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Characterization of sustainable concrete made from wastewater bottle caps using a machine learning and RSM-CCD: towards performance and optimization

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Abstract. The properties of concrete, a widely used building material across the globe, have changed due to technological breakthroughs. Cement, sand, coarse aggregate, and water are the four components used to build concrete. Technological improvements increase human comfort, yet the environment is also harmed. Therefore, recycling and reuse are vital to environmental engineers because they help reduce the amount of plastic bottle garbage disposed of as solid waste. In this study, water-cement ratios of 0.5, 0.55, and 0.6 are used in lieu of concrete in various percentages, including 0, 6, and 12% of coarse aggregate replaced by water bottle caps, to analyze the behavior of concrete's compressive strength experimentally. Based on experimental results, models based on artificial neural networks—Levenberg Marquardt and Response Surface Methodology—Central Composite Design models were developed to forecast the final compressive strength of concrete made in part from plastic water bottles. The results demonstrate that for accurately predicting the properties of concrete, the ANN-LM model yields the best result, R^2=0.98, which is close to 1 and R^2 = 0.85 for RSM-CCD, respectively.

Introduction

Concrete is widely employed as a building material. It may be utilized for all kinds of concrete constructions because it is versatile. Concrete is a composite building material primarily made of cement, water, and fine particles. Coarse aggregate can be partially substituted with plastic water bottle lids. With a global yearly use of 20–30 billion tones, it ranks second in materials consumed after water. Undoubtedly, one of the issues that will affect society the most in the future and that we must confront and solve in every manner possible is the recycling of waste materials of all types. Both the building and plastic recycling sectors benefit from developing plastic structural materials that use recycled plastic. Plastics are widely used, contributing to an ever-increasing volume of solid waste. The latter is obtained significantly from plastic bottles used as drink and mineral water storage containers [1]. Disposing of used plastic bottles and metal caps from soft drink bottles is a severe problem for environmental engineers and involves either recycling or reusing.

P.E.T. and metal bottle caps are added to the concrete at levels of 0, 5, 1, and 1.5% by volume of the entire mixture. Compressive, split tensile, and flexural strength are also analyzed, and the results are compared to conventional concrete. The findings demonstrate that standard concrete gains strength compared to various bottle cap percentages [2]. The workability of discarded plastic bottle caps that have been crushed has decreased. When 5% of the coarse aggregate is replaced with waste-crushed plastic bottle caps, the compressive strength increases by about 6.7%. When 15% of the coarse aggregate is replaced with waste-crushed plastic bottle caps, the strength decreases by about 27.6% using the water-cement ratio of 4.2 and 0.40. To increase concrete's compressive strength and flexural strength, it is feasible to mix discarded, crushed plastic bottle tops with cement [3].

Green construction is a crucial strategy to preserve natural resources and lessen the number of materials in our landfills. It is a worldwide issue that is becoming more and more essential. Recently, scientists looked at the feasibility of utilizing used bottle caps to partially replace coarse aggregate in the manufacturing of concrete [4]. The microstructure and mechanical properties of UHPC mixtures, including L.W.A., at high temperatures. Using a UHPC matrix containing different dosages of L.W.A., the effect of increasing temperature and L.W.A. concentration on the compressive and flexural strengths of the UHPC mixture was evaluated. Additionally, temperature exposure was applied to the UHPC combination before and after scanning electronic microscopy (S.E.M.) [5].

The ideal proportion for attaining the highest strength values is 10% cement substitution with B.L.A. to provide maximum compressive strength and durability against sulphate attack and water absorption [6]. The use of R.S.M. and ANN models revealed that they were accurate and valuable forecasts of the stiffness modulus and rutting of asphalt concrete mixes incorporating IWPET substitute aggregates [7]. Comparing the two statistical models revealed that, for the two responses taken into consideration, the ANN model performed better than the R.S.M. model due to its higher determination coefficient (R^2) and lower prediction errors (RMSE and M.R.E.) than the R.S.M. model [8]. The two model's comparison revealed that R.S.M. performed better than ANN, with an R^2 coefficient of determination of 0.9959, closer to 1 [9]. All R.S.M. prediction outcomes are within a 10% margin of experimental outcomes. However, three of the ANN model anticipated results fell outside the 10% limit [10].

