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A New Formulation to Estimate the Elastic Modulus of Recycled Concrete Based on Regression and ANN

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Abstract: A new formulation to estimate the elastic modulus of concrete containing recycled coarse aggregate is proposed in this work using artificial neural networks (ANN) and nonlinear regression. Up to six predictors variables were used to training 243 ANN. The models were generated based on results obtained from experimental campaigns. Feedforward neural network and Levenberg–Marquardt back propagation algorithm were used for training the ANN. The best ANN was found with the architecture 6-4-2-1 (input -1st hidden layer -2nd hidden layer -output), attaining a root-mean-square error of 2.4 GPa associated with a coefficient of determination of 0.91. Once the ANN model was established, 46,656 concrete samples were created. These were employed to formulate the model using nonlinear regression. The developed model showed a highly efficient performance to predict the elastic modulus. Lastly, considering the parametric study conducted, the results pointed out that the approach can be applied to predict the concrete elastic modulus and can indicate better mix proportions for concretes containing natural and/or recycled coarse aggregates, enabling its use as a simulation tool in the development of engineering projects focused on durability and sustainability.

Keywords: machine learning; artificial neural networks; nonlinear regression; elastic modulus; recycled aggregate concrete

1. Introduction

Civil construction is one of the sectors that most contribute to cities' development and economic growth. However, it also produces a large amount of waste and emits air pollutants. China, for example, generates an average of 2 billion tons of construction waste per year, followed by the United States of America, with an average ranging between 200–300 million tons per year [1,2]. Thus, alternative materials that minimize environmental damage are used, such as construction and demolition wastes (CDW) as aggregate to produce new concretes [3,4]. Nevertheless, its employability in structural components is reduced due to some differences in composition and properties of recycled aggregate (depending on the sorting process carried out at the CDW or on the recycling technique used) that alter the mechanical behavior of concrete and oppose the inherent sustainability benefits [5–7].

One of the main differences between recycled aggregate concrete (RAC) and natural aggregate concrete (NAC) is the greater porosity of RAC, which results in greater water absorption and interferes in the mortar quality adhered to the aggregate surface [8]. Mortar directly influences the mechanical properties of concrete, such as its compressive strength and elastic modulus [6,9].

The elastic modulus is considered one of the most important mechanical parameters. It is used to design concrete structures, in the same way that other parameters, such as the compressive strength and the Poisson coefficient, also are. The elastic modulus quantifies

the concrete's potential to deform elastically. In general, concretes with recycled aggregate present a lower elastic modulus than concretes with natural aggregate at the same water/cement ratio and proportions of the other constituent materials [10,11]. Conventional determination of concrete elastic modulus consists of a destructive technique in which material samples are subjected to loading tests to generate the stress–strain curve. Nowadays, there are alternative non-destructive techniques to estimate the elastic modulus, such as the ultrasonic pulse technique [12] and predictive formulations based on experimental results [13–24].

Most formulations and proposed models are based on regressions [13–20] or, in a more complex way, on solving equations that represent the mechanical behavior of composite materials [21–24]. More sophisticated models were developed using the theory of elasticity, concrete rheology, and mechanics of composite solids [25–29]. These models were determined considering concrete as a two/three-phase material.

With the computational advance, numerical models were developed throughout the years, reducing the uncertainties of analytical formulations and increasing their application's domain. In particular, over the last decade, the finite element method (FEM) started to be used in the analysis and modeling of the mechanical behavior of concrete structure in macro and/or mesoscale [30–38].

However, in some situations, it becomes difficult and complex to consider all the several factors that interfere with the elastic modulus. Added to that, when a larger number of parameters is applied, it results in a low-reliability modulus from extrapolation or in the generalization of the models. A viable and reliable alternative to circumvent the difficulties in evaluating the concrete elastic modulus is artificial neural networks (ANNs), since they can model complex problems, where multiple and nonlinear relationships between input and output are needed to map the problem [39,40].

Hammoudi et al. [41] and Kandiri et al. [42] report that efficient models to predict the elastic modulus of concrete with different aggregate types and distinct additions can be obtained by an ANN due to its ability to learn complex and nonlinear problems.

An ANN is described by a numerical structure similar to biological networks (Figure 1), which guarantees the ability to simulate basic characteristics of a nervous system, such as learning, patterns classification, and data processing [43].
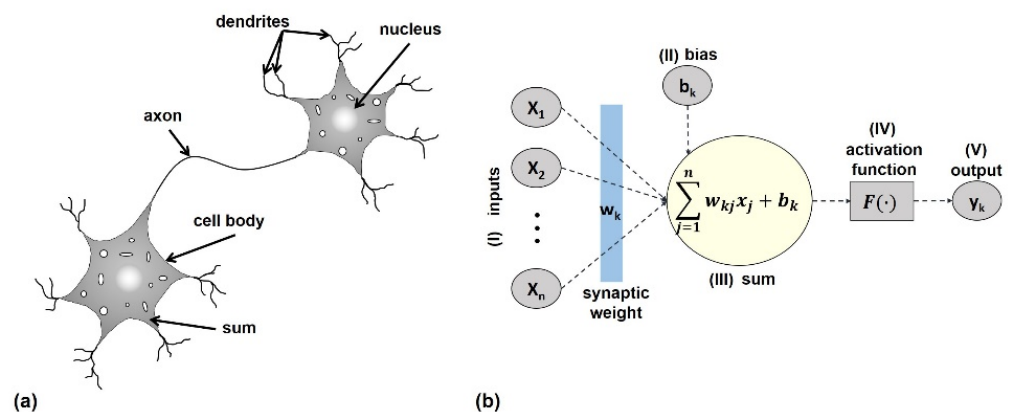

Figure 1. Representation of: (**a**) biological neuron and (**b**) perceptron artificial neural network.

One reason why neural networks spread out is the backpropagation training algorithm [44]. This algorithm can be easily implemented based on the downward gradient optimization technique. Due to its simplicity, most developed works in civil engineering employ it [45–50].

The first publication about machine learning in civil engineering was made by Adeli and Yeh [51]. The authors presented an artificial neural network of perceptron type (networks without hidden layers) to create a design model for steel beams. Many studies were published after that, most of them focused on pattern recognition and function mapping [52–59].

Moselhi et al. [52] analyzed the artificial neural networks' applicability to model problems related to the real estate market in different house flipping scenarios. Subsequently, in the same line of research, Chao and Skibniewski [53] and Li et al. [54] have shown that an ANN is capable of analyzing and estimating workforce productivity in the construction sector.

The largest number of ANN applications in civil engineering are found in structural engineering and materials science. In structural engineering, neural networks have been employed for the design and the analysis of structural components [55,56], in the study of structural optimization [57,58], dynamic analysis of structures due to earthquakes [45], and risk and damage monitoring [60,61].

In materials science, several studies have been developed to estimate mechanical properties, especially of concrete, such as compressive strength [62–64] and the elastic modulus [65–70].

