Compressive strength optimization and life cycle assessment of geopolymer concrete using machine learning techniques

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Abstract. Fly ash-based geopolymer concrete is studied in this research work for its compressive strength, life cycle and environmental impact assessment contribution to the construction environment. This is in line with the United Nations' sustainable development goals SDG9 and SDG11. However, the focus of this research paper is on the sustainability of geopolymer concrete and its overall environmental impact. The metaheuristic machine learning approaches have been deployed to predict the compressive strength (CS) of the GPC based on environmental impact considerations of the concrete constituent materials, which included fly ash, sodium silicate, sodium hydroxide, fine and coarse aggregates. The metaheuristic techniques include the k-Nearest Neighbour (kNN), support vector regression (SVR), and random forest regression (RFR), where all are optimized with the particle swarm (PSO). These metaheuristic techniques have been modified for this research work with new codes to enhance innovation in terms of run time and efficiency. The results of the life cycle assessment (LCA) evaluation of the GPC mixes based on the Ecoinvent 3 available in SimaPro and Eco-indicator 99 and CML 2001 modified in the framework of ReCiPe 2016 recent development show reduced potential of environmental acidification due to increased fly ash (FA) in the GPC mixes compared to previous results. The decisive CS and LCA predictive models, RFR-PSO and SVR-PSO respectively performed optimally above 90% and better than previous models from the literature. Overall, they present an innovative metaheuristic smart technology for the prediction of the GPC infrastructure behavior and performance integrity.

1 Introduction

In recent decades, concrete is known as the most applicable construction material. Ordinary Portland cement (OPC) is traditionally employed in the role of the precursor in the production of concrete [1]. With the boom in the construction industry, the manufacturing of OPC has faced a remarkable rise as well as the production of greenhouse gases. As a result, there has been a continuous investigation for alternative building and construction materials that have a lower carbon footprint [2]. When cement, the binding material in concrete, is manufactured, approximately the same amount of CO_2 is released into the environment. As a consequence of this, several researchers have experimented with various strategies that aim to reduce the amount of cement that is used in concrete, either partially or entirely [3]. Using geopolymer (GP) concrete is one of the most common ways to compensate for this adverse effect of OPC. It is appealing to note that OPC is totally substituted in GP concrete making it a more environmentally friendly building material than ordinary concrete [3]. Alkali activation of amorphous alumino-silicate material in the presence of a warm environment results in the formation of geopolymer, which serves as the binding material in geopolymer concrete. It has been said that the production of geopolymer concrete with a compressive strength of up to or even higher than 60 MPa might be accomplished with relative ease [4]. Because of its superior performance, such as resistance to acid and sulphate, geopolymer concrete is seen as a viable building material to replace cement concrete [4]. Previous studies have reported that the geopolymer can reduce CO_2 emission by 80-90 % compared to the OPC [4]. On the other hand, the effectiveness of geopolymer concrete as a construction material has been the subject

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of exhaustive research. According to the findings of Yip and colleagues [5], aluminosilicate gel (N-A-S-H) and C-S-H can both be found in geopolymer pastes that are based on MK/SG. This is pretty comparable to a geopolymer that is based on high levels of calcium FA and is activated in particular by sodium hydroxide (NaOH), as reported by Somna et al. [6]. The C-S-H and N-A-S-H components of concrete paste each contribute to the paste's overall strength. To put it another way, the alkalinity level of the activators that are utilized has a significant effect on the strength of geopolymer pastes. Additionally, it was observed that temperature has a very crucial effect on the activation of the aluminosilicates. According to the findings of several studies, the activation process in mixtures of FA and SG is predominated by SG activation at temperatures as low as roughly 27 degrees Celsius, but at temperatures as high as approximately 60 degrees Celsius, both FA and SG are activated. Despite this, the SG is making a positive contribution to the strength of pastes thanks to the compactness of its microstructure [6]. The production of C-S-H and C-A-S-H is responsible for the hardening of geopolymer that is based on FA/SG. The further creation of C-S-H, N-A-S-H, and C-A-S-H occurs after the hardening has taken place. On the other hand, the development of hydration gels is reliant on calcium ions as well as pH levels. The amount of alkali in the paste caused the compression strength of the geopolymer to rise. On the other hand, strength diminishes with increasing levels of silica. This is an impact of the SiO_2/R_2O ratio, which helps to contribute to the formation of the ring structure. Zhang et al. [7] found that activation alone by NaOH can create crystalline zeolite or nanosized crystals, depending on the Si/Na ratio. This was shown to be the case. The incorporation of sodium silicate has the potential to considerably lessen the production of crystallites.

