difference in predicted values and actual values regardless of the residuals' directions. Mathematically, the absolute value sign swallows the potentiality of negative signs having an effect. Consequently, all the individual differences in predictions and actual values have equal weight.

The formula for the Mean Absolute Error (MAE) is given by:

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |x_i - x|$$

Where:

- n = the number of errors,
- Σ = summation symbols (which means “add them all up”),
- $|x_i - x|$ = the absolute errors.

2. Root Mean Squared Error (RMSE)

RMSE is the most adopted and prioritised metric for evaluating models. It represents how far predictions are from actual values using Euclidean distance. RMSE is the square root of the average of squared differences of the target values from predicted values. It is a quadratic evaluation method that measures the average magnitude of the error. The reason for the wide adoption of RMSE over other scoring techniques is that it gives a comparatively high weight to large errors. This is very vital when dealing with the situation when large errors are very risky, costly, or undesirable.

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

$\hat{y}_1, \hat{y}_2, \dots, \hat{y}_n$ are predicted values

y_1, y_2, \dots, y_n are observed values

n is the number of observations

3. R squared (or Coefficient of determination)

R Squared is the measure of the best fit of the dependent variable explained by the independent variable. It means that the prediction from the models is approximately correlated with the real values. The range of values for the R squared score is between 0 and 1. An R^2 of 1 show that the model predictions is perfectly accurately. On the flip side, R Squared score of 0 means the model is very poor.

$$\begin{aligned} R^2 &= 1 - \frac{\text{sum squared regression (SSR)}}{\text{total sum of squares (SST)}}, \\ &= 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}. \end{aligned}$$

RESULT AND IMPLEMENTATION

To improve the physical and chemical properties of concrete, Nano silica (NS) and micro silica (MS); also known as silica fumes, were used in this research work. The implementation influencing variables were Curing time, % of NS and MS used in each mix, the water-cement ratio, and the compressive strength for each mix was then measured. The samples were prepared by adopting different percentages (with a maximum of 5%) replacement of cement by weight with Nano products. Cube samples of normal concrete and the concrete containing the percentage of the individual Nano products were prepared, and the compressive strength of the cubes was investigated at 3,7,14,21,28 days (Curing time). Each variable was recorded in each mix.

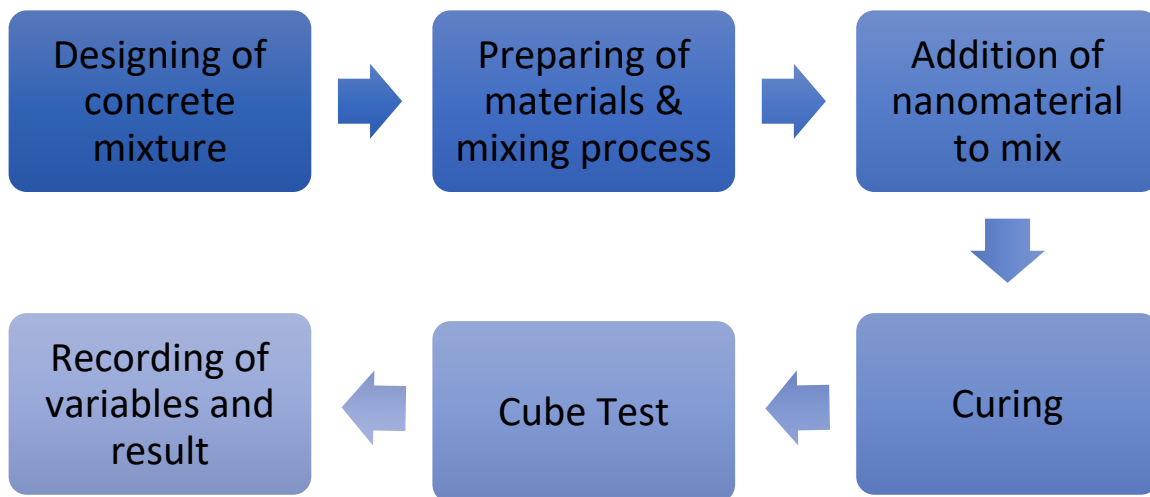


FIGURE 2: Flow chart showing the implementation process

The influencing variables were then recorded in the format below:

W/C	Curing time (Days)	Nanosilica (NS)	Microsilica (MS)	Compressive strength (Mpa)

EXPLORATORY DATA ANALYSIS

Exploratory Data Analysis (EDA) is the next stage in the application of machine learning for determining the compressive strength of concrete from nanoparticles. At this phase, trends are observed and documented. Patterns in the data are deduced as well. Here are some of the findings when carrying out the analysis.

1. **Water-Cement Ratio:** The data comprises experiments done with water to cement ratio of 0.5, closely followed by 0.4

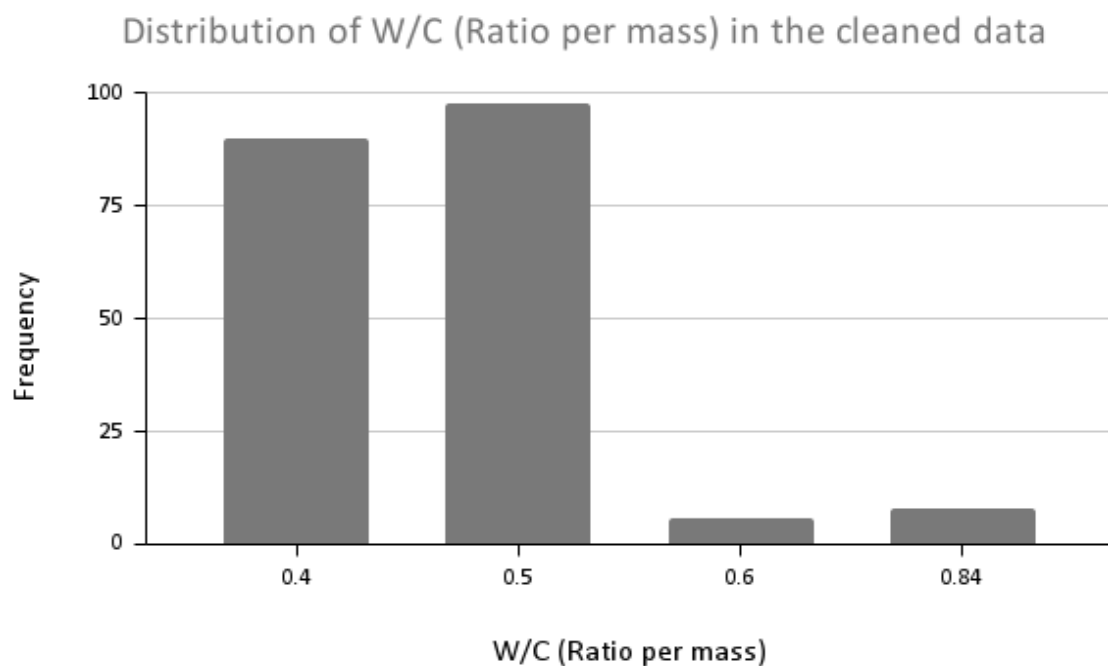


FIGURE 3: Distribution of W/C ratio per mass in the cleaned data

2. **Curing time:** The curing time in from the data ranges from 3, 7, 14, 21, and 28 days. Seven and twenty-eight days have the highest share, while three, seventeen, and twenty-one days have close-range representations.