Duan et al. [66] employed an artificial neural network to estimate the elastic modulus of concretes made with recycled aggregate. The authors used 324 data collected from different works and demonstrated the ANN's efficiency through comparison between predicted values and results from formulations in design standards.

Awoyera et al. [68] developed models based on machine learning to predict the elastic modulus of concretes made with geopolymer cements, in which they verified that the ANN was more efficient than other techniques.

Yoon et al. [69] used neural networks with a backpropagation training algorithm to obtain the elastic modulus of concretes made with lightweight recycled aggregate. The authors carried out a convergence analysis to select the best topology for the ANN and observed that, for this kind of problem, a maximum of four hidden layers were required. Moreover, they observed that the water/cement ratio, the cement consumption, and the aggregate/cement ratio have great influence on the network's learning.

Even though the use of ANNs to forecast the elastic modulus of concrete has increased, most of them are not used in practice by an engineer from the construction sector because they require prior knowledge about artificial neural networks. Therefore, some propose user-friendly software or even an analytical formulation based on a model generated by an ANN [70,71].

In this context, in this research, the possibility of applying machine learning coupled with nonlinear regression was evaluated in order to obtain a new formulation to estimate the elastic modulus of concretes containing recycled aggregate from construction and demolition waste, with a distinct replacement ratio (0–100%). Nonlinear regression is a form of regression analysis in which observational data are modeled by a function that is a nonlinear combination of the model parameters and depends on one or more independent variables. The data are fitted by a method of successive approximations.

Therefore, the possibility of applying machine learning coupled with nonlinear regression to obtain a new formulation to predict the elastic modulus of concretes containing natural and recycled aggregate was evaluated. Artificial neural networks, which have the best learning power among various machine learning models, were applied. The main novelty of this work refers to the methodology employed in the development of the analytical formulation, which uses artificial neural networks coupled with nonlinear regression. The regression modeling considered a dataset generated with the ANN that efficiently mapped the elastic modulus of concrete from the following predictor variables: cement consumption, water/cement ratio, replacement ratio of recycled coarse aggregate, fine aggregate/cement ratio, total aggregate/cement ratio, and coarse aggregate/cement ratio. The model was developed considering predictor parameters that are easy to obtain and do not require destructive testing.

In the second section, a brief description of artificial neural networks' main characteristics and functionalities is presented. In the third section, the methodology is detailed, and the process of ANN training and its use to generate the database for the development of the analytical formulation with nonlinear regression is described. In the fourth section,

the modeling results and the developed analytical formulations are presented. Finally, conclusions are presented in the fifth section.

2. Artificial Neural Networks

Artificial neural networks are inspired by biological neural networks and excel in data mining [72]. Artificial neural networks are parallel and distributed systems, composed of simple processing units called artificial neurons, similar to the structure of the human brain, which allow superior performance to that of conventional models [73].

Haykin [74] reports that an ANN presents five basic elements that resemble the biological ones:

I.   An input set x_j carrying its respective synaptic weight, w_{kj};
II.   An adder $\sum$ to the weighted input signals;
III.   An activation function, $F(\cdot)$, to bound the output amplitude;
IV.   A bias b_k to increase or decrease the net input of the activation function (a horizontal translation of the activation function graph);
V.   An output of the network y_k (see Figure 1b).

In general, a k neuron output of an ANN can be evaluated by Equation (1):

$$y_k = F\left(\sum_{j=1}^{n} w_{kj}x_j + b_k\right) \tag{1}$$

where y_k represents the k neuron output, F is the activation function, w_{kj} are the synaptic weights, x_j represents the inputs, and b_k refers to the bias.

Every network must go through a learning process to map and approximate a function, and the most used is the supervised learning process [75]. The name "supervised" holds for the network that is initially controlled by a supervisor, who presents the data to the ANN, which has the objective of finding a relation between input–output pairs.

The supervised training method used in this study was the "feedforward backpropagation" [74], the same training method used by Yoon et al. [69] to develop a model to predict the elastic modulus of concrete made with recycled aggregate. Considering a nonlinear mapping, in this work a multilayer perceptron (MLP) was utilized. The MLP is a supplement of feedforward neural networks that consists of three or more layers, as shown in Figure 2.
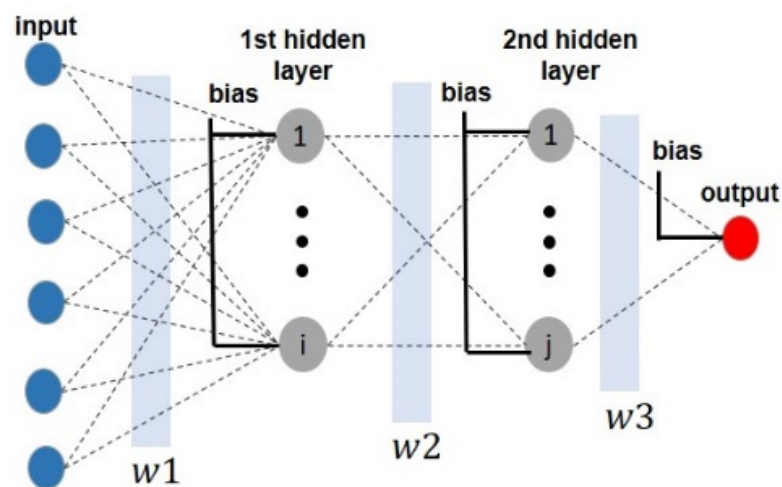

Figure 2. Representation of an MLP artificial neural network.

3. Model Development

In order to determine a predictive model for the elastic modulus of concretes containing natural and recycled aggregates, the methodology presented in the flowchart of