Portland Cement is the most popular building material used throughout the construction industry. cement consumption is also increasing as a result of rising urbanization in emerging nations [8-10]. Cement production has a lot of environmental consequences. The extraction of limestone, an important cement raw material, pollutes the environment, including the surrounding ecology and flora and fauna [11,12]. Portland Cement (PC) production releases an almost equivalent quantity of CO_2 into the atmosphere, resulting in air pollution [13]. Even while various activities exist to absorb CO_2, it still forms a major part of ecological contamination [14]. CO_2 emissions from cement manufacturing contribute to around 7% of total greenhouse gas emissions and contribute to about 4% of global warming [14].

As a result, studies have focused more on alternative construction materials in recent decades, such as increasing the use of low-carbon supplementary cementitious materials (SCMs) as a partial substitute for PC, developing alternative low-carbon binders, and increasing the use of recycled materials to reduce natural resource utilization [8]. Meanwhile, industrial waste disposals, such as fly ash (FA) and Ground Granulated Blast-Furnace Slag (GGBS), raise a number of difficulties. They cannot be dumped in the water, and dumping them on land pollutes the environment. This sparked interest in developing Geopolymer Concrete (GPC), an alternative building material generated from industrial waste [9]. GPC is a relatively innovative green building material that is gaining popularity. It is made by using alkali activators like water glass and NaOH to activate the cementitious properties of solid aluminosilicate materials like FA, ground granulated blast-furnace slag (GGBS), or metakaolin in an alkaline environment at a low curing temperature [13]. It has gotten a lot of attention because of its low carbon dioxide emissions, low embodied energy, chemical resistance, high thermal resistance, and great potential for recycling industrial waste to keep the environment clean and healthy [14]. As a renewable resource, geopolymer has an 80 percent reduced carbon footprint than Portland cement [14]. GPC compressive strength is influenced by the alkali activator to solid materials proportion, the silicate to hydroxide proportion, the alkali activator class, and the solid materials content [14].