The 3D microstructural investigation [11] suggested that the interfacial adhesion between the aggregates and the cementitious materials decreased with higher partial replacement. This reduction in interfacial adhesion results in unsatisfactory hardened characteristics. R.S.M. and ANN were used to assess the effects of adding fine glass aggregate and condensed milk can fiber (Sn) on the compressive and splitting tensile strength at three different curing ages. The inclusion of fiber and the substitution of fine glass aggregate for natural sand enhance the compressive strength of concrete from 14.15 to 16.05 MPa after seven days, 25.09 to 26.60 MPa after 28 days, and 32.12 to 34.14 MPa after 56 days, respectively, by 1% and 20%. The compressive strength of concrete diminishes as the quantity of both factors rises more [12]. Manufactured PE aggregates were utilized to replace fine natural aggregates, whereas P.E.T. aggregates were used to replace natural coarse aggregates at eight different volumetric replacement levels: 5%, 10%, 15%, 20%, 25%, 30%, 35%, and 40% [13]. R.S.M. is beneficial in forecasting the fresh and hardened characteristics of steel fiber-reinforced concrete because of its high predictive efficiency. This eliminates the tediousness of repeated laboratory experiments and enables quick decision-making for building applications [14].

The numerical method would be a potential advancement in this field since it delivers realistic and accurate forecasts while resolving most problems connected with the time-consuming, dangerous, and expensive experimental techniques required [15]. The current study uses plastic wastewater bottle caps in various percentages and water-cement ratios. After 28 days of curing, concrete samples are taken for a crushing test to determine the compressive strength of the concrete. Additionally, it is experimentally compared with traditional concrete. The model, prediction, optimization, and assessment were designed using the artificial neural network, Levenberg-Marquardt, response surface approach, and central composite design methodologies.

Methodology

Materials:

The cement utilized was ordinary Portland cement (O.P.C.), which an Eastern Cement Company makes. Initial and final settling durations are 120 and 280 mm, respectively, and cement has a standard consistency of 26% with a soundness test score of 0.9. Locally, the fine aggregate was sourced from a quarry site in the eastern province's Dammam Industrial District. Testing found that the fineness modulus was 2.93, and the specific gravity was 2.75. Therefore, the fine aggregate was considered based on a size of less than 4.75 mm. Basaltic rock that had been crushed was used as a coarse aggregate. The specific gravity was found to be 2.63, the aggregate size was 25 mm, and it will be more than 4.75 mm. Each of these elements and processes was tested following ASTM standards. The Prince Mohammad Bin Fahd University's civil engineering material laboratory is supplied with potable water that has undergone a thorough inspection to guarantee that it is free of bacteria and undesired material. All mixing and cures were done using this water. Waste plastic bottle caps provide an excellent recycling resource and may be purchased at the scrap market in the Dammam industrial district. By promoting the recycling of these caps, significant energy is saved, and the use of discarded plastic bottle caps in other sectors is brought into sharper focus.

The casting of concrete sample:

Concrete mix designs are carried out, and the material's physical characteristics are assessed in compliance with ASTM standards. The ratio of 1:1.7:3 was used for the concrete mix, and varied water-to-cement ratios of 0.50, 0.55, and 0.60 were used. As per ASTM standards, a mould with dimensions of 150x150x150 mm was employed. For simple concrete sample removal, oil was added to the surface of the moulds after they had been securely fastened with screws. Figure 1 shows the concrete mixing with partial replacement of concrete by plastic water bottle caps, casting, and crushing test of a concrete sample after 28 days of curing.

Figure 1 The mixing, casting and crushing test of concrete samples.

Crushing test of concrete sample specimen:

After being in the mould for 24 hours, the concrete sample was taken out and allowed to cure for 28 days. Following a 28-day curing period, the specimen sample was examined for compressive strength in a compression testing machine with a 2000 kN capacity in line with ASTM regulations. Table 1 compares the proportion of bottle caps, water cement ratio, coarse aggregate, fine aggregate, cement, water, and compressive strength to standard concrete.

Table 1 Compressive strength after 28 days.

Serial No:	(%) of Bottle Caps	Comp. Strength in (N/mm²)
1	0	26
2	6	27.2
3	12	28.3
4	6	27.5
5	12	28.8
6	0	27.8
7	6	27
8	12	27.3

Preparation of data sets for ANN-LM and RSM-CCD model optimization:
This method used eight experimental datasets to create the ANN-LM and RSM-CCD prediction models. Table 2 addresses the bottle cap concrete mix percentage.

