Gaussian process regression model for the prediction of the compressive strength of polyurethane-based polymer concrete for runway repair: A comparative approach

S.I. Haruna¹,³, Han Zhu¹,²*, I.K. Umar⁴, Jianwen Shao⁵, Musa Adamu³,⁵, Yasser E. Ibrahim⁵

¹School of Civil Engineering, Tianjin University, Tianjin 300350, China, ²Key Laboratory of Coast Civil structure Safety of the Ministry of Education, Tianjin University, Tianjin 300350, China. ³Department of Civil Engineering, Bayero University Kano, P.M.B 3011, Kano, Nigeria; ⁴Department of Civil Engineering Technology, Kano State Polytechnic, Nigeria; ⁵Engineering Management Department, College of Engineering, Prince Sultan University, Riyadh Saudi Arabia.

*Corresponding authors: hanzhu2000@tju.edu.cn, madamu.civ@buk.edu.ng

Abstract. Polyurethane (PU) composites have increasingly been used as construction materials to maintain civil engineering structures such as road pavement, runway, parking area, and floor systems in buildings. This study developed polyurethane polymer concrete (PC) mixtures by mixing aggregate-to-PU resin at 0.9: 0.1 and 0.85: 0.15 ratios by weight. The Machine Learning algorithms, including Gaussian Process Regression (GPR), Classification and Regression Tree (CART), and Support Vector Regression (SVR) model were employed to predict the compressive strength of PUPC mixtures as a repair material. The models were trained on the dataset of flexural strength (MPa), density (kg/m³), and PU composition (%), applied as input variables. The result revealed that the compressive stress-strain curves of PU-based polymer concrete exhibit linear elastic behavior under compression. The developed models demonstrate high prediction accuracy of PUPC’s strength. The Nash-Sutcliffe efficiency (NSE) was used to check the performance of each model, and the result obtained showed that the GPR model predicted the compressive strength with the highest accuracy with an NSE-value of 0.9619 and 0.9585 at the training and testing phase, respectively. The finding in this study could offer valuable insight into using these proposed models for compressive strength prediction of PU-based polymer concrete

1. Introduction

Polymer materials have been widely used in construction industries to maintenance civil engineering structures and other applications; these include rubber, Polyethylene (PE), Epoxy resins, Polyurethane (PU), Polystyrene (PS), Styrrene-Butadiene-styrene (SBS), block copolymer, and Ethyl Vinyl acetate (EVA) [1–4]. Moreover, among these polymer materials, polyurethane has increasingly attracted the attention of researchers to carry out studies on PU-based polymer or PU/cement-based composites [4–7]. Polyurethane is a class of polymer composed of carbamate group in their molecular structure, obtained by polymerization reaction between isocyanates and polyol [8]. PU demonstrate excellent performances such as high resistance to corrosion, resist impact and blast loads, extent elongation, resistance to chemical attack, and friendly use [4,9]. For these reasons, PU have broad applications in terms of thermosetting or thermoplastic, in rigid/complex form or flexible/soft form.
In the last decade, researchers have paid attention to evaluate the mechanical and impact resistance performance of polyurethane PC. For instance, Huang et al. [10] studied the mechanical performance of polyurethane PC modified with ground glass fiber (GGF) as a rapid repair of runway' material. Vasconcelos et al. [11] confirmed that wear and dynamic performance of polyurethane concrete was enhanced due to the inclusion of milled fiber. Another study by Haruna et al. [4] revealed significant improvement in impact resistance of polyurethane PC with increased PU resin content.

In the last decades, conventional linear and non-linear analyses were used to predict concrete mechanical performance. The statistical tools such as the design of the experiment were used for evaluating properties and optimizing the concrete mixture. For instance, regression analysis seems to be simple but has some drawbacks while involving several input variables; thus, led to a reduction of prediction accuracy. However, multiple regression analysis models can predict the parameter with high accuracy. Therefore, several studies have been conducted to employ computational, optimization, and prediction techniques in the engineering fields to solve complicated problems. These include Gaussian process regression [12], support vector regression [13], Emotional intelligence (EANN) and traditional FFNN [14], SVM, ANN, MLR and SWR model [15], and Hammerstein-Wiener and SVM model [16] are adopted. Malami et al. [17] analysed the concrete carbonation depth using hybrid and self-turning model. Adamu et al. [16] reported that Hammerstein-Wiener and SVM models predicted the concrete compressive strength containing Jujube seed with high accuracy. In related by Chou and Tsai [18] predicted concrete’ compressive strength of high-performance concrete using CART approach. Therefore, this study prepared polyurethane polymer concrete using two mixing ratios of aggregate-to-PU matrix at 0.85: 0.15 and 0.90: 0.1 by weight, the PC mixture were cast mechanical properties test. Moreover, machine learning algorithms including GPR, SVR, and CART were employed to predict the polyurethane PC’ compressive strength.