Engineers face a difficult challenge in predicting Geopolymer Concrete compressive strength since it varies owing to several circumstances. As a result, a numerical model capable of accurately estimating the strength performance of this concrete type is required, such as soft computing approaches [15]. Several studies looked at how the molar content of the NaOH solution, curing temperature, curing method, and duration of FA-based eco-friendly geopolymer concrete influenced compression strength. Several investigators have found that increasing the molarity of NaOH solution increases compression strength [14], whereas others have found that increasing the molarity has a detrimental influence on strength [14]. According to Van Jaarsveld et al. [14], particle size, calcium content, alkali metal content, amorphicity, and the form and provenance of the FA, all impacted the features of geopolymers. The calcium-fortified FA was discovered to have a crucial effect on the strength growth and ultimate compression strength, as more calcium concentration leads to faster strength performance and increased compression strength. They proposed two machine learning (ML) strategies for estimating the compression strength of FA-based GPC in this study. The data for training and validating methods was obtained through experimental work with 335 mixture ratios. In their research [16], Van Dao et al. suggested novel hybrid artificial intelligence (AI) meets to estimate the 28day compression strength of geopolymer concrete comprising 100 percent waste slag aggregates (WSA), namely a genetic algorithm (GA)-based adaptive network-based fuzzy inference system (GAANFIS) and a particle swarm optimization (PSO)-based adaptive network-based fuzzy inference system (PSOANFIS). A number of 21 distinct mixtures with 210 samples were prepared and tested to build and validate these models. To predict the compression strength of GPC, the mass proportion of alkaline activation solution to FA (Which varies from 0.4 to 0.5, and the mass ratio of Na_2SiO_3 to lye solution, which varies from 2 to 3, were utilized. The prediction algorithms employed the compression strength of the generated geopolymer concrete as an output parameter. Both the PSO-based ANFIS and the GA-based ANFIS performed well in predicting geopolymer concrete's 28-day compression strength, but the PSO-based ANFIS outperformed the GA-based adaptive network-based fuzzy inference system. Van Dao et al. [16] used two AI approaches, adaptive neuro-fuzzy inference (ANFIS) and artificial neural network (ANN), to evaluate the compression strength, with fine and coarse aggregate waste steel slag as materials. The produced mixes contained FA, NaOH in solid form, liquid glass, fine and coarse steel slag aggregates, and water, with four variables (FA, NaOH, liquid glass, and water) acting as independent factors for modeling. At a typical age of 28 days, 210 specimens were made with an intended compression strength of 25, 35, and 45 MPa. The two artificial intelligence prediction programs were given these values as targets. While both ANNs and ANFIS models have a reasonable probability of projecting geopolymer concrete compressive strength, the findings reveal that ANFIS outperforms ANNs. Nguyen et al. [17] looked at nine input parameters that include the following: FA, sodium silicate solution, NaOH solution, fine and coarse aggregate, H_2O, NaOH solution concentration, curing time, and curing temperature, with compression strength being the output. Three measures were used to assess the efficacy of the ML reaches: correlation coefficient (R), mean absolute error (MAE), and root mean square error (RMSE). There was a significant relationship between ML models and experimental outcomes. The presented models may be used to create a consistent mixture as well as to calculate the ratios of GPC based on FA. Nagajothi and Elavenil's work [18] findings that were obtained from the experimental and predictive research were used to determine the mechanical properties of Aluminosilicate materials such as GGBS and FA-based GPC samples. The amounts of GGBS and FA, and also the quantity of manufactured sand (m-sand) used to replace existing river sand in geopolymer concrete production, were the main focus of the experimental inquiry. The mechanical properties of the GPC that were investigated were compression strength, splitting tensile strength, and modulus of rupture. As the quantity of GGBS utilized in the tests rose, the mechanical properties of GPC improved. Furthermore, the test findings revealed that increasing the proportion of manufactured sand used boosted the mechanical qualities of the GPC until an optimal dose was reached, beyond which mechanical capabilities began to deteriorate. The mechanical characteristics of GPC predicted by an ANN were performed to validate agreement with test findings.

As a result of the above, the objective of this paper was to propose realistic models to predict the compressive strength of GPC, which are novel in terms of the materials employed and the methodology used to create them. This was carried out considering the environmental impact assessment evaluation of the GPC components.

2 Methodology

2.1 Geopolymer Concrete (GPC) Data Collection

The geopolymer concrete (GPC) database was collected from multiple data representing universal mixes of different sets of concrete reported by Nurul Aida Mohd Mortar et al. [19]. It was statistically analyzed and the result is presented in Tables 1 and 2.

Table 1. Statistical analysis of the GPC database.

	FA	SH	SS	FAg	CAg	LCA	CT	CP	CS
count	53	53	53	53	53	53	53	53	53
mean	452.18	73.92	147.29	669.21	1075.02	12.46	37.26	46.05	46.17
std	82.34	29.58	42.87	120.74	164.42	2.32	16.13	108.64	21.12
min	300	18	40.8	490	810	8.89	23	0.5	3.2
25%	400	57	132.6	576	936	11.1	25	28	35
50%	450	64	150	650	1080	12.2	28	28	47.3
75%	497	85	171.4	723	1200	13.5	60	28	62.8
max	640	160	228.6	990	1470	17.8	70	790	85

Table 2. The correlation of the database parameters.