Table 2 Concrete datasets with a mix of bottle caps for the ANN-LM and RSM-CCD models.

Serial No:	(%) of Bottle Caps	W/C ratio	C.A. (Kg/m³)	F.A. (Kg/m³)	O.P.C. (Kg/m³)	Water (Kg/m³)	Compressive Strength (N/mm²)
1	0	0.5	1200	850	310	160	26.0
2	6	0.5	1200	850	250	160	27.2
3	12	0.5	1200	850	190	160	28.3
4	6	0.55	1200	850	250	175	27.5
5	12	0.55	1200	850	190	175	28.8
6	0	0.6	1200	850	310	190	27.8
7	6	0.6	1200	850	250	190	27
8	12	0.6	1200	850	190	190	27.3

Development of ANN-LM and RSM-CCD prediction models:
Synthetic neural network, the model was created using MATLAB R2020b's Levenberg Marquardt backpropagation and Response Surface Methodology-Central Composite Design to forecast the compressive strength of partial substitution of coarse aggregate by plastic bottle caps [16]. Ordinary Portland cement, fine aggregate, coarse aggregate, water cement ratio, water content, and plastic bottle caps were the six variables used to create the model [17]. Additionally, the compressive strength of the concrete after the sample cured for 28 days was employed as the dependent or output variable [18]. In modeling, the datasets were split into 70% training data, 15% testing data, and 15% validation data [19]. Multiple neurons in 2 to 3 layers were used for testing and validation. For the prediction of the output factor, Design Expert version 11.1.2 (Stat-Ease) central composite design and face-centered approach were used [20]. The percentage of plastic bottle caps (%) was taken into account in this design model as a partial substitute for coarse aggregate codes (A) and (B) for the water-cement ratio, as indicated in table 3. The design used 2^n factorial runs (n=2), and the number of runs was calculated using the equation $2^n + 2n + n_c$ [21].

The model was designed with three different levels in mind: lower, middle, and higher [22]. The polynomial quadratic equation 1 establishes a relationship between input and output variables.

$$Y' = \beta_{o'} + \beta_{1'}A' + \beta_{2'}B' + \beta_{12'}AB' + \beta_{11'}A'^2 + \beta_{22'}B'^2 \quad (1)$$

Where Y = response variable, $\beta_{o'}$ is intercept, $\beta_{1'}$ and $\beta_{2'}$ were linear coefficients, β_{11}, and β_{22} were the quadratic coefficients, and β_{12} was the interaction between the coefficients.

Table 3. Experimental variables factors and coded levels in RSM-CCD design.

Factor	Name	Units	Type	Min.	Max.	Coded Low	Coded High
A	(%) of Bottle Caps	%	Numeric	-1.0	1.0	-1 ↔ -1.00	+1 ↔ 1.00
B	W/C Ratio		Numeric	-1.0	1.0	-1 ↔ -1.00	+1 ↔ 1.00

Results and Discussion

A well-trained model using the MATLAB tool ANN-LM was generated using the input parameters as the percentage of plastic water bottle caps and water-cement ratio with the number of hidden neurons varying from 10 to 30 [23]. The coefficient of correlation R^2 of regression analysis was employed to measure the model's accuracy, which shows the relationship between the estimated and measured variables. Figure 2 shows the highest relationship between the experimental vs. predicted response and the data fall along line 45º where the network outputs equal the targets [24]. It is found that the coefficient of determination (R^2) for the response allows the accurate prediction with $R^2 = 0.998$, which is close to 1.

