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To predict the compressive strength of self compacting concrete with recycled aggregates utilizing ensemble machine learning models

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A R T I C L E I N F O

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A B S T R A C T

This study aims to apply machine learning methods to predict the compression strength of self-compacting recycled aggregate concrete. To obtain this goal, the ensemble methods: Random Forest (RF), K-Nearest Neighbor (KNN), Extremely Randomized Trees (ERT), Extreme Gradient Boosting (XGB), Gradient Boosting (GB), Light Gradient Boosting Machine (LGBM), Category Boosting (CB) and the generalized additive models: Inverse Gaussian (GAM1) and Poisson (GAM2) were applied. For the development of the models, 515 research article samples were collected and divided into three subsets: training (360), validation (77), and testing (78). The SCC components: cement, water, mineral admixture, fine aggregates, coarse aggregates, and superplasticizers were taken as input variables and compression strength as output variables. To determine the ability of the models to project compressive strength, the following metrics were used: R^2, RMSE, MAE, and MAPE. The results indicate that the RF ($R^2 = 0.7128$, RMSE $= 0.0807$, MAE $= 0.06$) and GB ($R^2 = 0.6948$, RMSE $= 0.0832$, MAE $= 0.0569$) models have a strong potential to predict the compressive strength of SCC with recycled aggregates. The sensitivity analysis of the RF model indicates that cement and water are the variables that have the highest impact in predicting the compressive strength, while coarse aggregate has the lowest impact.

1. Introduction

Worldwide, the rapid development of the construction industry over the years has led to excessive consumption of natural resources, construction and demolition waste (C&DW) has been accumulated in a huge content, discarding the recycled aggregates (RA) in landfilling can result in environmental damage [1–4]. Particularly in the last decades, in the European Union, the construction industry has had exponential growth, and as a consequence of this growth, the production of C&DW has been increasing [5,6]. With this great development of the construction industry, the rate of demolition is increasing day by day, this makes it necessary to

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effectively reuse C&DW [7,8]. In general, this waste composition contains concrete, masonry, wood, metal asphalt, ceramic materials, among others [3,8]. This development of the construction industry makes concrete one of the most widely used products worldwide [3,9,10], due to its various advantages over other materials, e.g., integrity, durability, modularity, economy [11]. Concrete is mainly composed of fine aggregates (sand) and coarse aggregates (stone), these aggregates account for approximately 75% of the total concrete [3,12].

Since concrete is the most widely used construction material worldwide and intending to take advantage of this construction waste to minimize the environmental impact, the construction industry has developed advanced techniques for concrete design [8,10,13] thus achieving different types of concrete containing different mineral admixtures. Recently, the construction industry is widely applying a variety of specialty concrete, including self-compacting concrete (SCC) and high-performance concrete [10]. The introduction of SCC provides an allowable potential and attracts interest in exploiting substitute materials, waste, by-products, and secondary materials such as mineral admixtures.

Self-compacting concrete is a fluid concrete characterized by increased flow capacity, good segregation resistance and slump under its own weight. This is why this type of concrete allows the formwork to be filled without the need for mechanical vibration, so that it can be easily used in complicated formwork, reinforced structural elements and areas of difficult access. Thus, it avoids bleeding and segregation and maintains stability at the same time [14,15]. In this sense, it is used in the construction of civil works around the world, taking advantage of its ability to be compacted by the action of gravity [2,15–17].

The quality of SCC is generally established according to its compressive strength, which gives a general reference to the quality of concrete, since it is directly related to the structure of the hardened mixture [18]. Generally, the way to obtain the compressive strength of SCC is by physical experiments, which are expensive and time consuming to obtain results, so the working efficiency will be very low [11]. That is why, technological advances allow solving engineering problems at a lower cost by other methods, such as empirical regression, numerical simulation and the use of machine learning methods [11,19]. These methods allow predicting the compressive strength of SCC with the proportion of the designed mixture of different components (cement, admixture, water, coarse aggregates, fine aggregates and superplasticizers).

In this regard, there is a trend of using artificial intelligence through machine learning (ML) techniques to predict the compressive strength of SCC [3,9,20–22], these techniques can be used for various purposes, such as regression, classification, correlation, clustering. Therefore, with the development of ML techniques, it becomes easier to predict the compressive strength of SCC [19], as well as other mechanical properties of concrete [20,23]. Thus, to evaluate the mechanical properties of concrete with recycled aggregates Xu et al. [23] used multiple nonlinear regression and neural networks; Xu et al. [20] employed a probabilistic calibration method based on Bayesian theory and Markov Chain Monte Carlo (MCMC) method as well as Xu et al. [24] developed four different types of models: the multivariate regression (MNR) model and the two neural networks (i.e., BP-ANN and GA-ANN) to predict the behavior of RAC under triaxial loading.

Specifically the prediction of the compressive strength of self-compacting concrete is an application of the ML regression function, through the application of certain methods that can learn from the input data and provide very accurate results. Currently, a variety of ML methods are employed to predict the compressive strength of self-compacting concrete, including ensemble methods [21,25], neural networks [23,24], regression models [10,24,25] and generalized additive models (GAM) [25–27].

Therefore, the research objective of this work is to apply machine learning methods to predict the compressive strength of self-compacting concrete with recycled aggregates.

1.1. Self-compacting concrete (SCC) with recycled aggregates

Self-compacting concrete is defined as a special type of concrete able to be compacted by the action of its weight, which can settle in the highly reinforced and deep sections, filling the formworks and runs between difficult to access structures or complex molds, without the need for vibrating or any other compaction method [28–30]. This type of concrete, developed in Japan in the 1980 s with the advances in concrete technologies, has spread all over the world. Once hardened, it is dense, homogeneous, and has the same engineering properties and durability as traditional vibrated concrete [16,29,31,32], due to a studied dosage and the use of specific superplasticizer [28–30]. It presents the characteristic of being homogeneous as well as maintaining its cohesion during its placement, without segregation or bleeding, blockage of coarse aggregates, or exudation of the slurry [15,16,28,33].

For the preparation of the SCC mix, the same components are used as those used for conventional concrete: cement, fine aggregates, coarse aggregates, binder, and water [5,28,34–36], in the correct proportions to obtain a homogeneous mix. In addition to these materials, additives such as superplasticizers and modular viscosity additives (chemical admixture), in different proportions, are included in the preparation of SCC to help reduce segregation and exudation during pouring on-site as well as sensitivity to the variation of other elements of the mix [4,25,30].

The rapid development of the construction industry has generated a great demand for concrete, resulting in excessive use of natural assets, as is the case of natural stone aggregates, the material used in the production of concrete, as well as an increase in construction and demolition waste. For this reason, the construction industry has seen the need to exploit less natural resources, reduce the environmental impact and take advantage of C&DW, which has been achieved thanks to the use of recycled aggregates from concrete waste [1,2,16,37,38].