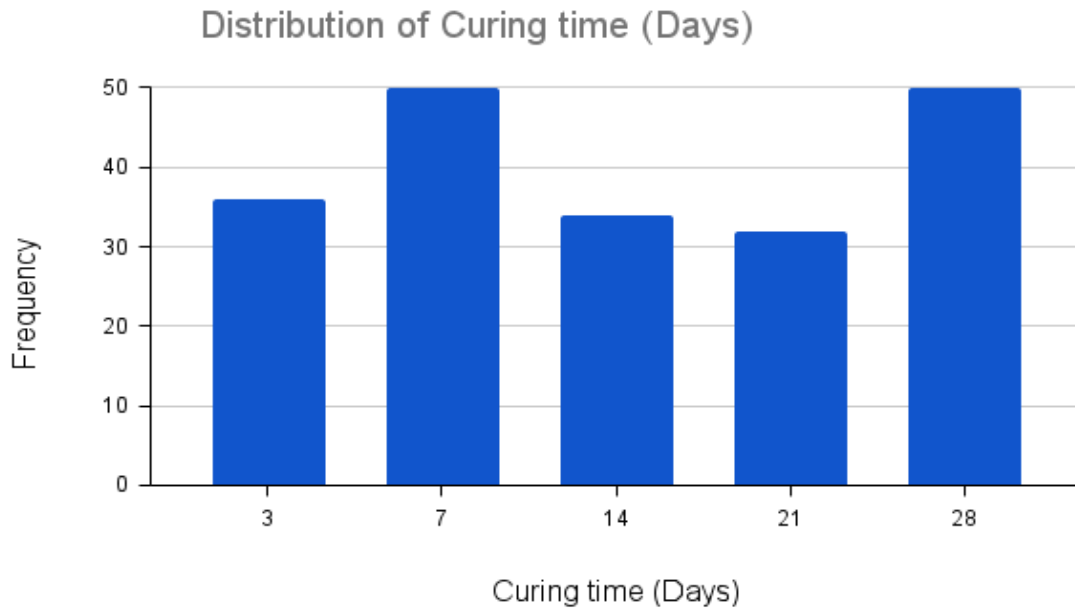


FIGURE 4: Distribution of curing time in the cleaned data

The results were classified based on the number of curing days, 3 days, 7 days, 14 days, 21 days, and 28 days. The resulting compressive strengths were grouped into:

- **Low compressive strength:** Less than 17 Mpa.
- **Moderate Compressive strength:** Between 17 and 30MPa.
- **High compressive strength:** Between 30 and 50MPa.
- **Very high compressive strength:** Above 50MPa.

The results were analysed and visualised using data analysis tools.

THREE DAYS CURING

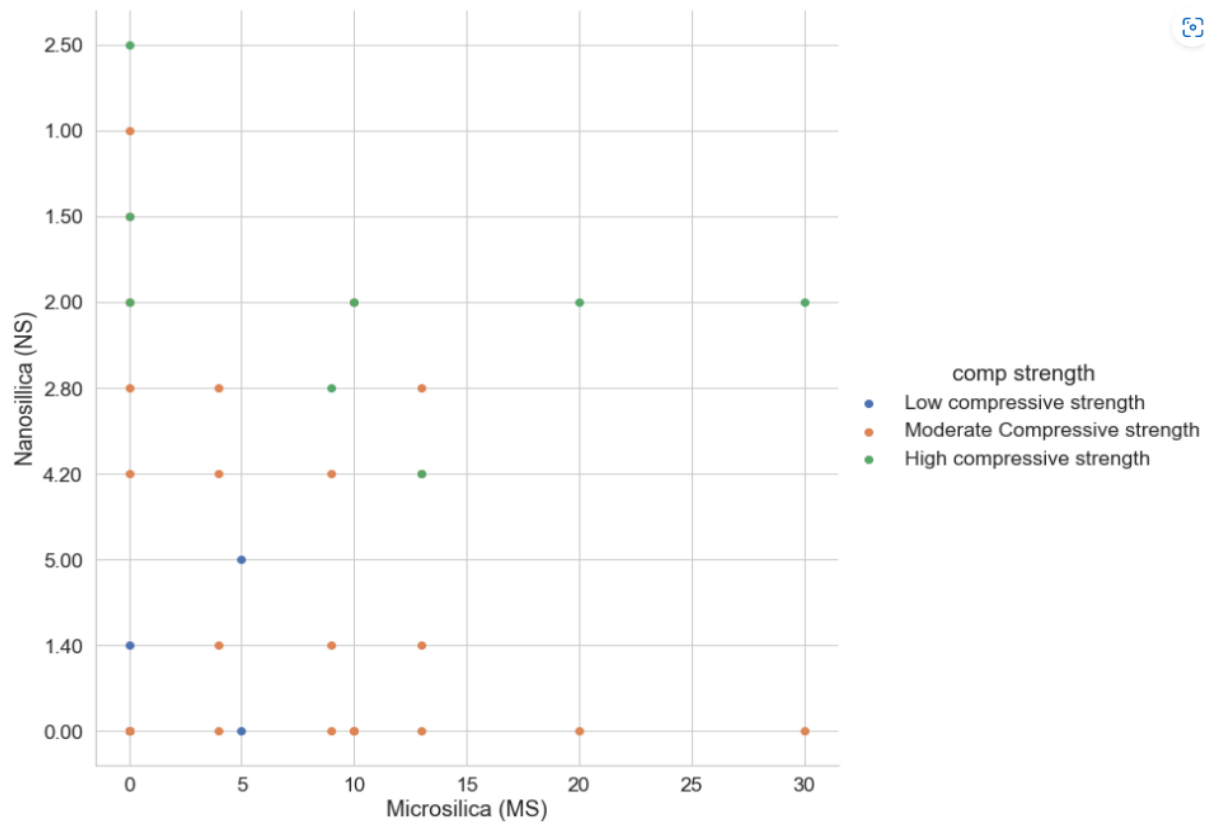


FIGURE 5: Three day curing results

It can be seen in the figure above that after three days, none of the cubes produced a very high compressive strength i.e. a compressive strength of above 50MPa. The percentage of nano silica with the highest number of high compressive strengths (between 30 and 50MPa) was 2%, and all percentages of micro silica mixed with 2% nano silica had little or no change in the compressive strength, as they were all classified as high compressive strengths.