Figure 3 was followed. A program developed in C++, which has already been validated and employed in other work by the authors [47,48,50], was used to train the ANN.
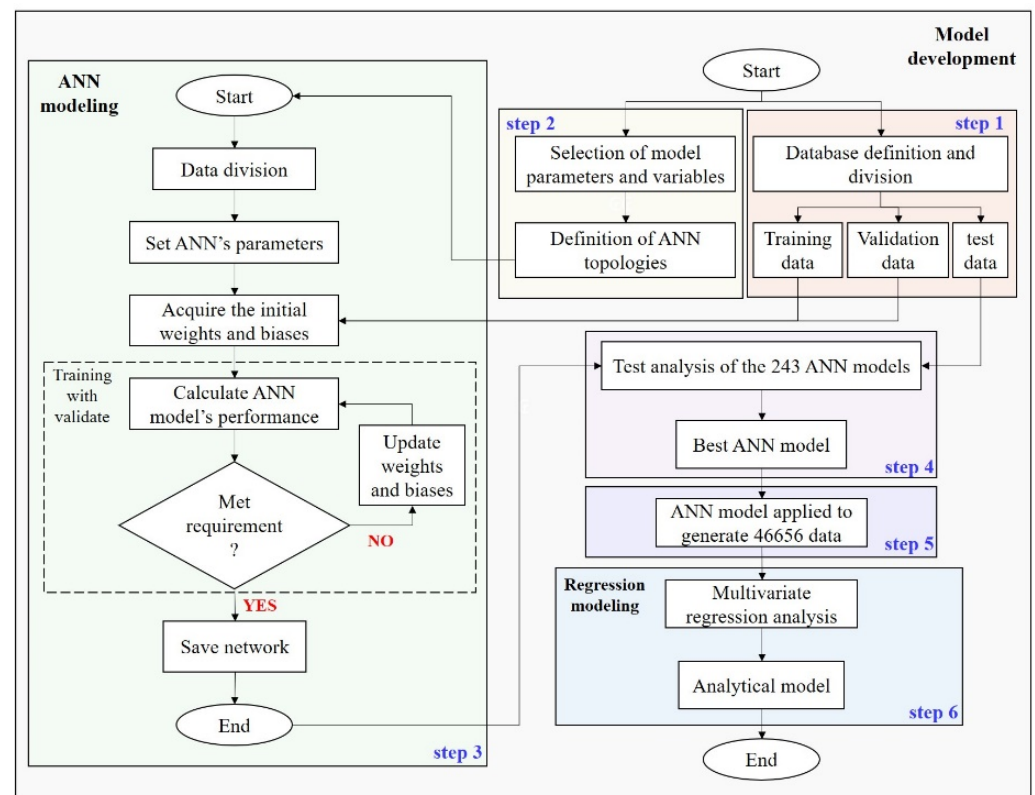

Figure 3. Flowchart of the adopted methodology.

As seen in Figure 3, in the first step, a database was created from experimental data available from several references [11,20,76–103] regarding the elastic modulus of concrete made with coarse aggregate from construction and demolition waste (CDW). The database is divided into three sets: the training set (60% of the database), the validation set (20% of the database), and the testing set (20% of the database). Training, validation, and testing data were randomly selected, and no changes were made afterwards. In the second step, a statistical analysis was carried out to evaluate the data distribution. The input parameters were selected, and three ANN topologies were proposed for the training process.

In the third step, training and validation of the selected networks were carried out. The network with the best performance was identified in the fourth step. Afterwards, in the fifth step, input parameters were randomly generated following statistical distribution built in the second stage. The network selected in the fourth step is used to establish the associated outputs. Thus, a new and large dataset is generated.

At last, the new dataset is used to formulate an analytical model by multivariable and nonlinear regression in the sixth step. The proposed model is then evaluated in a parametric study and compared with the initial dataset.

3.1. Database Definition

The first and main stage for the development of an ANN model is the definition of a consistent database with reliable and representative data. Thus, the database of this study was assembled considering thirty experimental campaigns of the last 20 years [11,20,76–103]. All the concrete samples were produced with Portland cement and cured under normal conditions for 28 days, when the value of the elastic modulus of the concrete was determined.

In this study, the effect of fine aggregate replacement by recycled aggregate as well as the influence of supplementary cementitious materials in the concrete mix proportions were not considered. The following characterizes the concrete mixture proportions: cement consumption (CC), water/cement ratio (WCR), replacement of natural aggregate by recycled coarse aggregate ratio (RCA), fine aggregate/cement ratio (FACR), total aggregate/cement ratio (TACR), and coarse aggregate/cement ratio (CACR). FACR, TACR, and CACR were defined in weight ratio, and the RCA was defined as a volume replacement of natural aggregate by recycled aggregate, following Behnood et al. [3].

It is well known that the characteristics of the natural and recycled aggregate are relevant to the value of elastic modulus, as indicated by Butler et al. [96] and Etxeberria et al. [80]. Butler et al. [96], for instance, showed that the recycled coarse aggregate from different sources could have different effects on the properties of concrete made with recycled coarse aggregate. Additionally, the amount of impurity in the recycled aggregate, the processing condition, and the moisture condition could affect the mechanical properties of the concrete produced with these aggregates. However, a regression analysis was conducted, considering that the dataset used in the present study showed that the amount and type of impurities were not significant. Similar results were found by Behnood et al. [3]. These results pointed out that the amount and type of aggregate impurities were not statistically significant when generating their predictive model for the elastic modulus of concrete made with recycled aggregate. Results in this sense should be analyzed thoroughly, especially in practical applications, as shown in Gao et al. [104], where the authors developed a study in which a framework was proposed to overcome industry barriers to producing recycled mixture.

The database containing 412 records of concretes produced with natural or recycled coarse aggregates (from CDW) and with elastic modulus between 20 and 45 GPa was divided into three subsets: one for training (60% of the data), one for validation (20% of the data), and another for testing and performance assessment (20% of the data). This subdivision aimed to minimize network overtraining and to increase the model's applicability domain. All these datasets were created considering fixed data from the experimental database.

3.2. Statistical Analysis of the Data

Throughout the modeling process, the proper compilation of the model's variables is extremely important since inappropriate selection could prevent the ANN from process information, including mapping input and output data [74,75].

Therefore, a dispersion analysis on the database of the elastic modulus (E_c) was carried out, considering the influence of the available parameters, such as CC, WCR, RCA, FACR, TACR, and CACR. In every analysis, correlation coefficients of Pearson "P" (Equation (2)) and Spearman "S" (Equation (3)) were determined, as well as the average, the standard deviation, the minimum value (Min), the first quartile (Q1), the median, the third quartile (Q3), and the maximum value (Max). Table 1 presents the statistical parameters and Figure 4 shows the frequency distribution curves.

$$\rho = \frac{\sum_{i=1}^{n}(x_i - x_m)(y_i - y_m)}{\sqrt{\sum_{i=1}^{n}(x_i - x_m)^2}\sqrt{\sum_{i=1}^{n}(y_i - y_m)^2}} \tag{2}$$

$$\rho_s = \frac{cov(rg_X, rg_Y)}{\sigma(rg_X)\sigma(rg_Y)} \tag{3}$$

where x_i and y_i are the variables analyzed, x_m and y_m are the average values, $cov(\circ, \circ)$ is the covariance function, $\sigma(\circ)$ is the standard deviation function, and rg_X and rg_Y are the rank variables of X and Y.

Table 1. Statistical parameters.