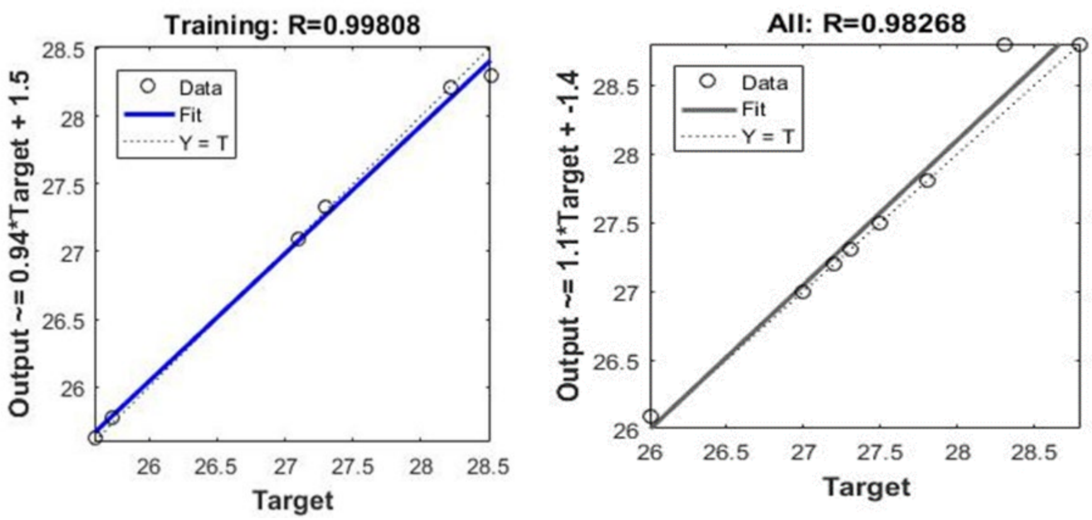

Figure 2 Experimental vs. Predicted values relationship for the response.

A central composite design and face-centered technique in response methodology were used to assess the experimental outcomes of a total of 8 runs with randomized type. The input factors' individual interface and quadratic impacts affect the prediction of the compressive strength of sustainable concrete, and an analysis of variance was conducted [25]. The R^2 predicted value was found to be 0.85. Figures 3(a) and (b) display the 3D plot between the input and output factor and prediction vs. actual experimental variables.

Analysis of variance (ANOVA) in design expert R.S.M. was used to look at the relationship between the inputs and outcome variables. The 5.36 model F-value suggests that the model terms are essential. A and B are important model terms in this instance. Model terms are insignificant if the value is higher than 0.10 [26].

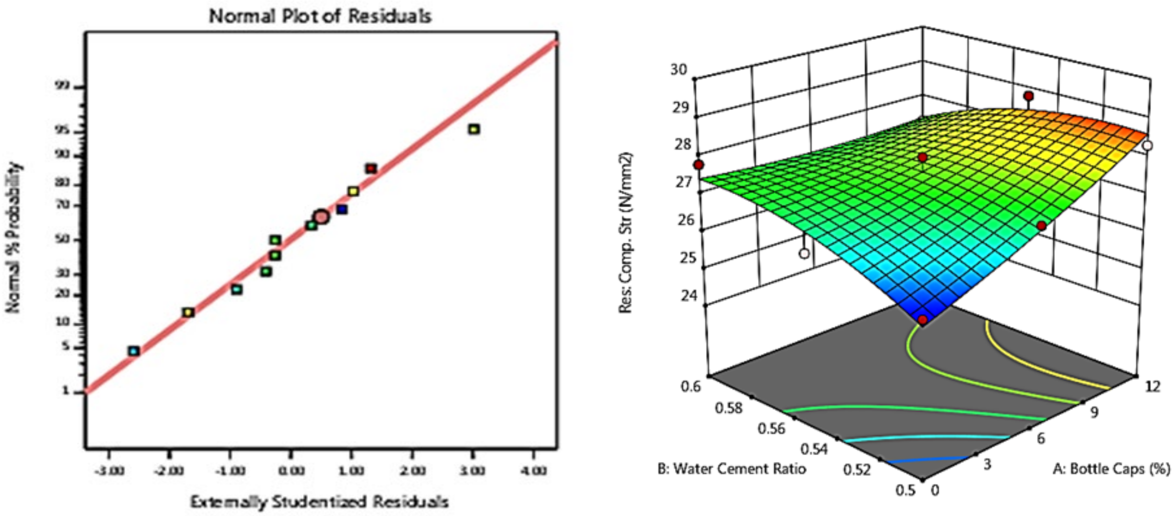

Figure 3 (left) A 3D plot and predicted vs. actual response (right) 3D surface plot

The lack of fit is implied to be insignificant compared to the pure mistake by the lack of fit F-value of 3.27. A significant lack of fit F-value has a noise probability of 24.28% occurring. The findings, which further corroborated the finding that allowed the null hypotheses of the two inputs to be rejected, reveal that the model's p-value is less than 0.05 [27]. Equations (2) and (3) show real and coded factors for response prediction. The coded factors may be used to predict responses based on independent factors using the coded factors. By comparing the factor coefficients, the quadratic equation in coded form proved extremely helpful in determining the relative importance of the elements [28]. The predictions may be made using the same equations in relation to the actual components.