	FA	SH	SS	FAg	CAg	LCA	CT	CP	CS
FA	1.000	0.244	0.745	-0.401	-0.483	0.966	-0.100	-0.014	0.406
SH	0.244	1.000	-0.223	-0.250	-0.201	0.214	-0.052	-0.258	-0.113
SS	0.745	-0.223	1.000	-0.379	-0.309	0.862	-0.152	-0.031	0.355
FAg	-0.401	-0.250	-0.379	1.000	-0.436	-0.459	-0.196	0.227	0.075
CAg	-0.483	-0.201	-0.309	-0.436	1.000	-0.453	0.226	-0.239	-0.353

LCA	0.966	0.214	0.862	-0.459	-0.453	1.000	-0.145	-0.074	0.375
CT	-0.100	-0.052	-0.152	-0.196	0.226	-0.145	1.000	0.152	-0.315
CP	-0.014	-0.258	-0.031	0.227	-0.239	-0.074	0.152	1.000	0.099
CS	0.406	-0.113	0.355	0.075	-0.353	0.375	-0.315	0.099	1.000

2.2 Life Cycle and Environment Impact Assessment

The term "geopolymer" is used to describe an inorganic polymer produced by alumino-silicate-rich raw materials. which are greener materials than cement since they emit fewer greenhouse gases and may use waste by-products from other industries as raw materials, such as coal fly ash [20].

Countries all over the globe are aggressively acting to minimize energy consumption and emissions to successfully mitigate the negative effect of the building sector on global warming. Silicate cement is one of the most widely utilized modern building materials since it is a key component of concrete materials. The industrial manufacturing of cement uses a large amount of materials and energy, accounting for 10% of world energy consumption [21]. The calcination of raw materials generates a lot of CO_2 and other hazardous gases, which causes a lot of pollution in the environment. Geopolymer concrete (GPC) has been identified as an excellent new ecologically friendly building material, decreasing the usage of energy-intensive, emission-intensive cement and, as a result, lowering the environmental effect to some extent. Nowadays, life cycle assessment (LCA) is regarded as one of the most methodical and scientifically based environmental assessment methodologies for evaluating building materials across their whole life cycle [22], as detailed in IS014040. Most LCA studies, on the other hand, concentrate on the environmental effect of ordinary Portland cement (OPC) or mixed cement concrete. The large environmental burden of OPC concrete was shown to be mostly related to the cement's high energy utilization and gas emissions [23].

The LCA of GPC is only mentioned in a few papers. Turner [24] calculated that CO_2 emissions from the mining used to create GPC concrete were about 9% lower than those from OPC concrete. When compared to OPC concrete, the metakaolin-based geopolymer might reduce CO2 emissions by 27–45 percent. The compressive strength of alkali-activated binary concrete was equivalent to or greater than that of OPC concrete, and it had a significant environmental benefit, since its carbon footprint was 44.7 percent lower. The production of the alkali activators differs somewhat, as does the need for increased temperature curing of GPC to obtain appropriate strength. A comprehensive environmental evaluation of GPC manufacturing in Australia was carried out by McLellan [25]. When compared to OPC, it can cut greenhouse gas emissions by about 44–64 percent. Chen [26] reached the same conclusion. The "cradle to gate" model, which is often employed in LCA, does not account for environmental effects beyond the gate and can only be used to compare GPC and OPC production. The LCA of ternary blended AAM was explored by Faridmehr [27]. The “cradle to gate” system's border is expanded to encompass AAM's sulfate and mechanical resistance, according to the performance standards. In the AAM combination comprising high-volume FA and GBF, the modified LCA with regard to CS demonstrated a decreased intensity of normalized CO_2 emissions. The maximum intensity of normalized CO_2 emissions is seen in AAM combinations including POFA, due to the comparatively low CS, and a large amount of power is needed for oven drying of POFA.