Parameter	Average	Standard Deviation	Min	Q1 (25%)	Median	Q3 (75%)	Max	p	S
CC (kg/m³)	376.60	59.96	247.00	333.63	380.00	401.00	512.50	0.27	0.27
WCR (-)	0.49	0.07	0.25	0.45	0.50	0.55	0.68	−0.42	−0.37
CACR (-)	2.81	0.54	1.47	2.48	2.70	3.18	4.28	−0.08	−0.07
RCA (%)	51.67	20.18	0.00	18.19	48.60	79.10	100.00	−0.52	−0.54
FACR (-)	1.98	0.54	0.97	1.64	1.94	2.20	4.17	−0.19	−0.17
TACR (-)	4.79	0.94	3.01	4.19	4.52	5.30	7.40	−0.16	−0.15
E_c (GPa)	29.40	4.93	19.93	25.81	28.86	32.30	44.66	-	-
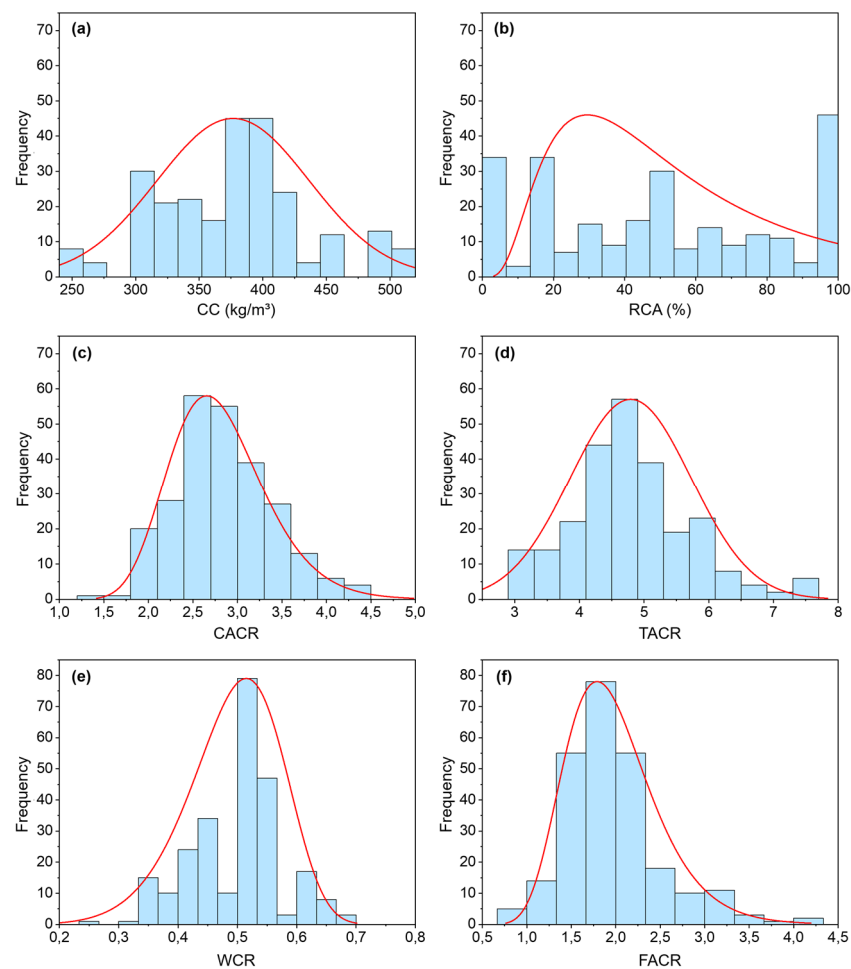
Figure 4. Distribution of: (**a**) CC, (**b**) RCA, (**c**) CACR, (**d**) TACR, (**e**) WCR, and (**f**) FACR.

The data dispersion and the correlation coefficients presented in Figure 4 and Table 1 enable a description of how to spread out a set of data and suggest whether they could be represented by simple functions, such as normal, log-normal, logistic, and exponential functions. Thus, the data dispersion and the correlation coefficients identified (i) an inverse relationship between the WCR and the elastic modulus; (ii) increases in the elastic modulus as the CC increases; (iii) a small inverse correlation of the TACR with the elastic modulus; and (iv) an inverse relation of 0.52 between the elastic modulus and the RCA, therefore indicating that as the RCA increases, the mechanical property decreases.

It was noticeable that the WCR, the RCA, and the CC would have a great influence on the predictive model, as indicated by the values of the correlation coefficients presented in Table 1. However, since neural networks can map complex and nonlinear relations, all variables at disposal in the database were used, letting the neural network choose the best parameters.

3.3. ANN Training and Parameters Definition

For network training and, consequently, mapping of the elastic modulus of concrete, some ANN topologies were created with different numbers of neurons in the input layer (from four up to six input parameters) and by the number of neurons present in each of the two hidden layers used (from one up to nine), as recommended by Felix at al. [50], in which the authors relate that no more than two hidden layers containing up to nine neurons are necessary to map complex problems, such as the mechanical parameters of concrete. All the ANN topologies utilized in the training process can be seen in Figure 5.
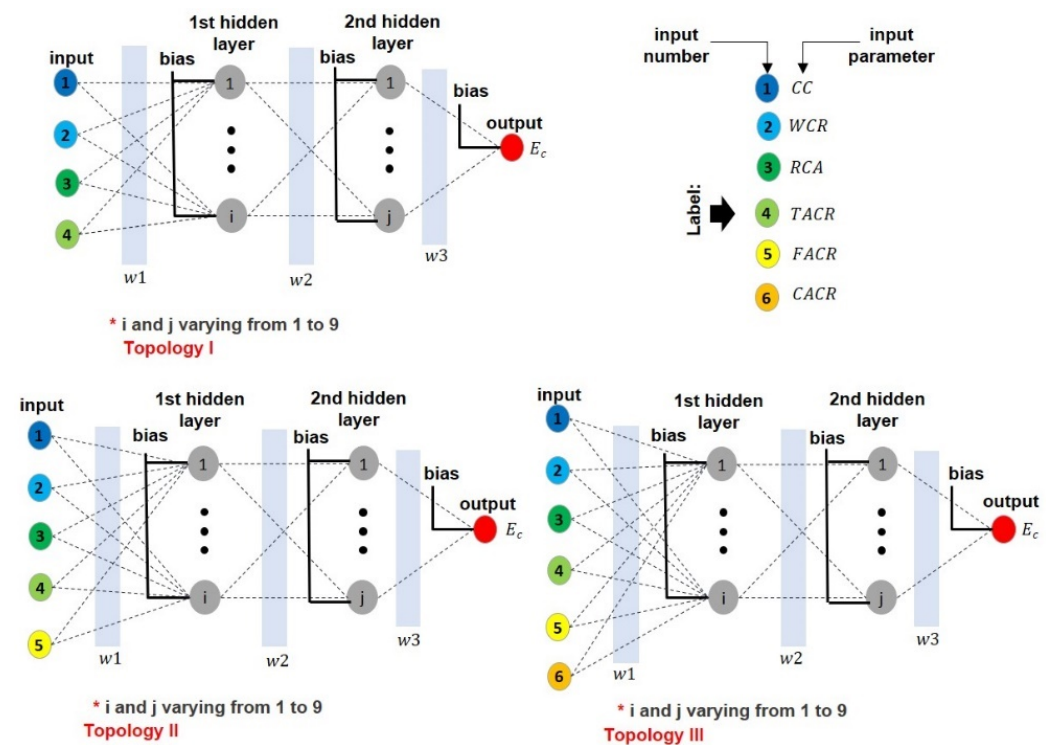

Figure 5. ANN topologies adopted in the training process.