2. Experimental program

2.1 Material

The finer aggregates sieved from the natural river sand are used for production of polyurethane PC mixtures. The fineness modulus of the material is 2.06. The particles size of coarse aggregate is in the range of 1.18 to 2.26 mm and that of fine aggregate is 0.3 to 0.6 mm. The aggregates were combined by 2:1 mixing ratio. Fig. 1 depicts the aggregate used and its particles distribution curve.

The bio-based polyurethane (castor oil) and polyaryl polymethylene isocyanate (PAPI) were bought from Guangzhou Jibisheng Technology Industry Co. Ltd China, and an alkylene carbonate served as a diluent was purchased from Zhangjiagang Yuanbang Chemical Material Co., Ltd China.

2.2 Sample fabrication

The schematic production process of polyurethane PC mixtures was depicted in Fig. 2. The polyurethane mixtures were cast for flexural and compressive strength tests. Two groups of the specimen were prepared using mixing ratio between the aggregate to PU resin at 0.85: 0.15 and 0.9: 0.1 by weight were adopted. The polyurethane PC mixtures were cast in prismatic specimens, removed after 1 day, and cured for 3 days at room temperature for 3 days. Table 1 summarizes the polyurethane PC mix proportion formulation used to prepare the PC mixture.
Fig. 1. Materials (a) coarse aggregate, (b) fine aggregate, and (c) particles distribution curve of aggregates

![Materials](image1)

![Particle distribution curve](image2)

Fig. 2. Schematic diagram for forward production of polyurethane PC mixtures

![Schematic diagram](image3)

Table 1. Formulation of polyurethane PC mixtures.

| Specimen ID | PU: Aggregate (weight ratio) | PU resin | Castor oil (g) | PAPI (g) | Solvent (g) | Defoamer (g) |
|-------------|-----------------------------|----------|----------------|---------|-------------|--------------|
| PUPC-0.15   | 0.15: 0.85                  | 167.00   | 33.00          | 10.00   | 0.40        |
| PUPC-0.10   | 0.1: 0.9                    | 167.00   | 33.00          | 10.00   | 0.40        |

2.3 Testing procedure
2.3.1 Compression test

The compressive test of polyurethane PC concrete was performed to evaluate the strength and elastic modulus. Three cubes 50 x 50 x 50 mm were prepared for the compression test. The 20-tonnes load capacity UTM (WDW 200E) was used to obtain the stress-strain relationship. 0.2 mm/s loading rate was adopted for this test following the international standard [4]. The specimens were loaded to failure. The modulus of elasticity was derived from the stress-strain curves using Eq.

\[ E = \frac{\sigma_2 - \sigma_1}{\epsilon_2 - 0.0005} \]  

(1)

Where \( E \) is the young modulus (MPa), \( \sigma_2 \) is the compressive stress equivalent to 40% of the peak stress (MPa), \( \sigma_1 \) is the stress at 0.0005 (MPa), \( \epsilon_2 \) is the corresponding strain of \( \sigma_2 \).
2.3.2 Flexural Test

The flexural strength was performed according to GB/T 17671-1999 [5], using 20-tonnes load capacity UTM (WDW 200E). The speed rate of the UTM was kept at 0.2 mm/s. The prismatic samples (40×40×160 mm) were subjected to flexural loading (3-point bending loading). The samples were placed and positioned on two identical supports with a clear distance of 100 mm. Thus, the flexural load and deflection were monitored until the sample failed in flexure. Thus, Eq. (2) was used calculate the flexural strength.

\[
\sigma_f = \frac{3FL}{2bd^2}
\]  

(2)

Where \(\sigma_f\), \(F\), \(L\), \(d\), and \(h\) are the flexural strength, ultimate load, clear span, width, and specimen depth, respectively.

2.4 AI-based model

2.4.1 Gaussian process regression

GPR applied to a robust non-linear prediction model, probabilistic, nonparametric, supervised, and unsupervised learning method that generalizes the non-linear and complex function mapping on the dataset. Recently, GPR has increasingly attracted the attention of researchers from different engineering fields. [19,20]. Due to the application of kernel functions, GPR can handle non-linear data. In addition it can give reliable result to input data [21].