The recycling of C&DW for the preparation of recycled aggregates, to replace natural aggregates, allows the elaboration of SCC with recycled aggregates [5,30,39,40], which has been recognized as a way to reduce construction waste and conserve the environment, in addition to a decrease in the cost of construction Works [16,37].

The mechanical properties of SCC with recycled aggregates, such as compressive strength, tensile strength, elasticity, flexural strength, are hardly affected concerning those of conventional concrete [5,39,40]. Martínez-García [5] points out that a 20% substitution of recycled aggregates has little impact on the properties and characteristics of concrete with recycled aggregates compared to those of conventional concrete. EHE-8 [28] recommends the 20% weight proportion of recycled aggregates as the maximum allowable weight limit of the use of recycled aggregates in the concrete mix.

1.2. Compressive strength

Compressive strength is one of the main mechanical characteristics of concrete. Compressive strength is calculated by the ultimate load divided by the cross-sectional area resisting the load and is expressed in megapascals (MPa) [41]. It is considered a conventional value established through a standardized test and referred to as the stress for which exhaustion is reached. The concrete compression strength of concrete is subject to the proportion of recycled aggregates incorporated in the mix [18,38,42] so its proper dosage has a considerable impact on the compression strength.

1.3. Machine learning

Machine Learning (ML) is one of the key approaches to artificial intelligence (AI). Machine learning is currently used in several research fields. It is characterized by the ability to improve behavior, called learning, based on previous experience. This improvement consists of establishing logical rules that lead a given system to make more assertive decisions for a given context. Machine learning deals with systems that are trained from data rather than explicitly programmed; it uses algorithms to learn from data patterns [43,45]. Machine learning methods allow the analysis of large amounts of data, being exceptionally systematic in terms of computing and progressing time [1,46], providing faster and more accurate results, thus reducing error rates to negligible levels. Machine learning methods can be divided into 3 categories: supervised learning; unsupervised learning (Clustering algorithms, Principal Component Analysis, among others), and reinforcement Learning [44,47]. Supervised learning methods are exposed to large amounts of labeled data, including input and output variables. The algorithm finds patterns among the data, learns from the observations, and generates predictions until the error has been sufficiently minimized. Supervised learning is divided into two types: classification and regression [48]. Classification uses algorithms to recognize specific patterns within the data set to define predictions. Among the most common classification algorithms are: ensemble methods, Decision trees, Nearest neighbors. Regression is utilized to understand the relationship between dependent and independent variables and is often used to make projections. Among the most common regression algorithms are: generalized linear models (GLM), generalized additive models (GAM), logistic regression, among others. Unsupervised learning methods employ data sets that are not classified with the aim of finding patterns in data fragments by recognizing similarities and grouping data by categories [48].

Reinforcement methods are trial-and-error learning. The system interacts with its environment producing actions that discover errors, the algorithms automatically determine the ideal behavior within a specific context seeking to maximize its performance [48]. Particularly in this paper, to predict the compressive strength of SCC with recycled aggregates supervised learning methods are used, specifically nine ensemble methods: Random Forest (RF), K-Nearest Neighbor (KNN), Extremely Randomized Trees (ERT), Gradient Boosting (GB), Light Gradient Boosting Machine (LGBM), Extreme Gradient Boosting (XGB), Category Boosting (CB) and the generalized additive models: Inverse Gaussian (GAM1) and Poisson (GAM2).

1.3.1. Ensemble methods

Ensemble Methods are learning algorithms that combine multiple differential machine learning models to improve prediction performance [49–51]. The result is a final model that performs better than individual models Among the ensemble methods are: Boosting and Bagging.

Bagging (bootstrap aggregating), seeks to improve classification by combining the prediction results of independently trained models into randomly generated training sets. In Bagging methods, the idea is to construct several independent estimators and calculate the mean of the predictions. This results in an estimator with a lower variance compared to independent estimators. Among the Bagging methods proposed are K-Neighbor Regressor (KNN), Random Forest (RF), and Extretrees Regressor (ERT) [19,25,47,52–54]. K-Neighbor Regressor (KNN) seeks to explore a set of training specimens close to a new query point and predict its value [55]. Random Forest (RF) is a method that takes into account several random decision trees and fits them based on several subsamples of the training data. RF uses the average of the decision trees to better predict and control overfitting [56]. Extretrees Regressor (ERT) is similar to RF, differing only in the way random splits are performed on the trees [57].

Boosting is an ensemble meta-algorithm that combines a set of weak classifiers to create a strong classifier. It builds an ensemble incrementally by iteratively training a new model to emphasize misclassified training samples from previous models. Estimators are built sequentially while seeking to decrease the bias of the final combined estimator. Among the methods employed are Gradient Boosting (GB), Light Gradient Boosting Machine (LGBM), Extreme Gradient Boosting (XGB), and Category Boosting (CB) [49,52,53]. GB progressively builds a model using differentiable loss function optimization [58]. At each step, a regression tree is fitted following the negative gradient of the loss function. LGBM is a variation of GB that uses trees based on learning algorithms. As a result, LGBM has a speed value at the training stage, ensuring higher efficiency [59]. XGB is a variation of GB and has an optimization algorithm for splitting trees integrated with a regularization component (to avoid overfitting) [60]. CB is also a variation of GB, which: uses symmetric trees to provide faster execution, allows the use of parallel processing, and uses ordered boosting to avoid overfitting [61].

1.3.2. Generalized additive models

Generalized additive models (GAM) are an extension of generalized linear models. The GAM is a generalized linear model, in which the output variable is given by a linear combination of unknown smooth functions of some predictor variables. GAM models do not restrict the relationship between the response variable and the explanatory variable to the linear form, but allow this relationship to have an unknown form, using Exponential Family distributions for the response variable. In this paper, the Inverse Gaussian (GAM1) and Poisson (GAM2) exponential distributions are used to build the GAM model [48,62,63].

2. Materials and methods

2.1. Experimental database

The data collected through the research article search contains the results of 515 samples of SCC hardened with recycled aggregates. Table 1 summarizes the database including the amount of data (no.) contributed by each article as well as its proportion (percentage) in the data.

From these published papers on the compression strength of SCC with RA, Table 2 shows the average, minimum and maximum values of the input (Cement, Mineral Admixture, Water, Fine aggregate, Coarse aggregate, Superplastificizer) and output (Feature compression know) variables used for modeling the compression strength of SCC with RA, through the use of Machine Learning techniques.