Equation of compressive strength at 28 days in coded factors (N/mm^2) = $+27.61 + 0.6833(A) + 0.10(B) - 0.70(A.B.) + 0.1237(A^2) - 0.4263(B^2)$ (2)

Equation according to actual factors (N/mm^2) = $- 33.33 + 1.355(A) + 203.578(B) - 2.334(AB) + 0.00343(A^2) - 170.526(B^2)$ (3)

Where, A and B are input factors of the percentage of bottle caps and water cement ratio. Optimizing the mix proportion of bottle cap partial replacement of concrete was carried out using the optimization tool in the R.S.M. application [29]. In this tool setting, the maximum compressive strength of concrete on the 28^{th} day predicted was found to be 28.6287 N/mm^2 at a percentage of bottle caps 12 % and water cement ratio of 0.5148 with the desirability of 0.961 1 out of 8 solutions as shown in figure 4 ramp diagram. Table 4 shows the compressive strength of concrete for the prediction by ANN-LM and RSM-CCD application.

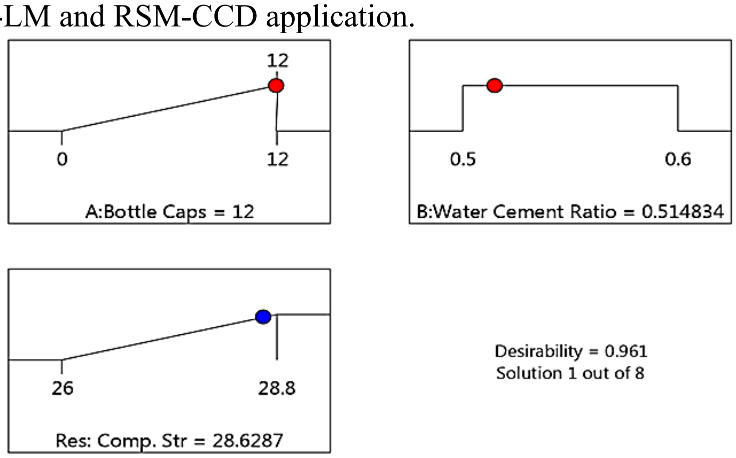

Figure 4 The desirability function of solution 1 out of 8

Table 4 Compressive strength of concrete by Expt., ANN-LM and RSM-CCD

Serial No:	Exp. Values (N/mm^2)	ANN-LM		RSM-CCD	
		Pred. Comp. Strength (N/mm^2)	(%) Error	Pred. Comp. Strength (N/mm^2)	(%) Error
1	26	26.09	-0.340	25.82	0.697
2	27.20	27.20	-0.100	27.08	0.443
3	28.30	28.80	-1.736	28.6	-1.049
4	27.5	27.51	0.036	27.61	-0.362
5	28.8	28.82	-0.035	28.42	1.407
6	27.80	27.82	-0.036	27.42	1.458
7	27	27.00	-0.917	27.28	-1.026
8	27.3	27.30	-0.365	27.39	-0.328

Conclusion
This method involved designing a concrete mix with various water-to-cement ratios and various percentages of plastic bottle tops to replace some of the coarse material. To ascertain the concrete sample's compressive strength, the experimental concrete mix was cast and examined after 28 days. For the prediction of concrete's compressive strength, software like RSM-CCD and ANN-LM were applied. The coefficient of determination of R^2 was determined to be 0.998 via ANN-LM. While the highest optimum value of concrete's compressive strength was determined to be 28.629 N/mm^2 at 12% of a 0.515 water-cement ratio, RSM-CCD was found to be 0.85. When predicting the compressive strength of concrete, ANN-LM and RSM-CCD are contrasted. Compared to RSM-CCD, ANN-LM modeling prediction was shown to have better values.

Conflict of Interest
The authors do not have any conflict of interest.

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