For a trained set \(M = \{(h_i, y_i) | i = 1,...,n\}\), the input data \(H \in R^{M \times n}\) is known as the designated matrix and \(y \in R^n\) is the vector of the independent variables. The primary assumption of the GPR model is that the output \(y\) is evaluated as

\[
y = f(h) + \epsilon
\]  

(3)

where, \(\epsilon \sim N(0, \sigma^2)\), \(\epsilon R\) is the homoscedastic noise of all samples \(x_i\).

2.4.2 Support vector regression

SVR is a machine learning algorithm with several benefits such as high learning and excellent performance ability, and good noise-tolerating [23,24]. SVR used a kernel function for mapping the data from the sample space into a greater dimensional space. This regression model could transform a nonlinear to a linear problem by learning the complicated relationships between dependent and independent variables. The SVR models have been employed in several regression analyses in the engineering field [25].

Consider training database with \(n\) points. \(\{(h_1, y_1), (h_2, y_2), (h_3, y_3), ......., (h_n, y_n)\}\) Where \(h_i \in R^n\) are the input variables, \(y_i \in R^n\) are the target variables of \(h_i\). \(N\) is the number of datasets, determine the mapping function \(f(h) \in R^n\) to explain the correlation of independent values \(h = \{h_1, h_2, h_3, ......., h_n\}\) and dependent values \(y = \{y_1, y_2, y_3, ......., y_n\}\) is the regression problem. Therefore, linear SVR algorithm was expressed in Eq. (4).

\[
f(h) = w\phi(h) + b
\]  

(4)

where \(\phi(h)\) defined the non-linear mapping function, \(w\) is the weight vector, \(b\) is the bias.

2.4.3 Classification and regression tree

CART was first developed by Breiman et al. [26]. CART is a decision tree-based model that was proven to be a strong tool for classification problems [27]. CART has been widely used in several engineering fields such as medical science, ecology, computer science etc. However, its application is limited to civil engineering. However, CART is effective in decision trees capable of constructing complex trees for solving complex problems involving large datasets. In the study, CART was used to prediction of PUPC’ compressive strength. Fig. 3 shows the flowchart for the development models used in our study.
The combination of input variables used for the development of machine learning models is depicted in Eq. 5.

$$
\sigma_c (MPa) = \begin{cases} 
M_{SVR} = f (PU + \rho + \sigma_f) \\
M_{GPR} = f (PU + \rho + \sigma_f) \\
M_{CART} = f (PU + \rho + \sigma_f)
\end{cases} \tag{5}
$$

Where $\sigma_c$ is the compressive strength, $M_{SVR}$, $M_{GPR}$, and $M_{CART}$ are the proposed model’s combination for support vector regression, Gaussian process regression, and classification and regression tree model, respectively, $f$ is the function of input variables, $\sigma_f$, $PU$, and $\rho$ are the flexural strength, PU binder content, and dry density, respectively.

The experimental dataset was normalized using Eq. (6).

$$
y_i = \frac{y - y_{\text{min}}}{y_{\text{max}} - y_{\text{min}}} \tag{6}
$$

where $y_i$ is the normalized value, $y$ is the observed value, $y_{\text{min}}$ and $y_{\text{max}}$ are the minimum, and maximum values of the data set, respectively.
2.4.4 Performance criteria

Four statistical indicators were used to determine the model prediction accuracy, which includes root means square error (RMSE), Nash-sutcliffe efficiency (NSE), Relative root mean square error (RRMSE), and percent mean bias (PBIAS), as given in Eq. 7-10.

I. Root mean square error

\[
RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\sigma_{Oi} - \sigma_{Pi})^2}
\]  
(7)

II. Nash-sutcliffe efficiency

\[
NSE = \frac{\sum_{i=1}^{N} (\sigma_{Oi} - \sigma_{Pi})^2}{\sum_{i=1}^{N} (\sigma_{Oi} - \sigma_{\bar{O}})^2}
\]  
(8)

III. Relative root mean square error

\[
RRMSE = \frac{RMSE}{\max_{i=1..N}(\sigma_{Pi}) - \min_{i=1..N}(\sigma_{Pi})}
\]  
(9)

IV. Percent mean bias

\[
PBIAS = 100 \times \frac{\sum_{i=1}^{N} (\sigma_{Oi} - \sigma_{Pi})}{\sum_{i=1}^{N} \sigma_{Oi}}
\]  
(10)

Where \( \sigma \) is the compressive strength (MPa), \( \sigma_{Oi}, \sigma_{Pi}, \) and \( \sigma_{\bar{O}} \) indicates observed and predicted \( \sigma \) values and means value of \( \sigma \), respectively.