SEVEN DAYS CURING

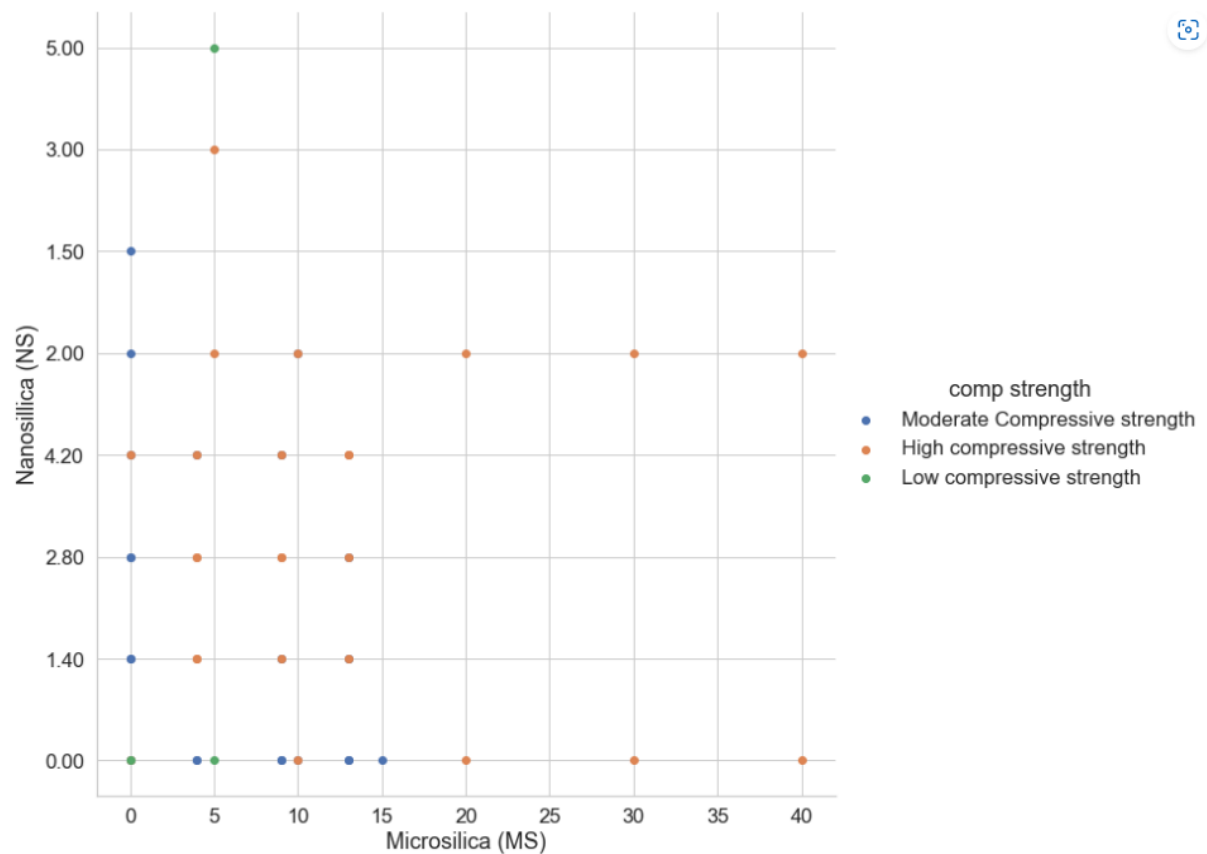


FIGURE 6: Seven day curing results

The results after seven days of curing produced almost the same results as the three-day curing, as 2% Nano silica was found to be the optimal percentage for high compressive strength. 4.2% Nanosilica with 0%,5%,8%, and 13% micro silica also produced high compressive strengths, with 5% Nanosilica producing a very low compressive strength.

FOURTEEN DAYS CURING

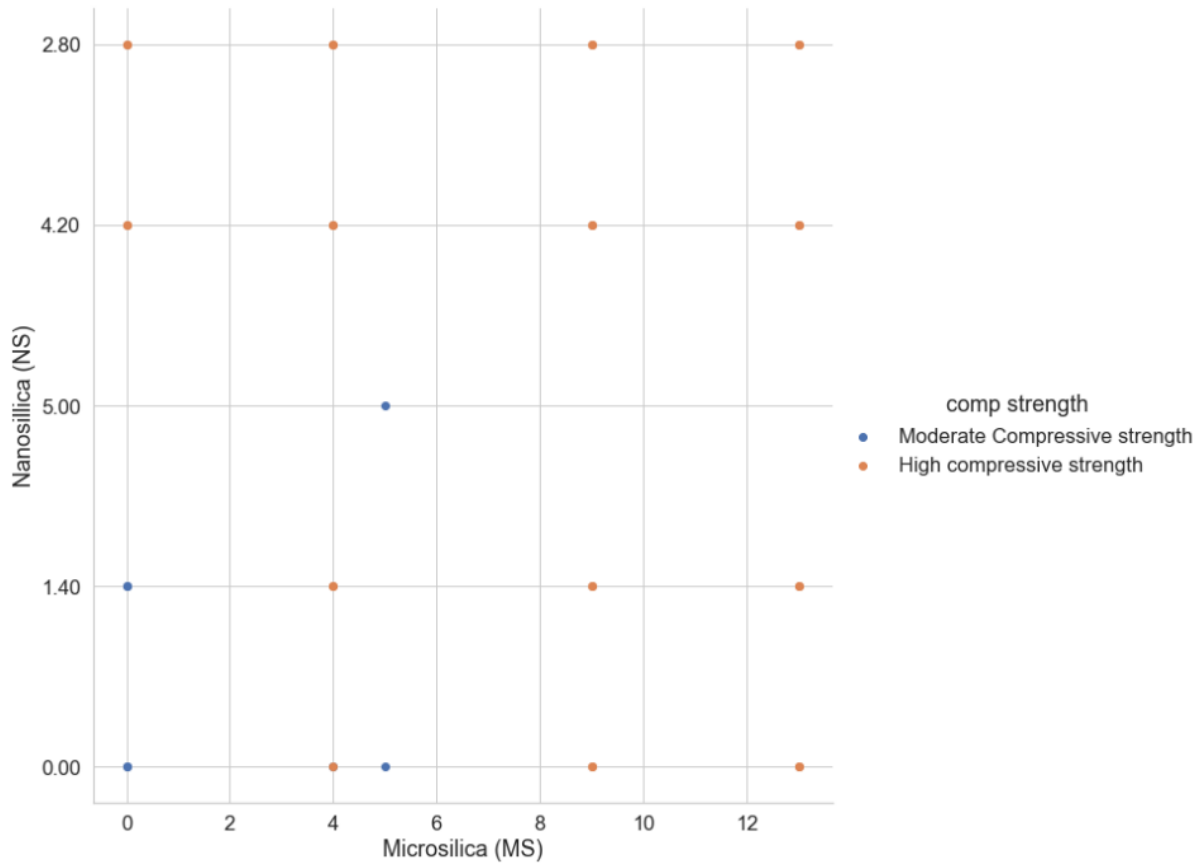


FIGURE 7: Fourteen day curing results

After fourteen days, no low compressive strengths were recorded, and no very high compressive strengths were recorded either. 2.8% and 4.2% Nanosilica produces high compressive strengths.