3 Results and Discussion

3.1 Life Cycle and Environment Impact Assessment of Geopolymer Concrete Mix Data

In this section, the LCA approach is used to detect the environmental influence of producing 50 different GPC mixtures at various stages of their life cycle, including raw material extraction, ingredient production and transportation to the production site, and concrete manufacturing. According to Habert et al. [28], the structural function has a major influence on the environmental impact during the use stage. As a result, the primary goal of this investigation is to define the concrete type. As a result, the waste materials consumption and disposal phases were ignored since various kinds of concretes were expected to have similar effects at these stages. This form of partial analysis is helpful in the larger-scale creation of entire life cycles for particular types of concrete. Furthermore, the effect of the remaining life cycle, such as maintenance and destruction, is assumed to be identical for the 50 combinations after the concrete is poured. Throughout the investigation, the database (Ecoinvent 3) available in SimaPro was used. More than 10,000 public processes are included in this database [28, 29]. Materials and procedures were chosen from the SimaPro data set based on facts on the status of raw material availability as well as expert views. 16-32-ton trucks with EURO3 fuel standards were used to examine the environmental implications of the transport stage in the LCA method of concrete manufacturing. The CO_2 emission factor was calculated to be 0.0033-kilogram CO_2 eq per m^3 of GPC throughout the production and transportation phases. Additionally, 0.009 kg/m^3 [24] was assigned to the element that includes structural temporary support and access throughout the manufacturing phase. The energy used in the production of LWC was measured in terms of mixing time and mixer power consumption. The LCA technique was based on ReCiPe 2016. Although its development is based on Eco-indicator 99 and CML 2001, ReCiPe is a relatively recent LCA approach. It features 22 impact categories with midpoint normalization and characterization factors, as well as three endpoint category indicators with normalization factors, all of which measure damage to specific protective zones [30]. The ReCiPe is made up of two groups of impact categories, each with its own set of characterization elements. At the midpoint level, there are 22 impact categories, and most of these midpoint impact categories are multiplied by damage factors and grouped into 3 endpoint categories at the endpoint level. Human health, ecosystems, and resources are the endpoint characterization elements employed in ReCiPe. It's worth noting that human health is measured in terms of the number of life years lost as well as the number of years spent incapacitated. Disability Adjusted Life is the result of combining these factors. These are integrated as Disability Adjusted Life Years (DALYs), whereas ecosystem loss is defined as the loss of species through time and space. Similarly, "resources" is defined as the excess costs of future resource output over an indefinite time horizon (assuming constant yearly production) with a discount rate of 3% [28-30]. The unit is 2000 US dollars. The values of the impact category were separated into reference values during normalization so that all groups could be compared at the same time. SimaPro's normalization numbers are adjusted per citizen. The EU25 +3 population was used as the default figure in SimaPro, and the global population was used as the default value based on the ReCiPe 2016 technique. The primary purpose of normalization is to determine the importance of each product and its respective outcome ranges.

3.2 Machine Learning Analysis of GPC Mix and LCA Impact

3.2.1 Machine Learning Analysis of GPC Mix and LCA Impact

For the LAC, the following variables were used as regressors; fly ash (FA), sodium silicate (SS), sodium hydroxide (SH), fine aggregate (FAg), and coarse aggregate (CAg). The kNN, SVR and RFR optimized using meta-heuristic algorithms of the Particle Swarm Optimization (PSO) and Differential Evolution (DE) to enhance their overall performance were deployed. Figure 1 shows the outcome of the kNN-PSO model of the LCA with performance indices; R^2 0.766, MAE 0.556, MSE 0.791, and RMSE 0.889. It can be observed that the predicted and observed values matched with a good fit. Figure 2 shows the SVR-PSO model of the LCA outcome. This shows that the model performed with the indices; R^2 0.999, MAE 0.054, MSE 0.004, and RMSE 0.060. It can further be observed that the linear kernel SVR-PSO model possessed good fit and correlation in terms of observed and predicted values. Figure 3 shows the model performance of the RFR-PSO on the prediction of the LCA of the GPC. The results show that the R^2 is 0.980, MAE 0.245, MSE 0.074, and RMSE 0.273. It further shows a relatively good fit between the observed and predicted values.