3 Result and Discussion

3.1 Compression test of polyurethane PC

Fig. 4 shows the compressive stress vs strain relationships of the PUPC specimens prepared according to the mixing conditions. To achieve more reliable response, three specimens were tested from each group. As can be seen from Fig. 4, the plots reveal that PC specimens exhibit elastic behavior when subjected to a compression test. The result indicates that the average compressive strength of PUPC-0.15 specimens is 16.9 MPa, which is slightly higher than the values obtained for the samples prepared with aggregate content of 90%. Moreover, the specimens prepared with a 0.9: 0.1 mixing ratio revealed similar behavior compared with samples of 0.85: 0.15 mix ratio, presumably caused by adopting aggregates larger than one utilized in literature [10,28]. This can produce a cost-effective polyurethane PC for runway repair materials. The average young modulus of PUPC-0.15 and PUPC-0.10 specimens was 233 MPa and 221.7 MPa, respectively.

![Fig. 4. Compression stress-strain curve of: (a) PUPC-0.15 specimens (b) PUPC-0.10 specimens.](image-url)
3.2 Flexural test of polyurethane PC

The flexural strength result of polyurethane concrete according to the mixing variable was shown in Fig. 5. The plots are representative of those other specimens in the two groups. Similar behavior was also observed in terms of flexural strength; despite the variation of PU matrix contents in the two groups, the flexural strength revealed moderate increment. The average flexural strength of PUPC-0.15 was found to be 6.63 MPa, which is 29.5% higher than that of the PUPC-0.1 specimen. The effect of PU matrix on the flexural performance of the polyurethane concrete in terms of deflection capability was observed, which showed that the specimen with higher content of PU matrix tends to deflect more than that of the specimen with a 10% PU matrix. The result showed that the deflection of PUPC-0.15 is 29.2% higher than that of specimen PUPC-0.1.

![Fig. 5. Flexural stress-deflection curve of: (a) PUPC-0.15 specimens (b) PUPC-0.1 specimens](image)

4 Modelling result

The artificial intelligent models perform based learning process, recognition of data set (linear and non-linear). The prediction of compressive strength of polyurethane PC from the data set that containing a regression problem aimed at predicting the compressive strength $\sigma_c$ (MPa). The dataset was used to develop AI-based models, including SVR, GPR, and CART models. For the modelling works, Table 2 summarized the input variables which includes polyurethane content, flexural strength, and density.

The dataset was normalized using Eq. (6) and then proportioning to training and testing phases before the modeling. This is to achieve a common scale of the dataset, minimize redundancy, and enhance the data quality. Additionally, correlation matrix was employed for sensitivity analysis to explore the most sensitive input variable to predict the compressive strength of polymer concrete, as shown in Table 2. The matrix describes the linear relationship that exists among the variables. Moreover, the single input-single output sensitivity analysis involving normalized RSME value using the SVR model was depicted in Fig. 6.
Fig. 6. The resulting increase in RMSE value after removing potential parameter

Tab. 3 shows the descriptive statistical parameters for the data set. These parameters are commonly used information in AI-based literature [4,29]. As can be seen, the mean values of the compressive strength, flexural strength, density, and PU composition are 19.2 MPa, 6.84 MPa, 2011.8 kg/m$^3$, and 12.63%, respectively. At the same time, the corresponding standard deviation is 4.2 MPa, 1.55 MPa, 46.52 kg/m$^3$, and 2.53%, respectively. Thus, the data set is suitable for AI-based model computation.