For the training process, a bipolar sigmoid function was adopted. As the network learning is supervised with the backpropagation training algorithm, a learning rate must be established since it is directly related to the network convergence. The learning rate adopted was 0.35, as indicated in Felix et al. [48]. Training and validation were performed simultaneously in order to prevent overtraining—when the network perfectly maps the training set data but is unable to interpolate the validation data, resulting in a low performance index [75,105,106]. Training and validation were performed using the same dataset for every ANN topology. As convergence criteria, root-mean-square error (RMSE—Equation (4)) was used. Additionally, training was interrupted when the number of interactions exceeded 105. The networks were created and trained using the computational package project-yapy, developed in C++ [107].

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - t_i)^2} \tag{4}$$

where y_i refers to network estimated values, t_i represents known values (targets), and n is the amount of data used in the analysis.

3.4. Regression

For the development of an analytical formulation to estimate the elastic modulus of concrete, multivariable statistical analysis using linear, polynomial, rational, and exponen-

tial regressions was adopted. This method was chosen to obtain nonlinear relationships among multiple variables at the same time—namely, the input variables and the elastic modulus [85–94].

A robust dataset (46,656 samples) was determined using the ANN model previously created, and it was employed in the nonlinear regression modeling. Input variables were randomly generated following its distribution (see Figure 4) to assemble a dataset similar to the experimental database.

A function base that represents the analytical formulation was defined considering the statistical analysis, which employed correlation coefficients between the selected input parameters and the concrete elastic modulus. It was verified that, when the RCA is combined with the CC, WCR, CACR, or FACR, the correlation with the elastic modulus increases. However, the TACR presented a better correlation with the elastic modulus when analyzed by itself (see Equation (5)).

$$
\begin{aligned}
E_c = \beta_0 + f_1(CC, RCA){\cdot}\beta_1 + f_2(WCR, RCA){\cdot}\beta_2 + \\
+ f_3(CACR, RCA){\cdot}\beta_3 + f_4(FACR, RCA){\cdot}\beta_4 + f_5(TACR){\cdot}\beta_5 + \varepsilon
\end{aligned}
\tag{5}
$$

where β_0 is a constant; $\beta_1, \beta_2, \beta_3, \beta_4$ and β_5 are parameters associated to the RCA, CC, WCR, CACR, FACR, and TACR, respectively; and ε represents the adjustment error. Functions f_1, f_2, f_3, f_4 and f_5 describe the relation of two parameters with the elastic modulus and were selected among the following functions: linear (Equation (6)), polynomial (Equation (7)), exponential (Equation (8)), rational (Equation (9)), or composite (Equations (10)–(12)).

$$
f(x,y) = \alpha_0 + \alpha_1 x + \alpha_2 y
\tag{6}
$$

$$
f(x,y) = \alpha_0 + \alpha_1 x + \alpha_2 y + \alpha_3 x^2 + \alpha_4 y^2
\tag{7}
$$

$$
f(x,y) = \alpha_0 + \alpha_1 e^{(\alpha_2 x)} + \alpha_3 e^{(\alpha_4 y)}
\tag{8}
$$

$$
f(x,y) = \frac{\alpha_0 + \alpha_1 x + \alpha_2 y}{\alpha_3 + \alpha_4 x + \alpha_5 y}
\tag{9}
$$

$$
f(x,y) = \alpha_0 + \frac{\alpha_1 x + \alpha_2 y + \alpha_3 x^2 + \alpha_4 y^2}{\alpha_5 + \alpha_6 x + \alpha_7 y + \alpha_8 x^2 + \alpha_9 y^2}
\tag{10}
$$

$$
f(x,y) = \frac{\alpha_0 + \alpha_1 e^{(\alpha_2 x)} + \alpha_3 e^{(\alpha_4 y)}}{\alpha_5 + \alpha_6 x + \alpha_7 y + \alpha_8 x^2 + \alpha_9 y^2}
\tag{11}
$$

$$
f(x,y) = \frac{\alpha_0 + \alpha_1 x + \alpha_2 y + \alpha_3 x^2 + \alpha_4 y^2}{\alpha_5 + \alpha_6 e^{(\alpha_7 x)} + \alpha_8 e^{(\alpha_9 y)}}
\tag{12}
$$

where α_i are parameters of the multivariable data analysis.

Figure 6 shows, in a simplified way, a flowchart of the multivariable regression analysis, a methodology similar to Santana et al. [108]. In the first step, the objective of the analysis is defined, which is to predict the elastic modulus of concretes made with natural and recycled aggregates. In this very same step, the variables and constraints are set up.

In the second step, the format of functions f_1 to f_5 in Equation (5) are defined using one of Equations (6)–(12). Whichever equation better represents the relation of the current parameter with the elastic modulus is selected. Adjustments to coefficients α_i and β_i are made in the third step using least squares and backward elimination [109]. Terms that do not contribute to the model are removed, as long as the removal does not decrease the accuracy of the adjustment. This step is repeated until the convergence of coefficients α_i and β_i. In the last stage, results obtained with the proposed model are compared with the experimental database [11,20,76–103].
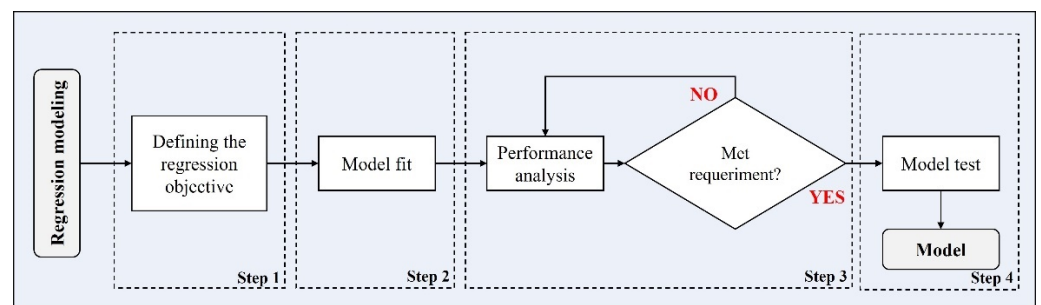
Figure 6. Flowchart of the multivariable regression process.

4. Results and Discussion

The development of the formulation was performed using two modeling techniques. ANN was first used to map the elastic modulus of concrete containing coarse recycled aggregate. Once trained and validated, many samples were generated. Then, this new dataset was employed to create an analytical formulation using multivariable and nonlinear regression. Hence, the results regarding the application of ANN and nonlinear and multivariable regression are presented below. Afterwards, a parametrical study of the proposed formulation is presented to demonstrate its applicability.

4.1. Analysis of the ANN Modeling

After ANN training, a performance analysis was conducted to select the optimum number of neurons in the hidden layer for each of the adopted topologies, represented in Figure 5. Fifteen models were selected regarding the RMSE obtained in training and validation stages. These results are shown in Table 2, where the maximum error (E_{max}) and coefficient of determination (R^2) are also included.