TWENTY-ONE DAYS CURING

At the 21-day mark, normal and high compressive strengths were obtained with no record of low or very high compressive strengths, with 4.2% Nanosilica being the dominating percentage.

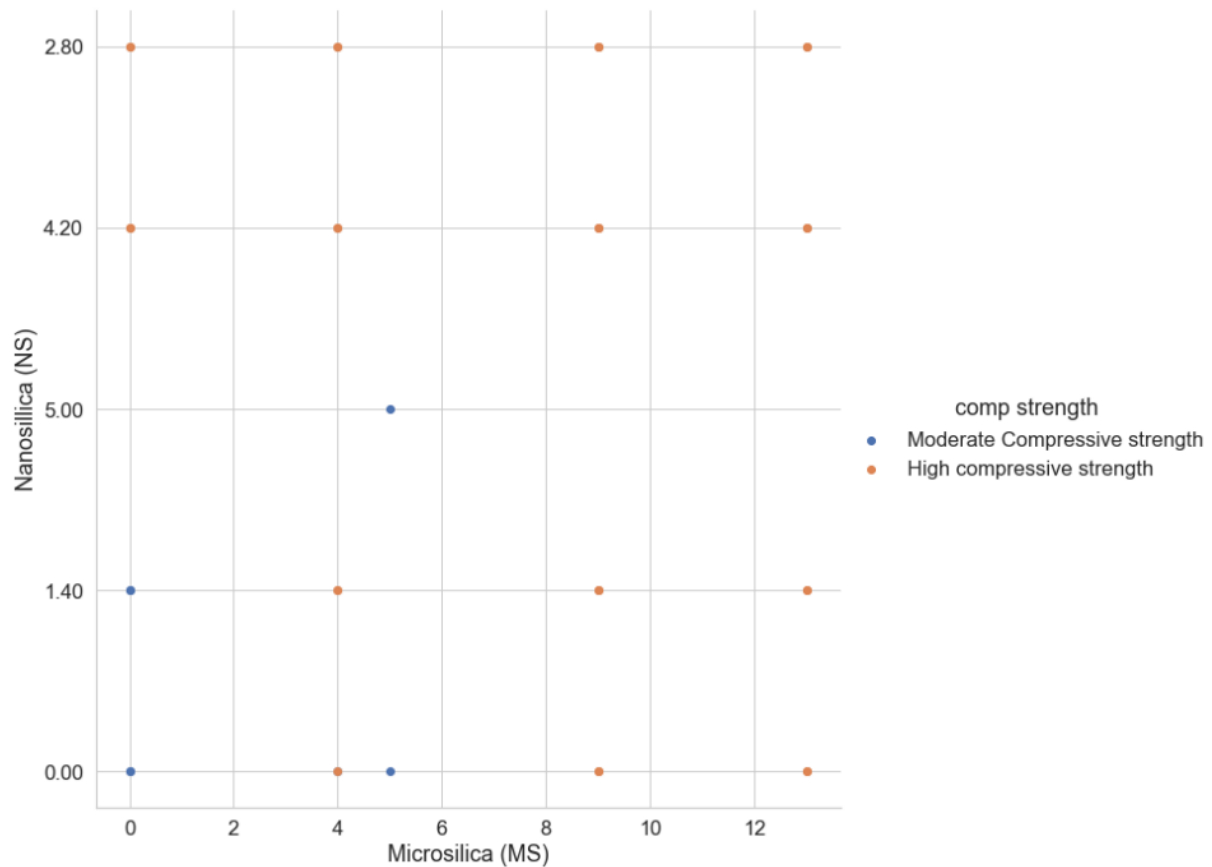


FIGURE 8: 21 day curing result

28 DAY CURING RESULTS

The 28-day results produced ranges of different compressive strength values: from normal to high to very high. Showing the different percentages of the nano products that were combined to give the compressive strengths.