2.2. Exploratory data analysis

The correlation coefficient (r) between the input variables: cement, mineral admixture, water, fine aggregate, coarse aggregate, and superplasticizer and the output variable feature compression know (fck) was calculated to evaluate the dependence of the variables on each other. A high absolute value of r between the variables would indicate that there is a correlation between them, so only one of them would be taken into account and the others would be excluded. For the calculation of r the following equation was used (1):

$$\boldsymbol{r} = \frac{\sum[(\boldsymbol{x}_i - \overline{\boldsymbol{x}})(\boldsymbol{y}_i - \overline{\boldsymbol{y}})]}{\sqrt{\sum(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^2 * \sum(\boldsymbol{y}_i - \overline{\boldsymbol{y}})^2}} \tag{1}$$

where, $\mathrm{x_i}$ = input variable, $\overline{x_i}$ = mean of input variable, $\mathrm{y_i}$ = fck(output variable), $\overline{y_i}$ = mean fck experimental, $i = 1, \ldots, n$ y n = Total data number.

A correlation (|r|>0.8) between input variables could point out the present multicollinearity between variables [116], which would

Table 1
Experimental database.

No	Reference	no.	percentage	No	Reference	no.	percentage
1	Ali et al. [64]	18	3.49	29	Nili et al. [65]	10	1.94
2	Aslani et al. [66]	15	2.91	30	Pan et al. [67]	6	1.17
3	Babalola et al. [68]	14	2.72	31	Pereira-de-Oliveira et al. [69]	4	0.78
4	Bahrami et al. [70]	10	1.94	32	Poongodi et al. [71]	9	1.75
5	Barroqueiro et al. [72]	6	1.17	33	Revathi et al. [73]	5	0.97
6	Behera et al. [74]	6	1.17	34	Revilla Cuesta et al. [75]	5	0.97
7	Bidabadi et al. [76]	11	2.13	35	Sadeghi-Nik et al. [77]	12	2.33
8	Chakkamalayath et al. [78]	6	1.17	36	Salesa et al. [79]	4	0.78
9	Duan et al. [80]	10	1.94	37	Sasanipour et al. [81]	5	0.97
10	Fiol et al. [82]	12	2.33	38	Sasanipour et al. [83]	5	0.97
11	Gesoglu et al. [84]	24	4.66	39	Señas et al. [2]	6	1.17
12	Grdic et al. [85]	3	0.58	40	Sharifi et al. [86]	6	1.17
13	Guneyisi et al. [87]	5	0.97	41	Silva et al. [88]	5	0.97
14	Guo et al. [89]	27	5.24	42	Singh et al. [90]	10	1.94
15	Kapoor et al. [91]	8	1.55	43	Singh et al. [92]	12	2.33
16	Katar et al. [37]	4	0.78	44	Sua-iam et al. [93]	20	3.88
17	Khafaga, S.A. [94]	10	2.91	45	Sun et al. [95]	10	1.94
18	Khodair et al.[96]	20	3.88	46	Surendar et al. [97]	7	1.36
19	Kou et al.[98]	13	2.52	47	Tang et al. [99]	5	0.97
20	Krishna et al. [100]	5	0.97	48	Thomas et al. [101]	4	0.78
21	Kumar et al. [102]	4	0.78	49	Tuyan et al. [103]	12	2.33
22	Li et al. [104]	4	0.78	50	Uygunoglu et al. [105]	8	1.55
23	Long et al. [106]	4	0.78	51	Wang et al. [107]	5	0.97
24	Mahakavi and Chitra, [108]	25	4.85	52	Yu et al. [109]	3	0.58
25	Manzi et al. [110]	4	0.78	53	Yu et al. [111]	6	1.17
26	Martínez-García et al. [6]	4	0.78	54	Yu et al. [112]	21	4.07
27	Mo et al. [113]	5	0.97	55	Zhou et al. [114]	6	1.17
28	Nieto et al. [115]	22	4.27	Total		515	100

Table 2
Mean, maximum and minimum values of input and output variables.

Variables		Abbreviation	Mean	Minimum	Maximum
Input	Cement (kg/m^3)	C	375.84	78.00	635.00
	Mineral Admixture (kg/m^3)	A	135.17	0.00	515.00
	Water (kg/m^3)	W	176.87	45.50	277.00
	Fine aggregate (kg/m^3)	FA	845.10	532.20	1200.00
	Coarse aggregate (kg/m^3)	CA	784.91	328.00	1170.00
	Superplasticizer (kg/m^3)	SP	4.50	0.00	16.00
Output	Feature compression know (MPa)	FCK	44.94	7.17	87.00

affect the modeling results, causing the model to be biased.

The heat map of the correlation coefficients is shown in Fig. 1. It can be seen that there is no significant correlation between the input variables and that no correlation is higher than 0.8, which indicates that there is no multicollinearity between the input variables.

2.3. Dataset splitting

Machine learning methods require data sets to be divided into subsets of training, validation, and testing, for benchmarking [1,9,25,52]. During the training process, the model performance is assessed with the validation dataset to optimize the hyperparameters of the model. Finally, to show the accuracy of the model in predicting the compressive strength, the test data set is used.

For the modeling of the compressive strength of self-compacting concrete with recycled aggregates, a total of 515 samples were randomly divided into: 360 samples (70%) for the training process, 77 samples (15%) for the validation process and 78 samples (15%) for the testing process. Table 3 shows the mean, minimum and maximum values of the input (Cement, Mineral Admixture, Water, Fine aggregate, Coarse aggregate, Superplasticizer) and output (Feature compression know) variables for the training, validation, and test data sets.

2.4. Models development

In this study, nine ML methods, described in Section 2.3 (KNN, RF, ERT, GB, LGBM, XGB, CB, GAM1, GAM2), were organized to project the compression strength of self-compacting concrete with recycled aggregates. After data preparation, the input variables are introduced into the learning methods. The training set containing 70% of the total data was used to develop a prediction model for each method selected in this research, while the validation set consisting of 15% of the data was used for hyperparameter fitting. It should be noted that, in the following sections, the best hyperparameter obtained for the validation data is highlighted in bold.