3.2.2 Prediction of the Compressive Strength (CS) of the GPC

For CS prediction, the following variables were used as regressors; fly ash (FA), sodium silicate (SS), sodium hydroxide (SH), fine aggregate (FAg), coarse aggregate (CAg), curing temperature (CT), and curing period (CP). Also, the kNN, SVR and RFR optimized using meta-heuristic algorithms of the Particle Swarm Optimization (PSO) and Differential Evolution (DE) to enhance their overall performance were deployed. Figure 4 shows the outcome of the kNN-PSO model of the CS with performance indices; R^2 0.630, MAE 11.060, MSE 146.595, and RMSE 12.108. It can be observed that the predicted and observed values matched with a good fit. Figure 5 shows the SVR-PSO model of the CS outcome. This shows that the model performed with the indices; R^2 0.445, MAE 11.944, MSE 219.551, and RMSE 14.817. It can further be observed that the linear kernel SVR-PSO model possessed not too good fit and correlation in terms of observed and predicted values. Figure 6 shows the model performance of the RFR-PSO on the prediction of the CS of the GPC. The results show that the R^2 is 0.915, MAE 0.731, MSE 1.829, and RMSE 1.352.

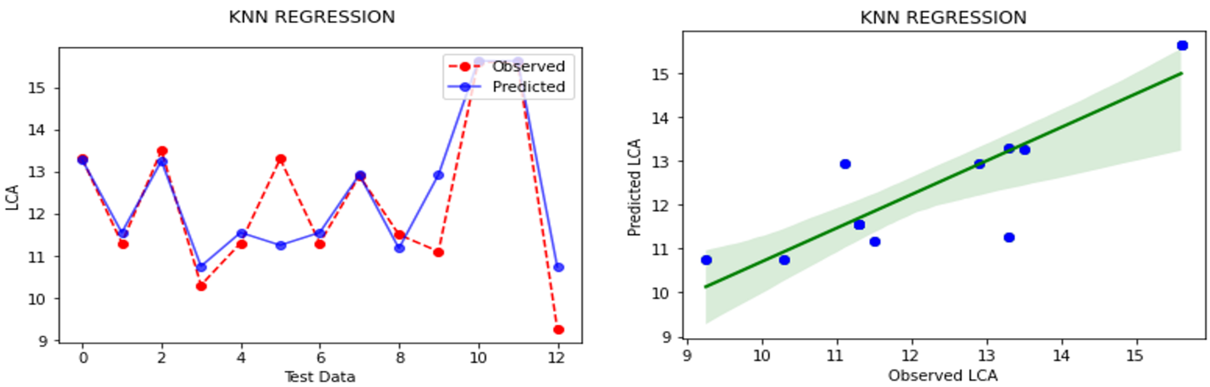

Fig. 1. LCA kNN-PSO model.