Table 2. ANN performance for training and validation stages.

Topology	Training			Validation		
	RMSE (GPa)	E_{max} (GPa)	R^2	RMSE (GPa)	E_{max} (GPa)	R^2
[4-6-2-1] *	3.62	4.74	0.96	3.60	5.28	0.87
[5-6-2-1] *	3.58	4.69	0.96	3.53	5.47	0.84
[5-3-2-1] *	3.61	5.31	0.89	3.49	5.05	0.87
[4-3-3-1] *	3.61	6.34	0.85	3.45	5.91	0.83
[5-4-2-1] *	3.72	5.33	0.90	3.29	4.86	0.89
[6-6-4-1] *	3.37	4.69	0.92	3.41	4.74	0.90
[6-7-3-1] *	3.29	4.28	0.96	3.18	4.30	0.91
[6-5-2-1] *	3.18	4.28	0.94	3.29	4.39	0.92
[6-6-3-1] *	3.23	4.23	0.96	3.19	5.03	0.83
[6-5-4-1] *	3.14	4.11	0.96	3.10	4.56	0.87
[6-5-3-1] *	3.09	4.07	0.95	3.12	4.52	0.87
[6-7-5-1] *	2.98	3.89	0.96	3.12	4.90	0.83
[6-4-3-1] *	2.97	3.88	0.96	3.05	4.96	0.82
[6-5-4-1] *	2.91	3.91	0.94	3.07	4.26	0.90
[6-4-2-1] *	2.81	3.79	0.95	2.48	3.20	0.92

* [x-y-w-z] 4-layer topology, where x indicates the input number, y the neuron number in the first hidden layer, w the neuron number in the second hidden layer, and z the output number.

Most ANNs presented good results for R^2, RMSE, and E_{max}, but their values worsen when training and validation stages are compared, as can be seen in Figure 7. This remarks the importance of cross-validation in any ANN training process.
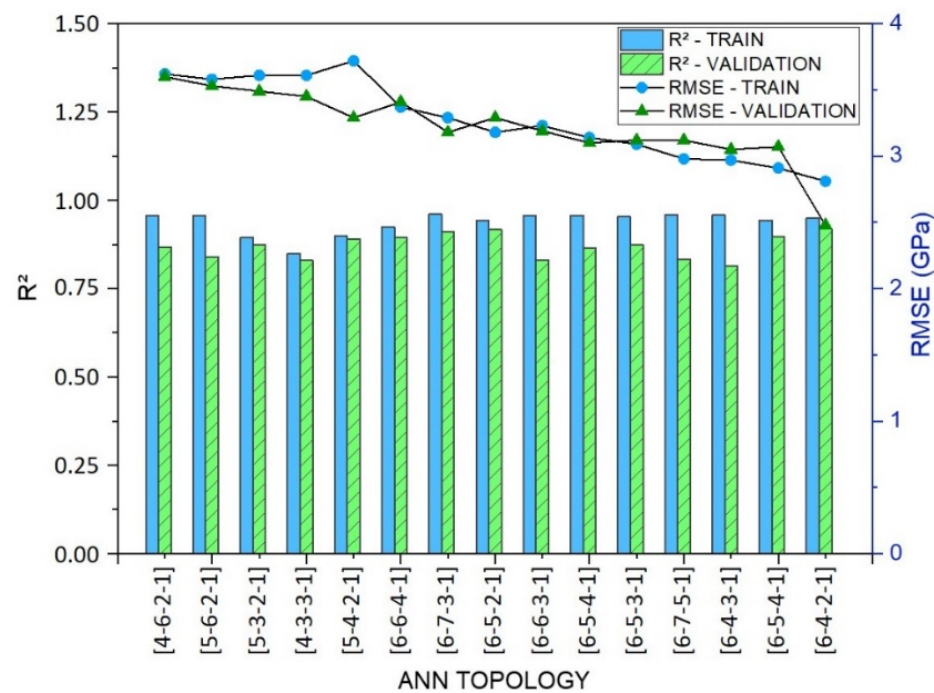
Figure 7. Performance in the training and validation stage to the 15 best ANN topologies.

As shown in Figure 7 and Table 2, the ANN achieved good performance in the training processes. The results point out that the variables cement consumption—CC, water/cement ratio—WCR, replacement of natural aggregate by recycled coarse aggregate ratio—RCA, and total aggregate cement ratio—TACR, would have a great influence on the prediction model and that they are very important to consider as predictor parameters of the prediction model. However, it is possible to observe that when more variables are introduced, such as the fine aggregate cement ratio—FACR and the coarse aggregate cement ratio—CACR, the results are improved, demonstrating that ANN performance can be improved when the number of predictor parameters increases since they are thus more representative.

Figure 8 shows the mapping performance for the best ANN of each basic topology used in this work (topologies that can be seen in Figure 5). Additionally, Figure 8 indicates the coefficient of determination of each ANN for the training and validation stages.

As seen in Figure 8, the ANN [4-3-3-1], [5-4-2-1], and [6-4-2-1] presented the optimum number of neurons in the hidden layer for the three basic topologies—those with a different number of input parameters, as shown in Figure 5. To select the topology that best maps the elastic modulus of concrete containing natural and recycled coarse aggregates, the results presented in Figure 8 and Table 2 were analyzed, where the performance parameters obtained in the training and validation stages were compared.

The ANN with the topology [6-4-2-1] was selected with the best performance, where the coefficient of determination was 0.95 and 0.92 in the stages of training and validation, respectively. The maximum error of this ANN was 3.79 and 3.20 GPa in the training and validation stages, respectively.