2.4.1. Bagging methods

KNN, The hyperparameters that were adjusted for this algorithm were: number of neighbors to be used for query, 'n_neighbors' =

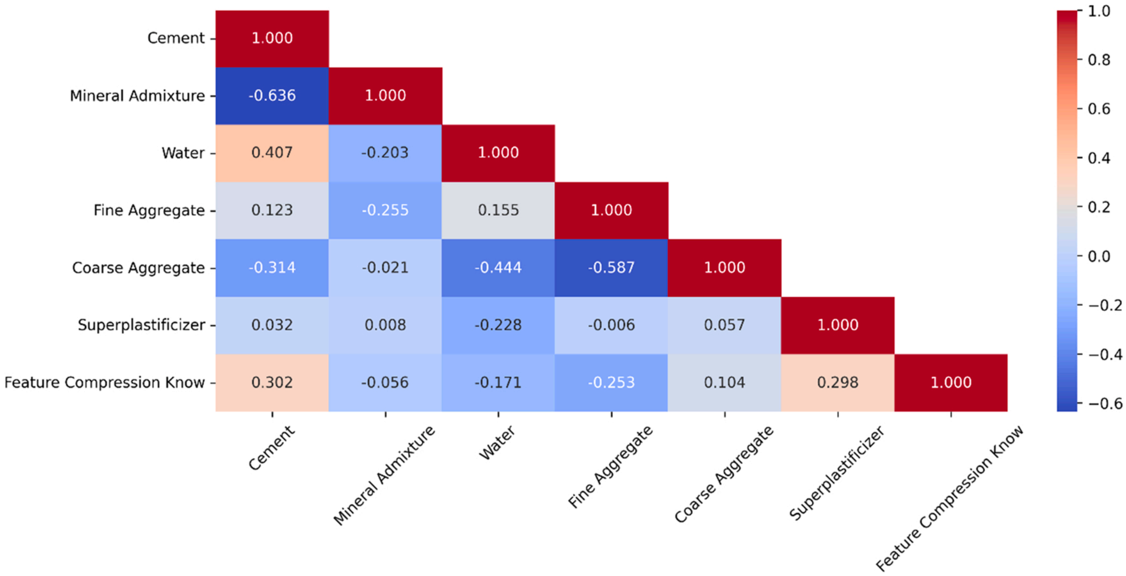

Fig. 1. Heat map for the correlation coefficient between the input and output variables.

Table 3
Mean, maximum and minimum values of the input (kg/m^3) and output (MPa) variables of the data sets: training, validation, and testing.

Split	Variables		Mean	Minimum	Maximum
Training	Input	Cement	377.78	94.00	635.00
		Mineral Admixture	131.42	0.00	390.00
		Water	176.15	45.50	277.00
		Fine aggregate	847.52	532.20	1200.00
		Coarse aggregate	786.41	328.00	1170.00
		Superplasticizer	4.61	0.00	16.00
	Output	Feature compression know (MPa)	45.01	7.17	87.00
Validation	Input	Cement	391.35	130.00	635.00
		Mineral Admixture	130.65	0.00	390.00
		Water	179.51	45.50	277.00
		Fine aggregate	846.37	532.20	1200.00
		Coarse aggregate	769.58	328.00	1170.00
		Superplasticizer	4.14	0.00	16.00
	Output	Feature compression know (MPa)	45.21	21.00	87.00
Testing	Input	Cement	351.56	78.00	635.00
		Mineral Admixture	156.98	0.00	515.00
		Water	177.59	45.50	277.00
		Fine aggregate	832.68	581.00	1200.00
		Coarse aggregate	793.12	502.10	1170.00
		Superplastificizer	4.36	0.00	14.00
	Output	Feature compression know (MPa)	44.34	12.07	78.00

[1–5,10,20,50]; query point weights, which can be uniform (the same for all points) and proportional to the inverse of the distance to the query point, weights = ['uniform', '**distance**']; algorithm used to compute the nearest neighbors, algorithm = ['auto', 'ball_tree', 'kd_tree', '**brute**'].

RF was developed with the following hyperparameters: the number of trees, n_estimators = [2,3,5,10,20,50,100,150,200]; the maximum depth of each tree, max_depth = [2,3,5,10,20,50,100,150,200]; function to measure the quality of splitting a tree, criterion = ['squared_error', '**absolute_error**', 'poisson'].

ERT was developed with the same hyperparameters that were used are RF: the number of trees, n_estimators = [2,3,5,10,20,50,100,150,200]; the maximum depth of each tree, max_depth = [2,3,5,10,20,50,100,150,200]; function to measure the quality of splitting a tree, criterion = ['**squared_error**', 'absolute_error', 'poisson'].

2.4.2. Boosting methods

GB was developed using the hyperparameters: number of boosting stages, n_estimators= [2,3,5,10,20,50,100,150,200,500]; maximum depth in order to limit the number of nodes in the tree, max_depth = [2,3,5,10,20,50,100,150,200]; the learning rate, learning_rate = [0.01, **0.1**, 0.5, 0.6, 0.65, 0.7, 1].

LGBM, the hyperparameters that were adjusted for this algorithm were: number of boosting stages, n_estimators = [5,10,20,50,90,120,200,300,400,500]; number of tree leaves, n_leaves = [5,10,20,50,100,150,200]; the learning rate, learning_rate = [0.01,0.1,**0.25**,0.5,0.75,1].

XGB was developed using the hyperparameters: number of boosting stages, estimators = [2,3,5,10,20,50,100,150,200]; the maximum depth, max_depth = [2,3,5,10,20,50,100,150,200]; the learning rate, learning_rate = [0.01, 0.1, **0.5**, 0.6, 0.65, 0.7, 1].

CB was developed using the hyperparameters: number of iterations of the algorithm, iterations = [50]; maximum tree depth, depth = [2,3,5,10,12,16]; the learning rate, learning_rate = [0.01,0.1,0.25,0.5,0.75,**1**].

2.4.3. GAM models

GAMs models, the hyperparameter used to fit the GAMs was the number of smooth functions, spline. For GAM1 we have n_spile = [5,10,20,50,100,150,200,300,500], and for GAM2 we have n_spile = [5,10,20,50,100,150,200,300,500].

2.5. Metrics for evaluating the performance of machine learning methods

Four statistical performance metrics were utilized to determine the efficiency and accuracy of the predictions of all the machine learning methods used to predict the compressive strength of self-compacting concrete with recycled aggregates: Coefficient of Determination (R^2) (Eq. (2)), Root Mean Square Error (RMSE) (Eq. (3)), Mean Absolute Percentage Error (MAPE) (Eq. (4)) and Mean Absolute Error (MAE) (Eq. (5)) [10,13,25,52].

$$\boldsymbol{R^2} = \mathbf{1} - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y}_i)^2} \tag{2}$$

$$\boldsymbol{RMSE} = \sqrt[2]{\frac{\mathbf{1}}{\boldsymbol{n}} \sum (y_i - \hat{y}_i)^2} \tag{3}$$

$$MAE = \frac{1}{n}\sum|(y_i - \hat{y}_i)| \tag{4}$$

$$MAPE = \frac{100}{n}\sum\left|\frac{(y_i - \hat{y}_i)}{y_i}\right| \tag{5}$$

where, y_i = fck(output variable), $\hat{y_i}$ = fck estimated, $\overline{y_i}$ = mean fck experimental and n = *Total data number*.