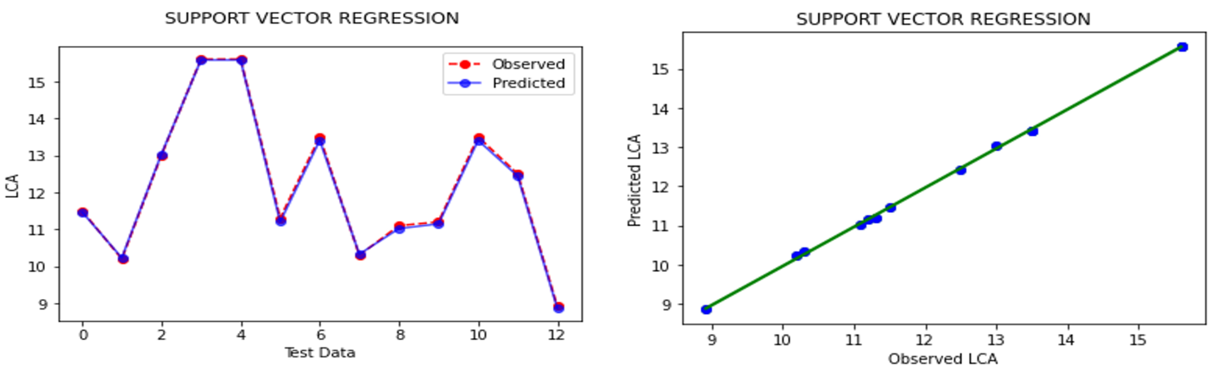

Fig. 2. LCA SVR-PSO model.

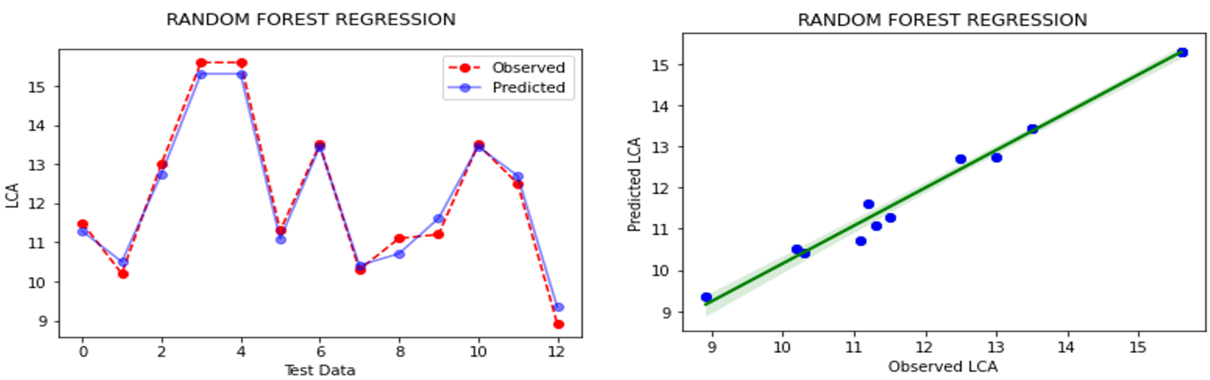

Fig. 3. LCA RFR-PSO model.

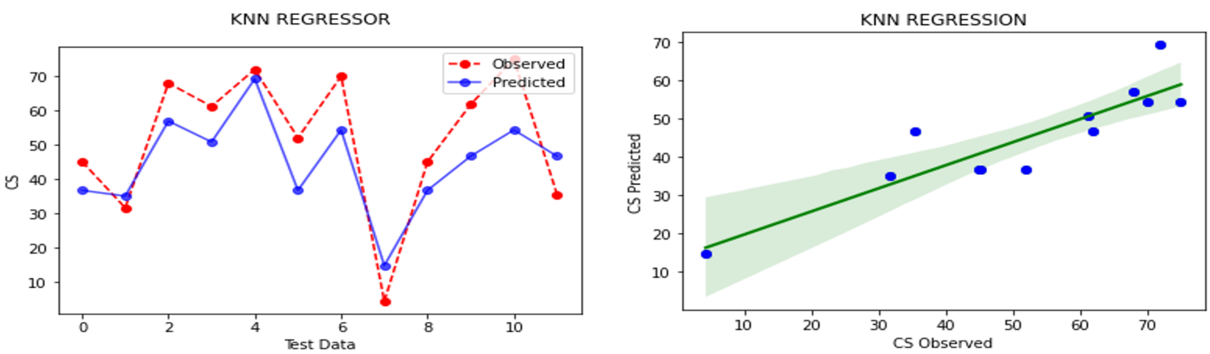

Fig. 4. CS kNN-PSO model.