Finally, is it necessary to test the model with regard to its potential for generalizability. Haykin [74] and Patterson [75] relate that if the ANN performs well on the data that it has not trained on, it can be said that it has generalized well to the given data. Considering that, Figure 9 shows the good performance obtained with the model application in the test analysis, where the analysis was performed with experimental results collected from the literature. The results point out the model's generalizability and that it is able to estimate the elastic modulus of concrete containing recycled aggregate from construction and demolition waste.
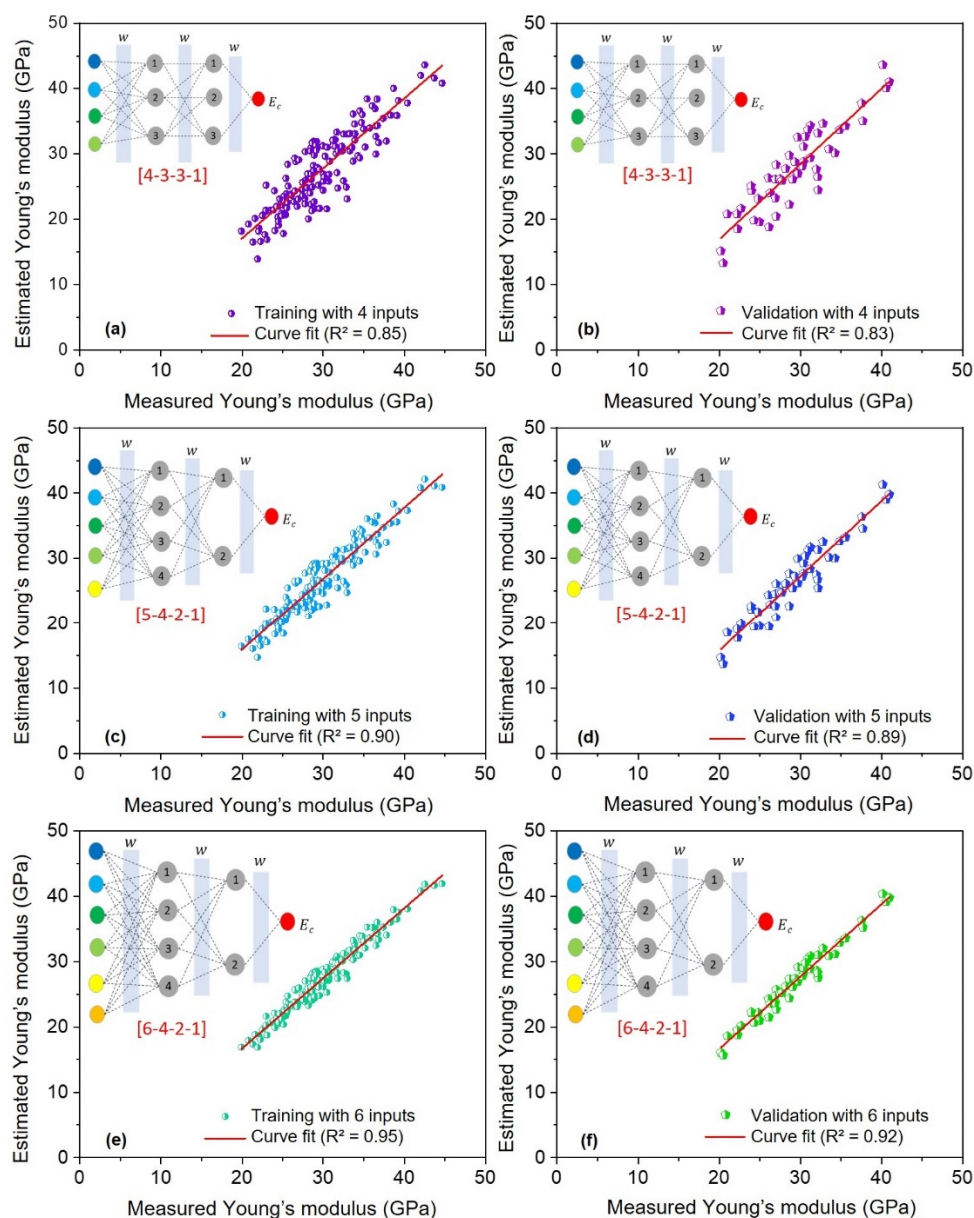
Figure 8. Coefficient of determination of: (**a**) training and (**b**) validation of ANN [4-3-3-1]; (**c**) training and (**d**) validation of ANN [5-4-2-1]; (**e**) training and (**f**) validation of ANN [6-4-2-1].
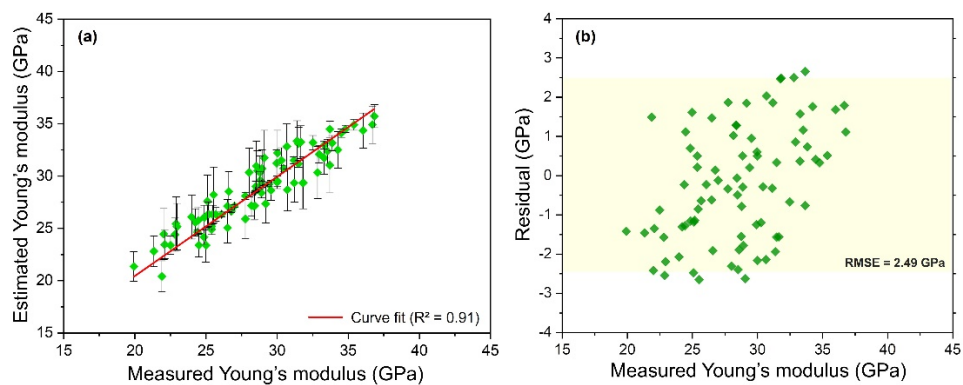

Figure 9. (**a**) Coefficient of determination and (**b**) RMSE and residuals of the [6-4-2-1] ANN.

4.2. Analysis of the Nonlinear Regression

ANN [6-4-2-1] was used to generate 46,656 datasets based on input variables randomly obtained based on their distribution (see Figure 4). Multivariable regression analysis using linear, polynomial, rational, and exponential functions according to Equations 6–12 was employed to propose a formulation to predict the elastic modulus. A backward process was used to set up the parameters for the prediction of the elastic modulus based on the following input variables: CC, WCR, CACR, FACR, TACR, and RCA. Table 3 shows the selected function and the required coefficients for each function. Null terms are omitted.

Table 3. Results of the multivariable regression.

Function	Equation Number	α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_9
$f_1(CC, RCA)$	8	-	19.02	7×10^{-4}	8.75	-0.017	-	-	-
$f_2(WCR, RCA)$	9	-1.448	1.00	-	-0.028	-	-7.9×10^{-5}	-	-
$f_3(CACR, RCA)$	9	-22.98	1.00	-	-0.608	-	-1.6×10^{-3}	-	-
$f_4(FACR, RCA)$	10	26.59	1.00	-	-	-	0.283	-	3.8×10^{-4}
$f_5(TACR)$	11	-	47.55	0.2225	-	-	-	1.00	-

Thus, the general form of the equation to predict the elastic modulus is given by:

$$E_c = -21.7 + 0.4 \cdot f_1 + 1.02 \cdot f_2 - 0.7 \cdot f_3 + 0.32 \cdot f_4 + 0.7 \cdot f_5 \tag{13}$$

where f_1, f_2, f_3, f_4 and f_5 establish the relation between input and output variables, written as:

$$f_1(CC, RCA) = 19.02 \cdot e^{(0.0007 CC)} + 8.75 \cdot e^{(-0.017 RCA)} \tag{14}$$

$$f_2(WCR, RCA) = \frac{-1.448 + (WCR)}{-0.028 - 0.000079 \cdot RCA} \tag{15}$$

$$f_3(CACR, RCA) = \frac{-22.98 + (CACR)}{-0.608 - 0.0016 \cdot RCA} \tag{16}$$

$$f_4(FACR, RCA) = 26.59 + \frac{(FACR)}{0.283 + 0.00038 \cdot (RCA)^2} \tag{17}$$

$$f_5(TACR) = \frac{47.55 \cdot e^{[0.2225 \cdot TACR]}}{(TACR)} \tag{18}$$

Following Santana et al. [108], normality, homoscedasticity, and independence from residuals of the proposed multivariable and nonlinear regression were evaluated. A Shapiro–Wilk test (of normality) resulted (p-value > 0.05) in 0.917, which indicates that the null hypothesis of the data being normally distributed is not rejected. A Durbin–Watson test (of independence) resulted in 0.803—values below 2.0 indicate that error terms have a positive autocorrelation. Additionally, a Breusch–Pagan test (for homoscedasticity) resulted in 0.286 for a significance level of 5%—low values indicate homoscedasticity. This behavior can be observed in Figure 10c, in which the residuals has a constant dispersion.