Particularly RMSE and MAE have the same units (Mpa) as compressive strength (FCK), while R^2 and MAPE are expressed in percent. The lower values of RMSE, MAE, and MAPE, as well as the higher values of R^2, indicate a good accuracy of the prediction result of the compressive strength prediction of SCC with RA using ML [9,11,33,51].

3. Results and discussion

The capacity of Bagging (KNN, RF, ERT), Boosting (GB, LGBM, XGB, CB), and GAM (GAM1, GAM2) methods to predict the compression strength of SCC with RA for training, validation, and test data set was thoroughly evaluated by the metrics: coefficient of determination (R^2), root mean square error (RMSE), mean absolute percentage error (MAPE) and mean absolute error (MAE). However, the R^2 value also known as the coefficient of determination is observed as the best of them for model assessment [46]. R^2 values from 0.60 and 0.75 indicate satisfactory results, values from 0.75 and 0.95 indicate good model prediction and values above 0.95 indicate excellent prediction, while values below 0.60 indicate unsatisfactory Results [13,52,117]. In addition, sensitivity analysis was also carried out. The results of these analyses are presented in detail in the following sections.

3.1. Predictive performance of machine learning models

3.1.1. Predictive performance of bagging models

Table 4 shows the results of R^2, RMSE, MAE, and MAPE for the training, validation, and test data set values of the Bagging models: K-Neighbor Regressor (KNN), Random Forest (RF), Extretrees Regressor (ERT), for the compression strength of SCC with RA. In general, the errors in the training data set present the adequacy of the developed model, while the errors in the test data present the generalization ability of the developed model. It can be observed that all models: KNN, RF, and ERT, show good concordance with the training data since the coefficients of determination R^2 are all higher than 90%, demonstrating that these models can predict the compressive strength of SCC with RA close to the experimentally determined values.

Comparing the metrics of the KNN, RF, and ERT methods for the test data, in Table 4, it can be observed that Random Forest (RF) outperforms the KNN and ERT models in terms of prediction accuracy and its ability to generalize, by observing a satisfactory value of R^2 = 0.7128, as well as low values of MAE = 0.060 and MAPE, = 13.0784, these are considered satisfactory results to select RF as a good model. Despite the fact that the statistical metrics of the KNN, RF, and ERT models on the testing data do not differ much, Fig. 2(a) shows that the RF model overcomes the other models. Regarding performance, RMSE and MAE values lower than 0.10 indicate a good fit (Fig. 2(b)) in compressive strength prediction [46,117–119].

In Fig. 3, it can be seen that the methods: KNN, RF, and ERT seem to predict well the actual measurements. However, it can be appreciated that for the model performed with RF the predicted values were quite similar to the measured data, this is reflected in the prediction graph where the values are grouped along the prediction line and present less dispersion compared to the KNN and ERT models. These results indicate that RF shas a strong capacity to learn from the training data. In general, it can be said that Random Forest (RF) can predict compressive strength, generating reliable results with a high degree of adequacy compared to the actual values, which is similar to the findings of previous studies [1,120]. The superior performance of the RF model can be attributed to its structure [1].

Table 4
Performance metrics of the proposed Bagging Methods.

Datasets	Metrics	Methods		
		KNN	RF	ERT
Training	R^2	0.9633	0.9388	0.9653
	RMSE	0.0322	0.0415	0.0313
	MAE	0.0130	0.0285	0.0121
	MAPE	2.9935	6.8785	3.0697
Validation	R^2	0.4155	0.5766	0.5066
	RMSE	0.1248	0.1062	0.1147
	MAE	0.0810	0.0739	0.0770
	MAPE	19.6506	17.6191	18.2424
Testing	R^2	0.6832	0.7128	0.6739
	RMSE	0.0848	0.0807	0.0860
	MAE	0.0582	0.0600	0.0586
	MAPE	12.8782	13.0784	13.0738

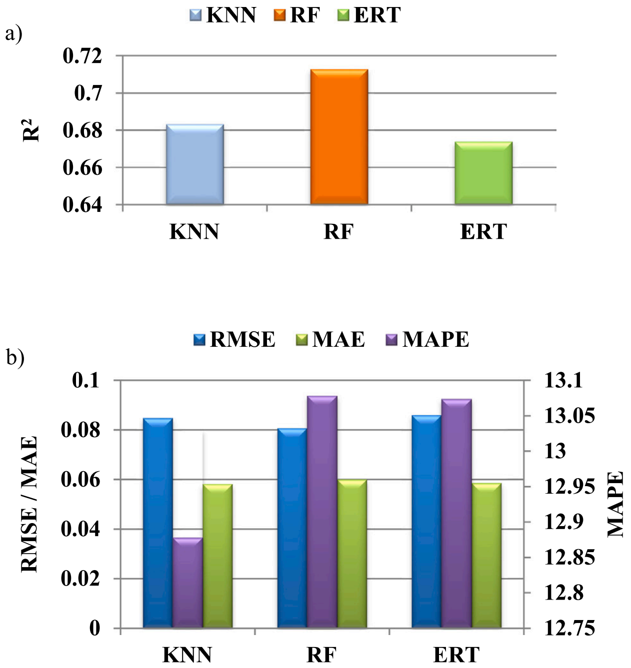

Fig. 2. R^2, RMSE, MAE and MAPE Bagging Methods: (a) R^2, (b) RMSE, MAE and MAPE.

3.1.2. *Predictive performance boosting models*

Table 5 presents a summary of the precision metrics of the Boosting models: Gradient Boosting (GB), Light Gradient Boosting Machine (LGBM), Extreme Gradient Boosting (XGB), Category Boosting (CB), from the training, validation, and test data sets. It can be seen that, in the training data set, the R^2 values for all models were greater than 0.95, so all models show good agreement with the training data. This indicates that these models can perform excellent [13,52,117] projection of the compression strength of SCC with RA.

Now, to evaluate the predictive performance of the model, the metrics are based on the test data set, which serves as a more objective basis for an unbiased evaluation of the model's accuracy in predicting compressive strength. Table 5 shows that, for the test data, in all four models the R^2 values are greater than 0.65, which indicates that these models predict the compressive strength satisfactorily. However, the GB model (Fig. 4) presents an $R^2 = 0.6948$ higher than that of the models: LGBM, XGB, and CB, as well as low values of RMSE = 0.0832, MAE = 0.0569 that indicate a good fit in the predictions by being lower than 0.10 [118,119].

These results can be corroborated in Fig. 5, where it can be seen that for the GB model the estimated values are quite close to the prediction line, these present a lower dispersion than in comparison with the LGBM, XGB, and CB models.