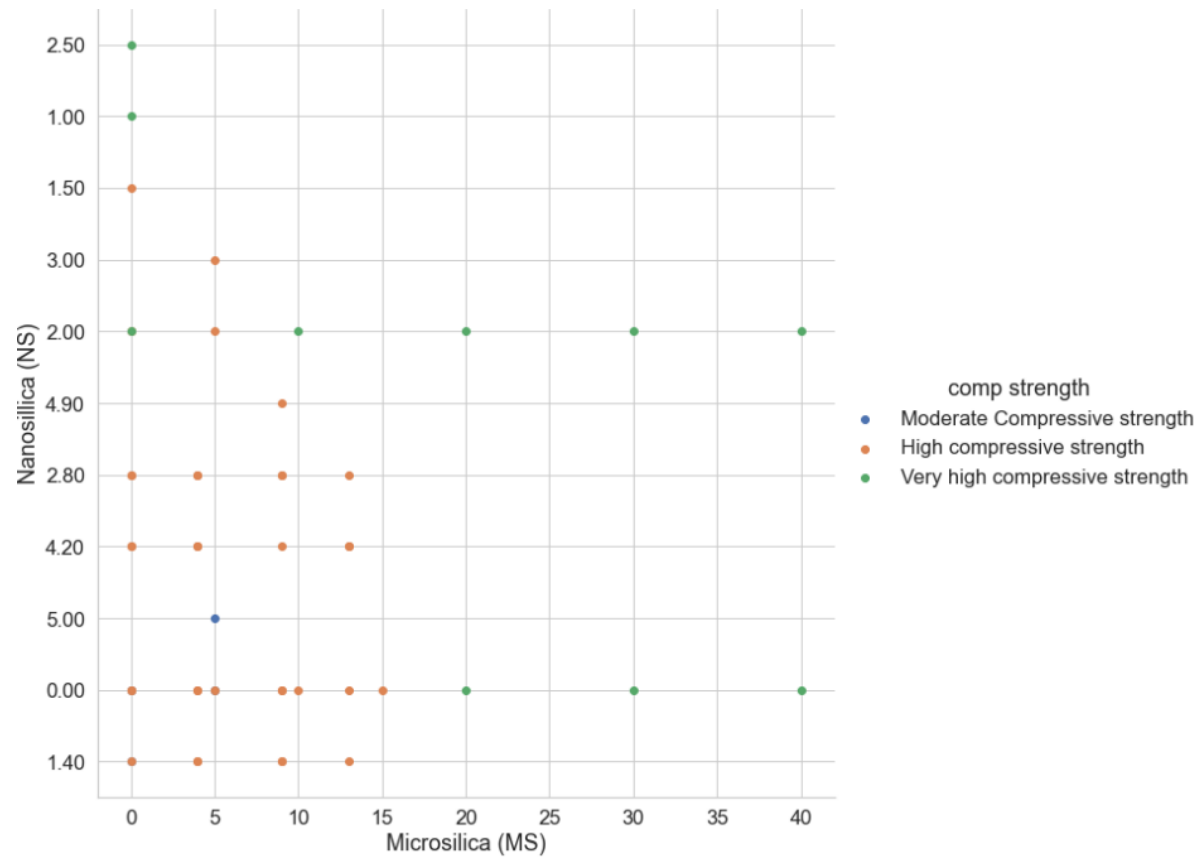


FIGURE 9: 28 day curing results

3. **Microsilica:** Concrete made without any percentage of microsilica had a good representation in the data. This allowed us to analytically explore the influence of addition of certain quantity of microsilica as additives at different percentages.

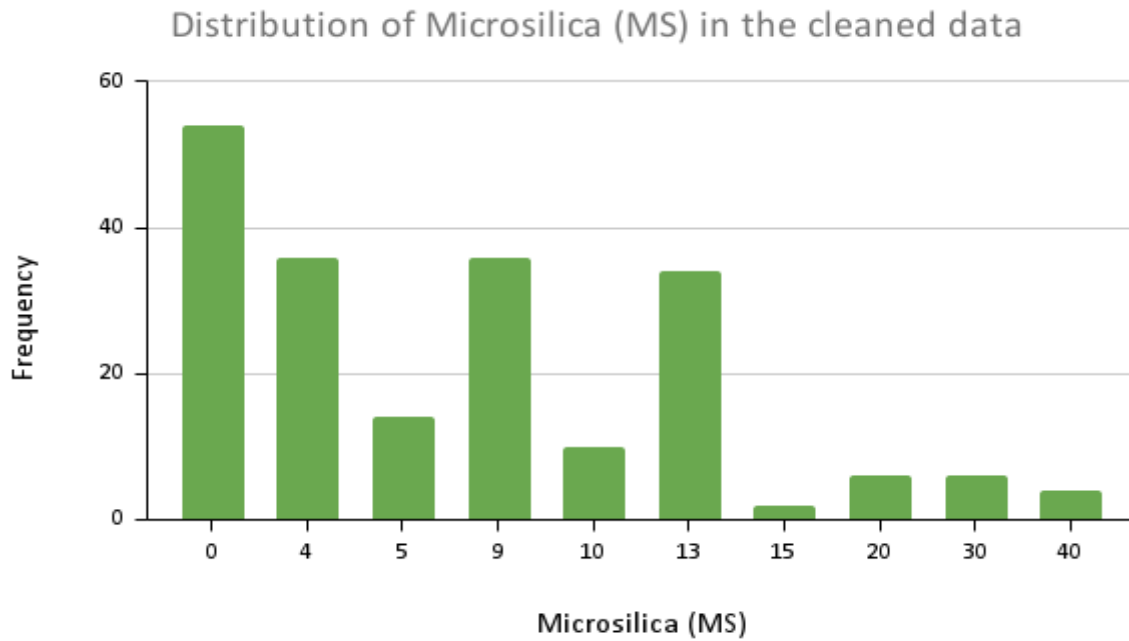


FIGURE 10: Distribution of microsilica in the cleaned data

4. **Nanosilica:** Nanosilica is the central focus of the study as its effect was intensively studied. This nanoparticle is the most essential component of nanocenet. A good number of the dataset had concrete made without nanosilica as additives. Hence, we could study the influence of addition of nanosilica at different percentages up to 5%. Further addition of nanosilica beyond 5% was not carried out because there was an observed decline in compressive strength of concrete as the addition of nanosilica approached 5%.

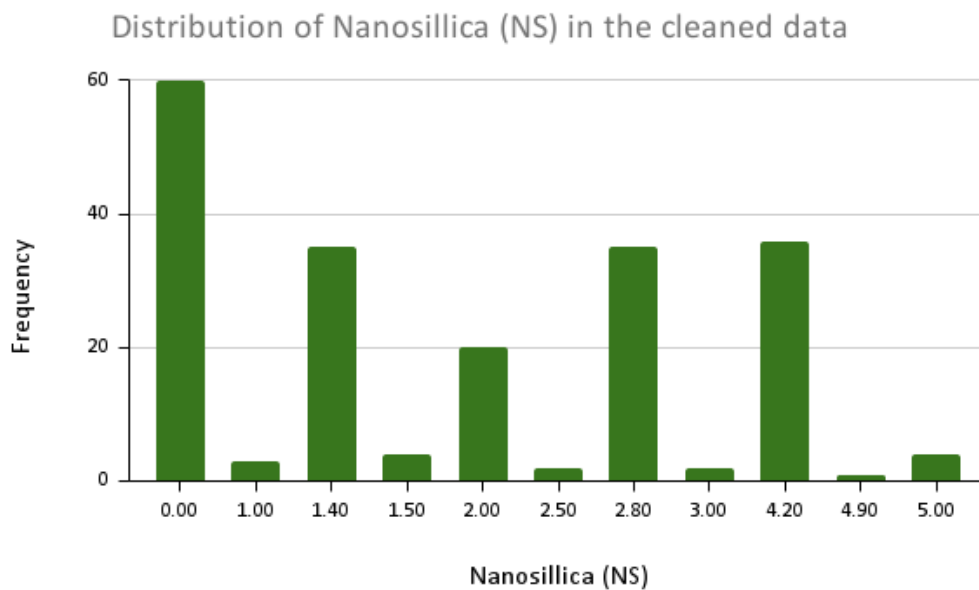


FIGURE 11: Distribution of nanosilica in the cleaned data

Correlation Heat Map

The correlation heat map is a two-dimensional plot of the correlation (linear relationship) between variables represented with varying intensity of colours. The varying intensity of colours shows the linear relationship of the features in the dataset which is positioned on the right side of the plot.