### Table 2: Correlation matrix

|              | PU content (%) | $\rho$ (kg/m$^3$) | $\sigma_f$ (MPa) | $\sigma_c$ (MPa) |
|--------------|----------------|-------------------|------------------|------------------|
| PU content (%) | 1              |                   |                  |                  |
| $\rho$ (kg/m$^3$) | 0.4385         | 1                 |                  |                  |
| $\sigma_f$ (MPa)  | 0.5736         | 0.6081            | 1                |                  |
| $\sigma_c$ (MPa)  | 0.5822         | 0.6627            | 0.9662           | 1                |

### Table 3: Descriptive statistics of the dataset

| Statistical parameter | PU content (%) | $\rho$ (kg/m$^3$) | $\sigma_f$ (MPa) | $\sigma_c$ (MPa) |
|-----------------------|----------------|-------------------|------------------|------------------|
| Mean                  | 12.63          | 2011.08           | 6.84             | 19.20            |
| Standard Deviation    | 2.53           | 46.53             | 1.55             | 4.20             |
| Minimum               | 10.00          | 1890.00           | 5.10             | 12.70            |
| Maximum               | 15.00          | 2082.00           | 10.30            | 28.30            |

Table 4 shows the evaluation matrices used to check the prediction efficiency of the developed model: GPR, SVR, and CART, which are sufficient to describe the efficiency of these model as translating errors and goodness of fit. The model with highest NSE value, lowest RMSE, RRMSE, and PBIAS values translates the best model. Therefore, the GPR model achieved high prediction accuracy with statistical criteria with an NSE value of 96.19%. However, all the proposed AI-based models demonstrate high prediction accuracy of the compressive strength of polyurethane PC considering the NSE values (>0.75) in training and testing phases, as can be seen in Table 4. In summary, all the models showed excellent prediction capability with NSE values higher than 90%.
Table 4: Modelling results

| Models | Training | Testing |
|--------|----------|---------|
|        | NSE      | RMSE    | RRMSE  | PBIAS | NSE      | RMSE    | RRMSE  | PBIAS |
| SVR    | 0.9466   | 0.0627  | 18.1749| 0.1343| 0.9364   | 0.0648  | 12.3801| 0.0971|
| GPR    | 0.9619   | 0.0530  | 15.3469| 0.1140| 0.9585   | 0.0524  | 10.0048| 0.0817|
| CART   | 0.9574   | 0.0530  | 10.1300| 0.0822| 0.9499   | 0.0608  | 17.5983| 0.1449|

Fig. 7 and 8 shows the scatter plots between the measured and predicted values at the training and testing stages, respectively. As can be seen from these plots, higher goodness of the fit was obtained in GPR models compared to SVR and CART models in both training and testing phase displaying best performance criteria of NSE value of 0.9619 and 0.9585, respectively. The goodness of fit of the models translates the ability of the model to handle the non-linearity of the dependent variables.

Fig. 7. Scatter plots measured vs computed compressive strength in training stages for a) SVR b) GPR c) CART

Fig. 8. Scatter plots measured vs computed compressive strength in testing stages for a) SVR b) GPR c) CART
Additionally, the Radar plot (Fig. 9) and Taylor diagram (Fig. 10) were used to compare the stability and check the model’s performance for the prediction of $\sigma_c$ (MPa), respectively. The radar plot compared the accuracy of the proposed models, the result showed the high accuracy of the GPR model, as can be seen in Fig. 9. Taylor diagram defined several statistical matrices such as RSME standard deviation and correlation coefficient ($R^2$). Therefore, the azimuthal position translates the correlation between the actual and predicted values indicating that the GPR model has the highest correlation value, approximately 99% nearest to the actual value, as shown in Fig. 10. This showed that the GPR model revealed higher fitness among the three AI-based models. Thus, the diagram confirmed that the developed machine learning algorithm revealed high prediction accuracy, which could be applied in modeling the $\sigma_c$ (MPa), of the mechanical properties of polyurethane PC.

**Fig. 9.** Radar plot showing stability of the developed models

**Fig. 10.** Comparing model’s performances using Taylor diagram

### 5. Conclusion
In this study, polyurethane PC were developed using two mixing ratio for the repair of road pavement, runway facilities. Three non-linear AI-based models were employed for the prediction of the compressive strength of polyurethane PC. The following conclusions can be drawn:

- The compressive and flexural strength of PUPC-0.15 specimen increase modestly compared with that of PUPC-0.10 specimens. This is attributed to the particle size of aggregate used in our work.
- The sensitivity analysis showed that the flexural strength of the polyurethane PC specimen appeared to be the most predominant variable for the compressive strength’ prediction.
- All the proposed models successfully predict the compressive strength of polyurethane PC with high accuracy. Moreover, the GPR algorithm predicted the compressive strength with the highest accuracy with an NSE-value of 0.9619 and 0.9585 at the training and testing phase, respectively, compared to other developed models.

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