3.1.3. *Predictive performance of GAM models*

Table 6 shows the precision metrics of the GAM models: Inverse Gaussian (GAM1) and Poisson (GAM2), for the training, validation, and test data sets. It can be appreciated that for the training data the GAM1 model presents an $R^2 = 0.3534$, the similar result presents GAM2 with an $R^2 = 0.3630$, these results are unsatisfactory to predict the compressive strength, being values lower than 0.6 [13,52, 117]. Therefore, models GAM1 and GAM2 are poor for projecting the compression strength of SCC with RA.

3.1.4. *Predictive performance of the best machine learning models*

Once the Bagging, Boosting, and GAM models were analyzed, it was obtained as results that the best models to project the compression strength of SCC with RA are the Gradient Boosting (GB) and Random Forest (RF) models. Table 7 presents the metrics of the GB and RF models, where it can be observed that for the training data, both models present R^2 values higher than 0.90, indicating that GB and RF are good predictors of compressive strength [13,52]. However, when evaluating the predictive performance of the models, through the comparison of the metrics for the test data, it can be appreciated that the RF model presents a value of $R^2 = 0.7128$ higher than GB (Fig. 6), as well as low values of MAE = 0.060 and RMSE = 0.0807 that indicate a good fit in the predictions of compressive strength [46,117,119].

Fig. 7 shows how in the RF model the estimated values are more similar to the experimental results, these are grouped along the prediction line, presenting less dispersion concerning the GB predictive model. In summary, the Random Forest (RF) model showed a better prediction capacity, therefore it is considered the best model to predict the compression strength of SCC with RA.

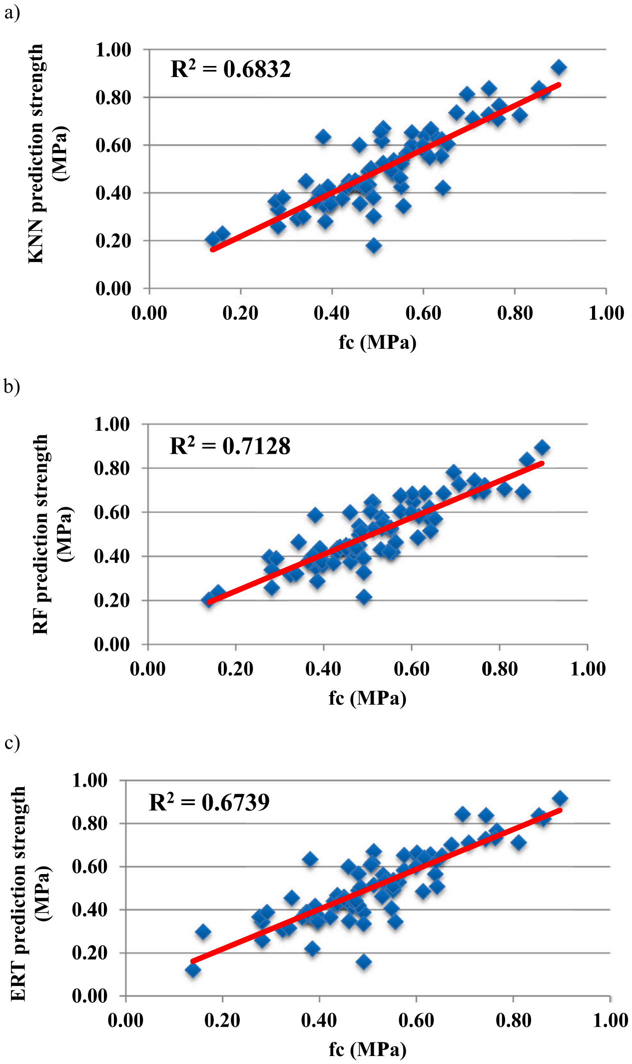

Fig. 3. Comparison of compressive strength prediction with Bagging Methods: (a) KNN, (b) RF, and (c) ERT, from the testing dataset.

Table 5
Performance metrics of the proposed Boosting methods.

Datasets	Metrics	Methods			
		GB	LGBM	XGB	CB
Training	R^2	0.9653	0.9530	0.9648	0.9644
	RMSE	0.0313	0.0364	0.0315	0.0317
	MAE	0.0134	0.0205	0.0148	0.0164
	MAPE	3.1342	4.4857	3.5297	3.8346
Validation	R^2	0.5257	0.5455	0.4783	0.4551
	RMSE	0.1124	0.1100	0.1179	0.1205
	MAE	0.0771	0.0788	0.0791	0.0833
	MAPE	18.2233	18.2537	18.7161	19.7652
Testing	R^2	0.6948	0.6905	0.6643	0.6837
	RMSE	0.0832	0.0838	0.0873	0.0847
	MAE	0.0569	0.0592	0.0595	0.0614
	MAPE	12.8259	13.2913	12.6654	13.6472

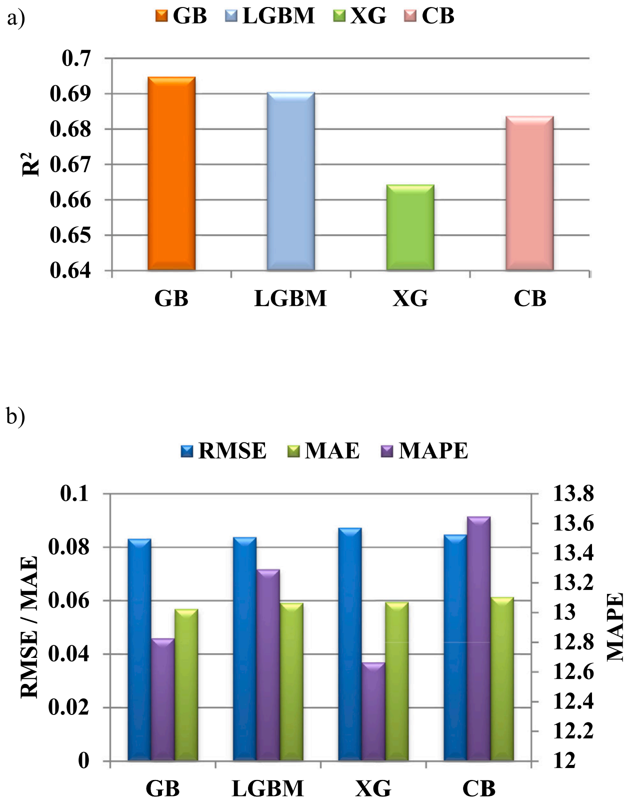

Fig. 4. R^2, RMSE, MAE and MAPE Boosting Methods: (a) R^2, (b) RMSE, MAE and MAPE.

3.2. Sensitivity analysis

Sensitivity analysis is the technique that helps to understand the impact of each input variable on the output variable. Input variables with high sensitivity values have a greater impact on the output variable. According to Ahmad et al. [13], the input variables have a considerable effect on the prediction of the output variable.