- From abs (0.8) – abs (1. 0) = strong correlation
- From abs (0.6) – abs (0.8) = fairly strong correlation
- From abs (0.4) – abs (0.6) = average correlation
- From abs (0.0) – abs (0.4) = weak correlation

NB: **abs** means absolute value, that is, either positive or negative values.

The correlation heat map for the dataset used in this study was done and the result is as shown below:

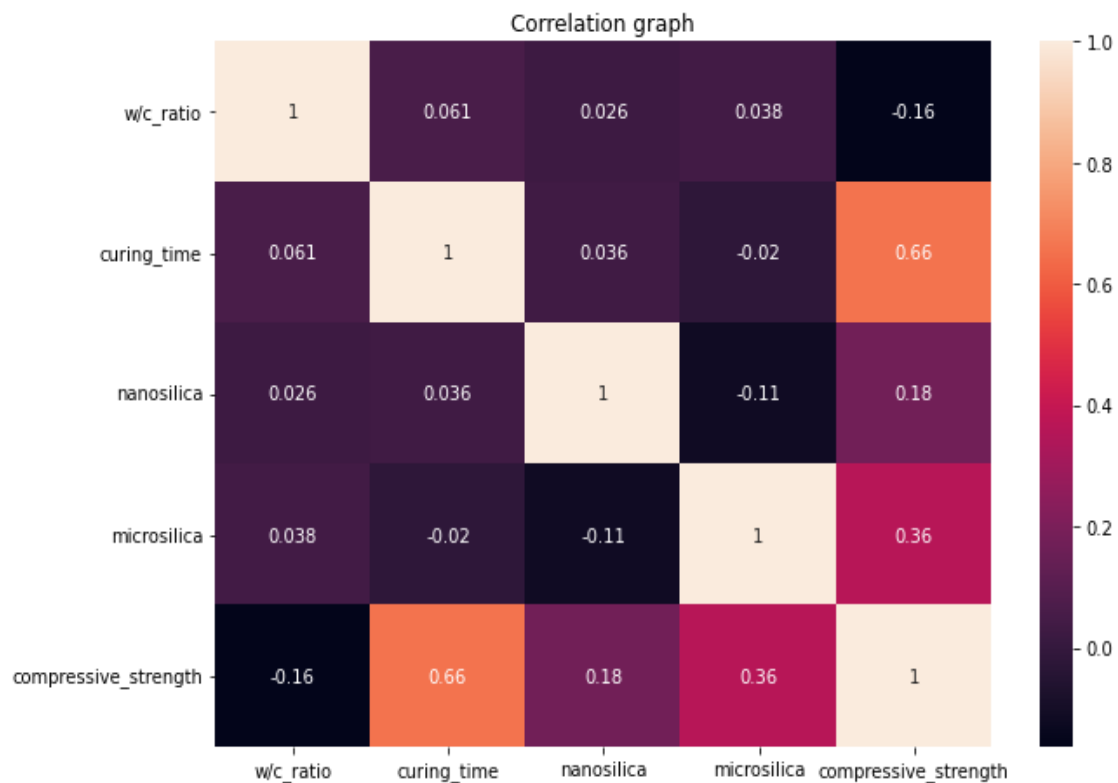


FIGURE 12: Correlation of the features and the label in the dataset

It can be seen that curing time (in days) has the highest correlation with compressive strength. Although this is not the central focus of the study, it could be deduced from the exploratory that as compressive strength increases, the compressive strength increases. On the contrary,

Nano silica and micro silica did not follow the same trend pattern, implying that the relationship between nano silica and micro silica is not a linear dependency.

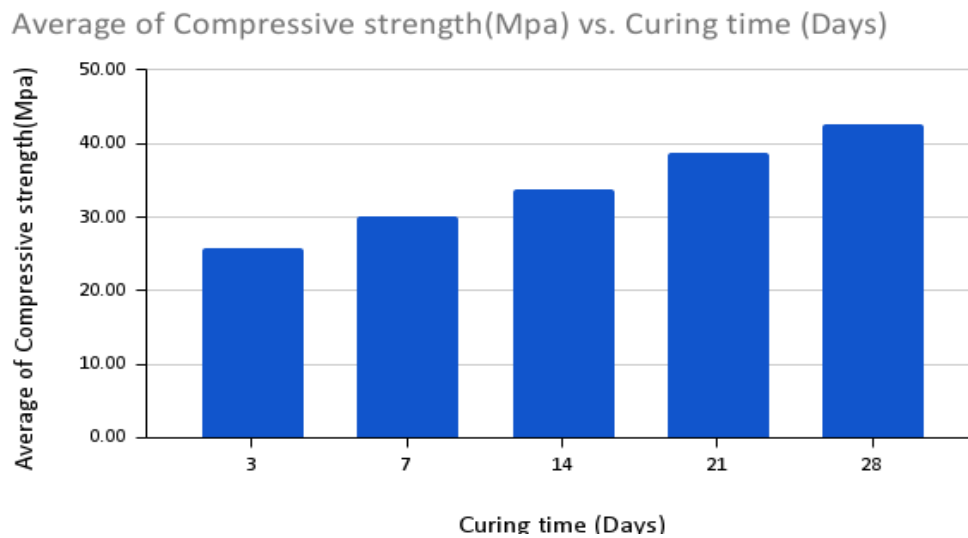


FIGURE 13: Average compressive strength of concrete against curing time (days)

RESULTS

In this study, XGBoost Regression gave the lowest mean absolute value of 2.319Mpa, followed closely by CatBoost Regression with 2.353MPa. Random Forest and K-Nearest Neighbour gave 3.051 and 3.289MPa mean absolute error respectively. This implies that XGBoost will have on average a 2.319MPa deviation from the actual value of compressive strength of concrete.