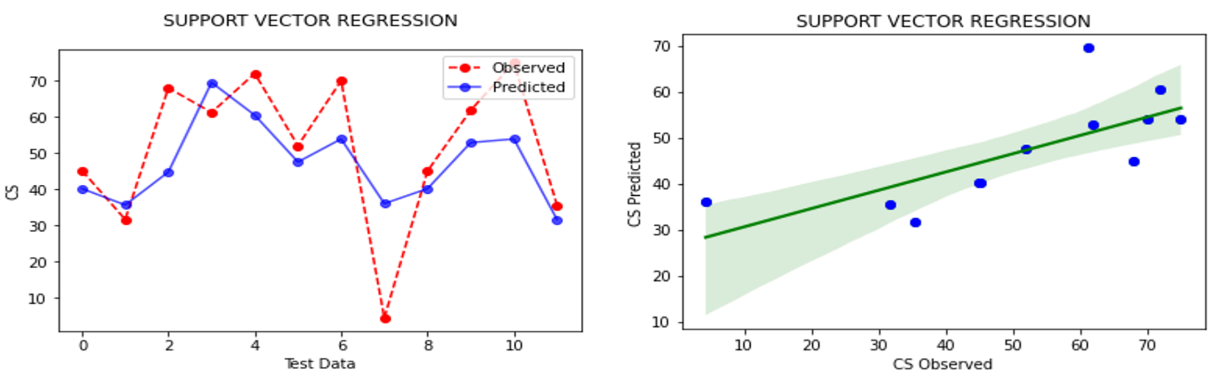

Fig. 5. CS SVR-PSO model.

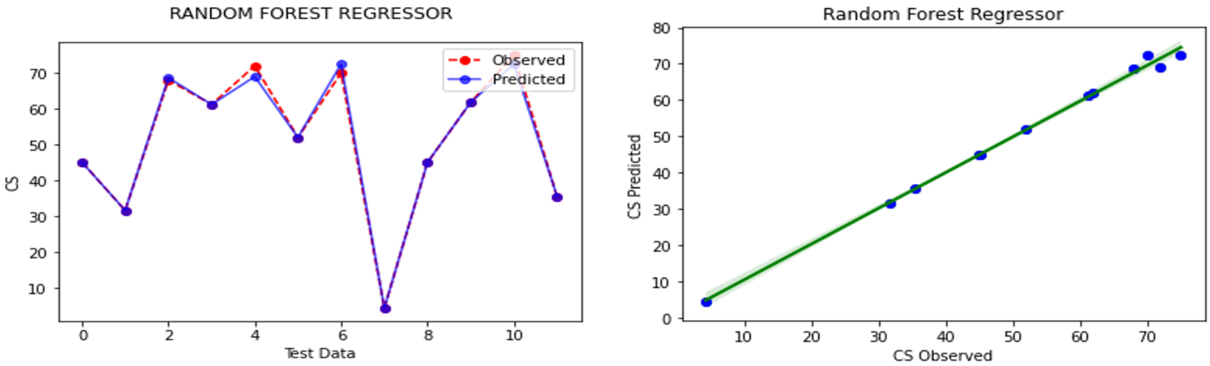

Fig. 6. LCA RFR-PSO model.

4 Conclusions

The metaheuristic machine learning techniques have been deployed to predict the compressive strength (CS) and life cycle assessment (LCA) points under environmental impact considerations of the concrete constituents. The following remarks can be concluded from the forgone exercise:

- Less CO_2 equivalent (CO_2 eq) per m^3 was released from the production and transportation of the GPC compared to the conventional concrete.
- The prediction of the GPC compressive strength (CS) showed that the random forest regression optimized with the particle swarm optimization (RFR-PSO) algorithm outclassed the kNN-PSO and the SVR-PSO with a very wide margin.
- The prediction of the life cycle assessment (LCA) points showed that the support vector regression optimized with particle swarm optimization (SVR-PSO) algorithm outclassed both the kNN-PSO and the RFR-PSO.
- Generally, the deciding models possessed the least errors and best fit between the optimized and measured values.

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