To evaluate the contribution of each of the input variables: cement, Mineral admixture, water, fine aggregates, coarse aggregates, and superplasticizers on the uncertainty of the output variable, compressive strength (fck), sensitivity analysis was employed. The sensitivity of compressive strength to each input variable was determined by Eqs. (6) and (7):

$$S_i = \frac{N_i}{\sum_{i=1}^{n} N_i} * 100 \tag{6}$$

$$N_i = f_{max}(x_i) - f_{min}(x_i) \quad , \quad i = 1, \ldots, \quad n \tag{7}$$

where, $f_{max}(x_i) and f_{min}(x_i)$ are the estimated maximum and minimum compressive strength concerning the input variable.

Each of the input variables: cement, mineral admixture, water, fine aggregates, coarse aggregates, and superplasticizers have a significant role in predicting the compression strength of SCC with RA. Fig. 8 shows the results of this sensitivity analysis, it can be seen that cement and water are the most influential input variables in predicting the compression strength of SCC with RA. Cement has a contribution of 28.39% and water of 23.47%. In this regard, Ahmad et al. [13] affirmed that cement is a decisive factor influencing the prediction of compressive strength. On the other hand, it can be appreciated that the input variables: mineral admixture, superplasticizer, and fine aggregates have a contribution in similar levels of 14.51%, 12.61%, and 11.79% respectively. The results of the analysis showed that coarse aggregates (9.23%) are the least effective variable in contributing to the prediction of compressive strength, these results agree with the findings of previous research [21].

4. Conclusion

For the projection of the compression strength of SCC with RA, six input variables were taken into account: cement, water, mineral admixture, fine aggregates, coarse aggregates, and superplasticizer. The predictive ability of the models was evaluated through the following metrics: R^2, RMSE, MAE, and MAPE.

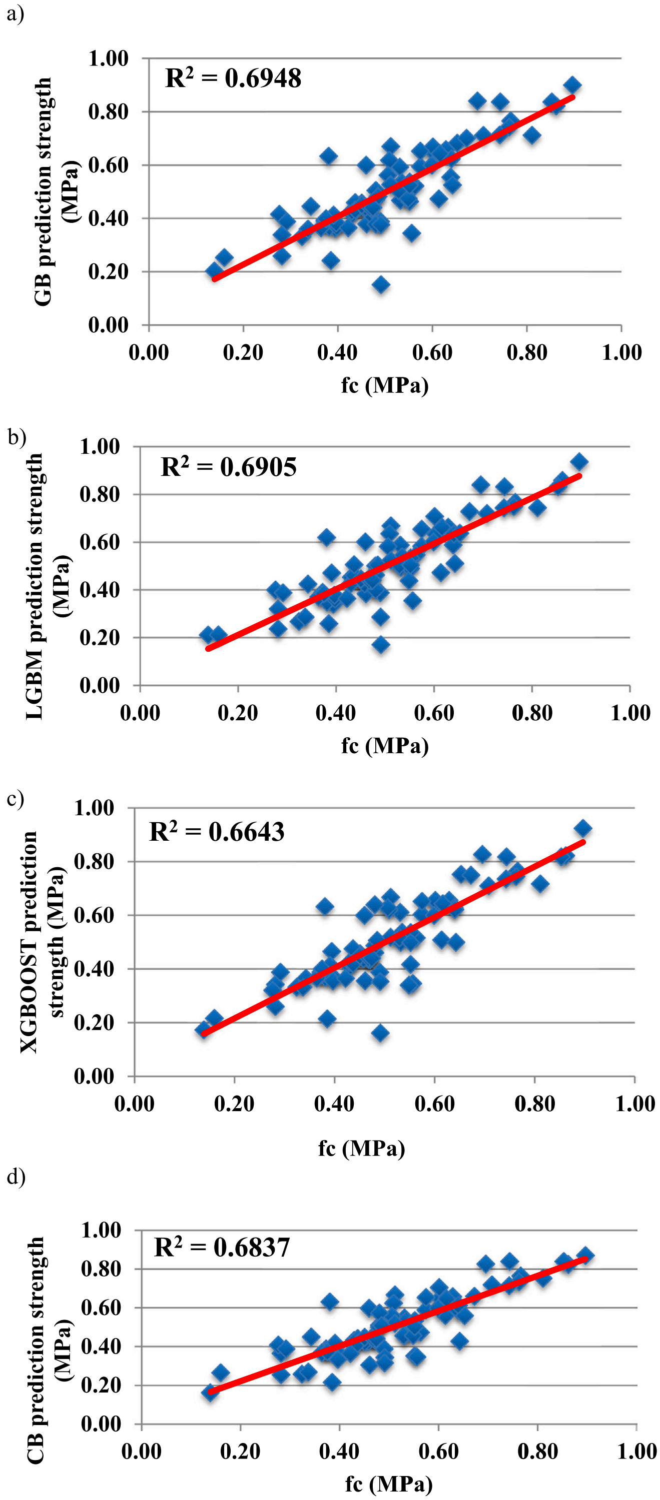

Fig. 5. Comparison of compressive strength prediction with Boosting Methods: (a) GB, (b) LGBM, (c) XGB, and (d) CB, from the testing dataset.

1. This study has described the application of the Bagging models: KNN, RF, and ERT; Boosting: GB, LGBM, XGB, and CB, as well as the GAM models: GAM1 and GAM2 for the projection of the compression strength of SCC with RA. For the development of these models, a database of 515 samples from various experimental studies was obtained and divided into 3 groups: training (70%), validation (15%), and test (%).

Table 6
Performance metrics of the proposed GAM Models.

Datasets	Metrics	Methods	
		GAM1	GAM2
Training	R^2	0.3534	0.3630
	RMSE	0.1351	0.1340
	MAE	0.1073	0.1070
	MAPE	24.8118	25.0538
Validation	R^2	0.2593	0.2755
	RMSE	0.1405	0.1389
	MAE	0.1124	0.1113
	MAPE	23.0691	23.0500
Testing	R^2	0.2722	0.2662
	RMSE	0.1285	0.1290
	MAE	0.0978	0.0989
	MAPE	23.7784	24.2997

Table 7
Performance metrics of the proposed Best Methods.