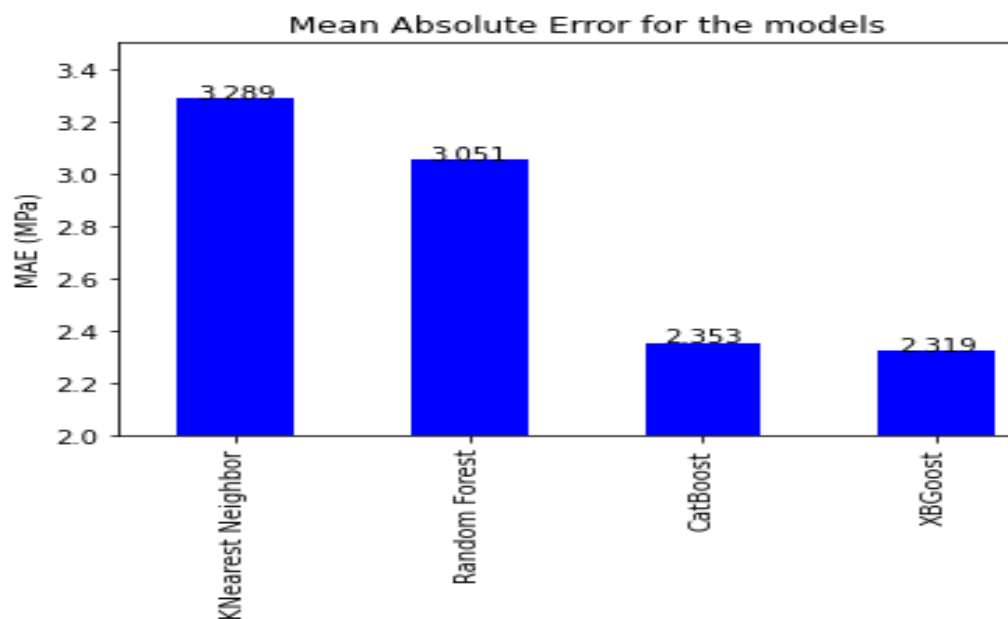


FIGURE 14: Mean absolute error for the models

In Figure 14, it could be seen that CatBoost Regression gave the lowest root mean squared error of 3.234MPa, followed closely by XGBoost Regression with 3.547MPa. Random Forest and K-Nearest Neighbour gave 4.053 and 4.179MPa root mean squared error respectively. This implies that CatBoost will have on average a 3.234MPa which makes it less susceptible to large errors, unlike XGBoost. This is the reason for going with CatBoost Regression as the best-performing model.

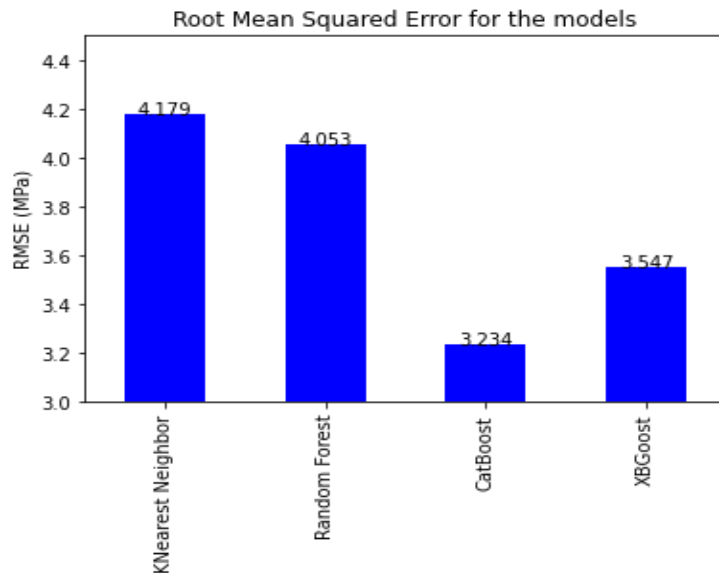


FIGURE 15: Root mean squared error for the models

Also, Figure 15 shows that CatBoost Regression gave the highest coefficient of determination on the test dataset with 0.919, followed by XGBoost Regression with 0.816. Random Forest and K-Nearest Neighbour had 0.773 and 0.759 scores respectively. This implies that CatBoost will have the best fit of predicted values real targets of unseen data.

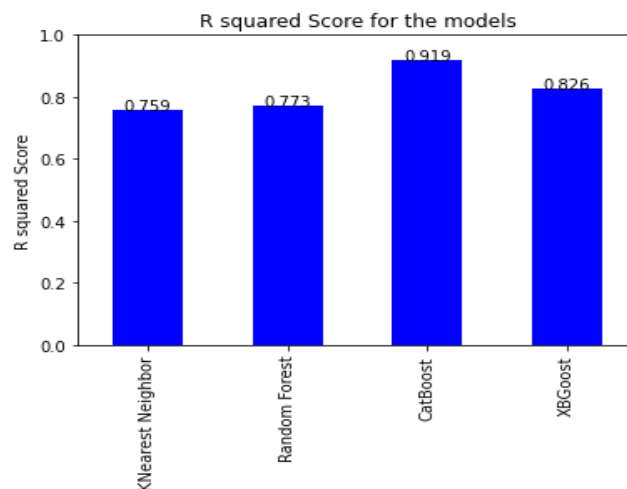



FIGURE 16: Coefficient of determination for the models

DEPLOYMENT OF THE MODEL

The CatBoost model after performing a series of hyperparameter tuning was saved as a pickle file using joblib. Afterward, the model was deployed on Heroku using FastAPI so that it can be used on the web². The codebase can be accessed on GitHub for further improvement on the model³.

**MODEL FOR PREDICTING COMPRESSIVE STRENGTH
OF CONCRETE FROM NANOPARTICLES**



W/C (Ratio per mass)

Curing time (Days)

Select an option

▼

% of NanoSilica (NS)

% of MicroSilica (MS)

Predict

FIGURE 17: Dashboard of the Web Interface

² The web interface can be accessed via <https://concrete-strength-predict.netlify.app>

³ The codebase can be accessed via https://bit.ly/github-repo_compressive-strength-of-concrete-app

CONCLUSION AND RECOMMENDATIONS

CONCLUSION

In this study, the partial replacement of cement with nano silica by 1.4%, 4.2%, and 2.8% increased the compressive strength of concrete by 8.64%, 52.16%, and 39.07%, respectively. Furthermore, the partial replacement of cement with micro silica by 4%, 9%, and 13% increased the compressive strength of concrete by 21.73%, 34.75%, and 52.16%, respectively, with a curing time of 7 days and a W/C ratio of 0.4. The study deduced that nanosilica had more effect on the compressive strength of concrete than micro silica. Also, curing time has a strong linear relationship with the compressive strength of concrete.

The dataset containing the features -W/C ratio, curing time, nano silica, micro silica, and compressive strength as the target, was trained using four different models. The CatBoost regressor was the best performing model with the highest R squared value (0.919), lowest RMSE (3.234), and second highest MAE (2.353). The boosting scheme of the CatBoost regressor reduced overfitting, which made the model the best choice among the four used.

Interestingly, this research paper provided a practical way of solving one of the most critical problems in the construction industry. It addressed cost-effectiveness through the elimination of physical determination of compressive strength of concrete and embracing the use of machine learning. Furthermore, it postulated that wastes like slag and fly ash can be used as nanoparticles to improve the technical properties of concrete. Essentially, the study addressed sustainability. Also, the rate of greenhouse gas emissions could be reduced by embracing the use of nanocement against the use of Ordinary Portland Cement.

Finally, the solutions postulated in this study could be employed by stakeholders in the construction industry to save cost in determining the compressive strength of concrete. Climate companies will benefit from this solution presented as well, the reason being that the study devised means of reducing greenhouse emissions. Furthermore, the research paper may offer opportunities to reduce the pressure on raw materials trading on renewable energy (Iavicoli et al., 2014).