Datasets	Metrics	Methods	
		GB	RF
Training	R^2	0.9653	0.9388
	RMSE	0.0313	0.0415
	MAE	0.0134	0.0285
	MAPE	3.1342	6.8785
Validation	R^2	0.5257	0.5766
	RMSE	0.1124	0.1062
	MAE	0.0771	0.0739
	MAPE	18.2233	17.6191
Testing	R^2	0.6948	0.7128
	RMSE	0.0832	0.0807
	MAE	0.0569	0.0600
	MAPE	12.8259	13.0784

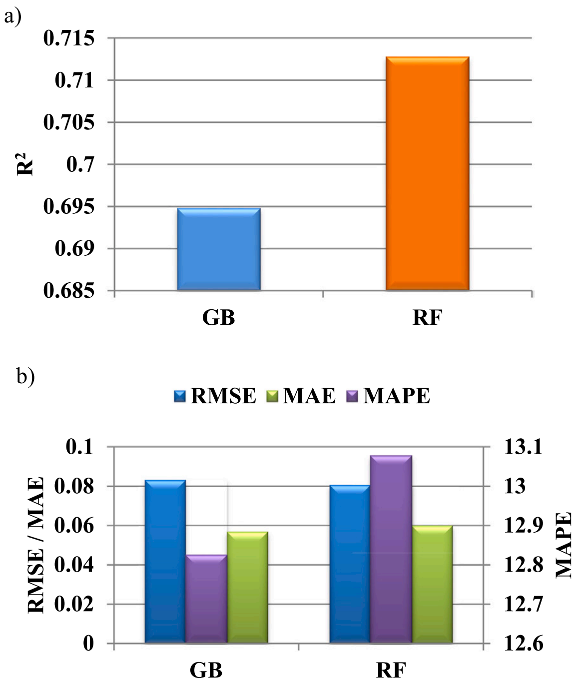

Fig. 6. R^2, RMSE, MAE and MAPE the best Models ML: (a) R^2, (b) RMSE, MAE and MAPE.

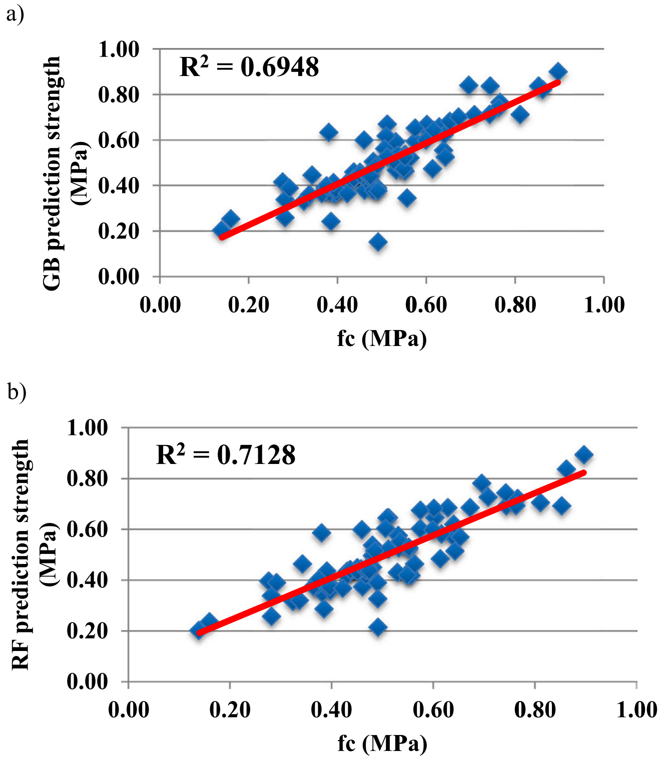

Fig. 7. Comparison of compressive strength prediction with best Models: (a) GB and (b) RF, from the testing dataset.

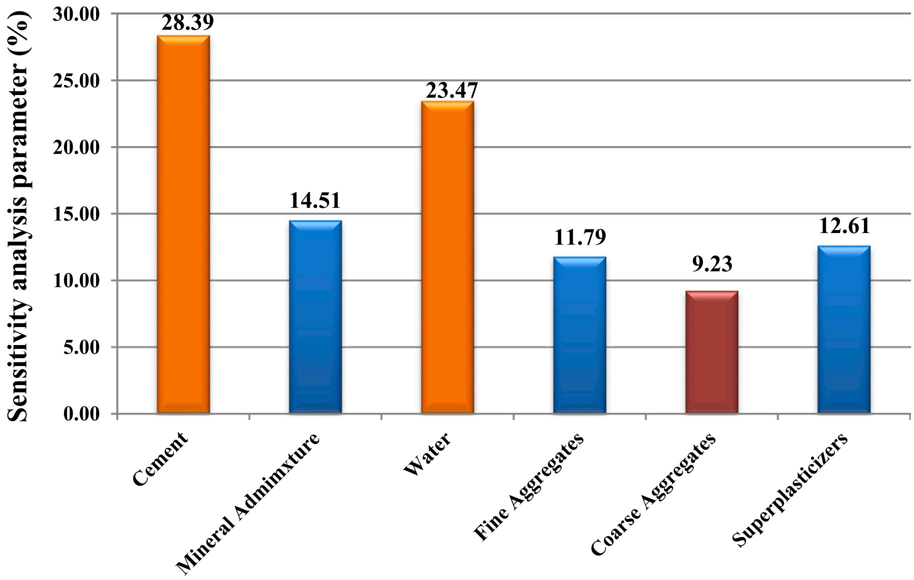

Fig. 8. Contributions of the input variables to compressive strength in the RF model.

2. The results of the test data set showed that the Bagging RF (R^2 = 0.7128, RMSE = 0.0807, MAE = 0.06) and Boosting GB (R^2 = 0.6948, RMSE = 0.0832, MAE = 0.0569) models presented the highest performance with high prediction accuracy. However, it was also evidenced that the GAM1 (R^2 = 0.2722) and GAM2 (R^2 = 0.27662) models are not good models for predicting compression strength, this was proven by the presented values of R^2 being much lower than 0.60.
3. The Random Forest (RF) model (R^2 = 0.7128, RMSE = 0.0807, MAE = 0.06) developed is the best model for the prediction of compression strength, compared to the other models.

4. The sensitivity analysis of the RF model indicates that cement with a contribution of 28.39% is the main variable influencing the compressive strength. In the same context, water is present with a contribution of 23.47% as another important variable in the prediction of compressive strength. On the other hand, the variable with the lowest incidence was coarse aggregate (9.23%). All this indicates that the compressive strength of SCC with RA increases more with cement and water, while coarse aggregate decreases it. On the other hand, mineral admixture, fine aggregates, and superplasticizers contribute modestly to the development of the RF model. Thus, the level of contribution of each input variable is identified by the RF model.

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CRediT authorship contribution statement

Jesús de-Prado-Gil: Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Covadonga Palencia:** Writing – review & editing, Supervision. **Neemias Silva-Monteiro:** Investigation, Writing – original draft, Writing – review & editing. **Rebeca Martínez-García:** Investigation, Writing – original draft, Writing – review & editing, Supervision. All authors have read and agreed to the published version of the manuscript.

Institutional review board statement

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Informed consent statement

Not applicable.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Not applicable.

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