RECOMMENDATION

1. Due to the rising discovery of the potencies in nanotechnology, stakeholders in the construction industry are encouraged to invest in funding research, especially in the field of nanotechnology, so that more solutions could be explored.
2. To increase the significance of nanotechnology research, universities should embrace collaboration programs and the use of technological skills among undergraduate students.
3. Regulations that will help to safeguard the lives of people against the health and safety effects of exposure to nanomaterials should be unapologetically enforced.

REFERENCES

1. Al-Jamimi, H. A., Al-Kutti, W. A., Alwahaishi, S., & Alotaibi, K. S. (2022). Prediction of compressive strength in plain and blended cement concretes using a hybrid artificial intelligence model. *Case Studies in Construction Materials*, 17, e01238. <https://doi.org/10.1016/j.cscm.2022.e01238>
2. Alyasri, S.A.H., Alkroosh, I.S. and Sarker, P.K., 2017. Feasibility of producing nano cement in a traditional cement factory in Iraq. *Case studies in construction materials*, 7, pp.91-101.
3. Aytekin, B., & Mardani-Aghabaglou, A. (2022). Sustainable Materials: A Review of Recycled Concrete Aggregate Utilization as Pavement Material. *Transportation Research Record: Journal of the Transportation Research Board*, 2676(3), 468–491. <https://doi.org/10.1177/03611981211052026>
4. Bhavya Khullar (2017). “Climate Change and Reduce Pollution.” <https://www.scientificamerican.com/article/nanomaterials-could-combat-climate-change-and-reduce-pollution/> [Accessed 18 September 2022].
5. Bickbau, M. Y. (2016). U.S. Patent No. 9,505,659. Washington, DC: U.S. Patent and Trademark Office.
6. Britannica (2022). Retrieved from <https://www.britannica.com/technology/cement-building-material/The-major-cements-composition-and-properties>. Accessed on September 11, 2022.
7. Czarnecki, L., 2013. Sustainable Concrete; Is Nanotechnology the Future of Concrete Polymer Composites? AMR 687, 3–11. <https://doi.org/10.4028/www.scientific.net/amr.687.3>
8. Firoozi, A., & Raihan Taha, M. (2014). Nanotechnology in civil engineering Road Stabilization View project Biosorbent View project. In *Article in Electronic Journal of Geotechnical Engineering*. <https://www.researchgate.net/publication/287283673>

9. Singh, G. B., & Subramaniam, K. V. (2019). Production and characterization of low-energy Portland composite cement from post-industrial waste. *Journal of Cleaner Production*, 239, 118024.
10. Helena Monteiro, Bruna Moura, Nelson Soares, “Advancements in nano-enabled cement and concrete: Innovative properties and environmental implications” *Journal of Building Engineering*, Volume 56, 2022, 104736, ISSN 2352-7102, <https://doi.org/10.1016/j.jobe.2022.104736>
11. Hossain, K. and Rameeja, S., 2015. Importance of nanotechnology in civil engineering. *European Journal of Sustainable Development*, 4(1), pp.161-161.
12. Iavicoli, I., Leso, V., Ricciardi, W. *et al.* Opportunities and challenges of nanotechnology in the green economy. *Environ Health* **13**, 78 (2014). <https://doi.org/10.1186/1476-069X-13-78>
13. Jeevanandam J, Barhoum A, Chan YS, Dufresne A, Danquah MK. Review on nanoparticles and nanostructured materials: history, sources, toxicity and regulations. *Beilstein J Nanotechnol*. 2018 Apr 3; 9:1050-1074. doi: 10.3762/bjnano.9.98. PMID: 29719757; PMCID: PMC5905289.
14. Jitendra Patil, Dr. Umesh Pendharkar (2016). Study of Effect of Nanomaterials as Cement Replacement on Physical Properties of Concrete. *International Research Journal of Engineering and Technology (IRJET)*. www.irjet.net
15. Jo, B. W., Chakraborty, S., & Yoon, K. W. (2014). “Synthesis of a cementitious material nanocement using bottom-up nanotechnology concept: An alternative approach to avoid CO₂ Emission during production of cement. *Journal of Nanomaterials*.”
16. Mitch Jacoby (2020). “Alternative materials could shrink concrete’s giant carbon footprint.” <https://cen.acs.org/materials/inorganic-chemistry/Alternative-materials-shrink-concretes-giant/98/i45> [Accessed 19 September 2022]

17. Parva Chhantyal, 2020.” The Advantages of using Nanoparticles in Cement Mortar.” Retrieved from <https://www.azonano.com/article.aspx?ArticleID=5506>. Accessed on September 11, 2022.
18. Pendharkar, U & Patil, J. (2016). Study of Effect of Nanomaterials as Cement Replacement on Physical Properties of Concrete. *International Research Journal of Engineering and Technology*. www.irjet.net
19. Rahimzadeh, C. Y., Salih, A., & Barzinjy, A. A. (2022). Systematic Multiscale Models to Predict the Compressive Strength of Cement Paste as a Function of Microsilica and Nanosilica Contents, Water/Cement Ratio, and Curing Ages. *Sustainability (Switzerland)*, 14(3). <https://doi.org/10.3390/su14031723>
20. Sada, Lecture & Abd Alkhaliq Alyasri (2014). The use of Nanotechnology in construction sector. *Al-Qadisiyah Journal for Engineering Sciences*. 7. 68.
21. Sadeghi-Nik, A., Berenjian, J., Bahari, A., Safaei, A.S. and Dehestani, M., 2017. Modification of microstructure and mechanical properties of cement by nanoparticles through a sustainable development approach. *Construction and Building Materials*, 155, pp.880-891.
22. Saloma, Amrinsyah Nasution, Iswandi Imran, Mikrajuddin Abdullah. Improvement of concrete durability by nanomaterials. *Procedia Engineering* 125 (2015) 608 – 612. The 5th International Conference of Euro Asia Civil Engineering Forum (EACEF-5).
23. Srivastava, T., 2022. *K Nearest Neighbor / KNN Algorithm / KNN in Python & R*. [online] Analytics Vidhya. Available at: <https://www.analyticsvidhya.com/blog/2018/03/introduction-k-neighbours-algorithm-clustering/> [Accessed 19 September 2022].
24. S. P. Dunuweera, R. M. G. Rajapakse, "Cement Types, Composition, Uses and Advantages of Nanocement, Environmental Impact on Cement Production, and

Possible Solutions", *Advances in Materials Science and Engineering*, vol. 2018, Article ID 4158682, 11 pages, 2018. <https://doi.org/10.1155/2018/4158682>.