Figure 10 also shows other performance indicators: R^2 (Figure 10a), the sum of squares error "SQE" (Figure 10b), the *PRESS* (prediction error sum of squares) (Figure 10b), the *RMSE* (Figure 10c), the E_{max} (Figure 10c), and the percentage residuals (Figure 10d). Additionally, a coefficient of determination of 0.88 was obtained, pointing out its estimation capacity. The *PRESS* value of 463.51 has the same magnitude as the sum of squares error (391.18), an indication of model validity. Errors have a normal distribution with an average close to zero. Ninety-seven percent of the predicted values presented errors below the *RMSE*, thus indicating this value as the model error. The results indicate that the model was coherently developed and can predict the elastic modulus of concretes made with natural and recycled aggregates.
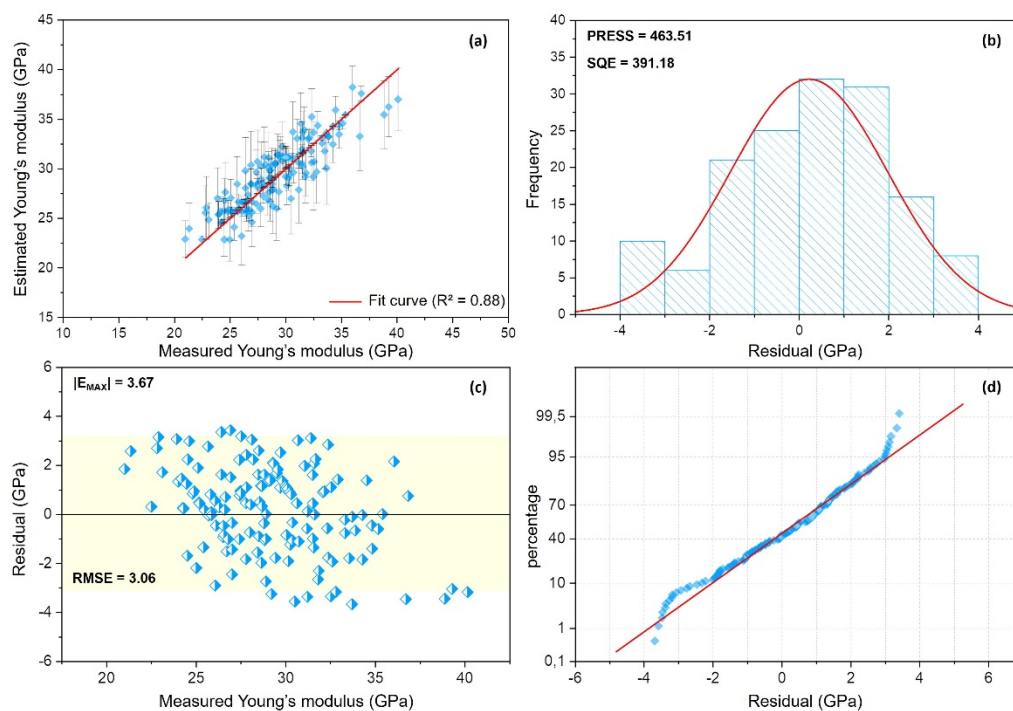
Figure 10. Performance parameters obtained with the proposed model: (**a**) coefficient of determination, (**b**) residual distribution, (**c**) RMSE, and (**d**) percentage residual.

Therefore, the results point out the model's applicability and that it is able to estimate the elastic modulus of concrete containing recycled aggregate from construction and demolition waste, with distinct replacement ratio (0–100%), water/cement ratio varying from 0.25 to 0.68, and cement consumption (in kg/m^3) varying from 247.00 to 512.50.

4.3. Parametric Analysis

In order to assess whether the developed formulation consistently represents the influence of each variable considered in the model and whether the formulation efficiently maps the concrete elastic modulus, a parametric analysis was conducted, and the results obtained were compared with the results available in the literature.

Five analyses were performed considering the combination of two input variables and their effects on the elastic modulus.

A reference scenario with the average values of model input parameters was set up, according to Table 1. The applicability domain was used to establish the range of the variables, as also shown in Table 1.

Initially, the mutual influence of the WCR and the RCA is presented in Figure 11. There is an inverse relation between the WCR and elastic modulus, regardless of the RCA.
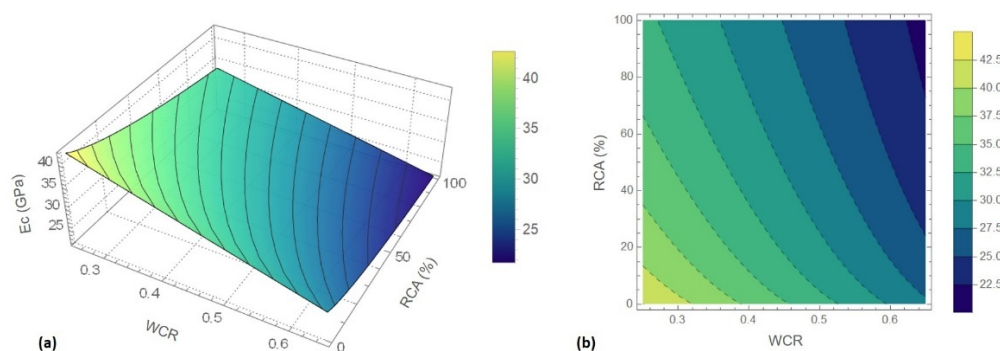

Figure 11. Effect of the WCR and the RCA in the elastic modulus in (**a**) 3D and (**b**) isoline.

The results of the analytical model proposed in this work indicate a reduction of 7% in elastic modulus for concretes made with 100% recycled aggregate when the WCR increased 25%. On the other hand, when analyzing concrete produced only with natural aggregate, an increase of 25% in the WCR generates a 13% of reduction on the concrete elastic modulus. This is explained by the porosity of the cement matrix, which increases, as the WCR also does. Gómez-Soberón [76] studied the influence of saturation degree in concretes made with recycled aggregate and observed that as the RCA increases, porosity also increases, which directly influences material stiffness.

Figure 12 presents the influence of the CC and the WCR. Higher CC associated with low WCR improves the elastic modulus. However, by fixing the WCR, only a small increment in the elastic modulus is seen when the CC is increased.
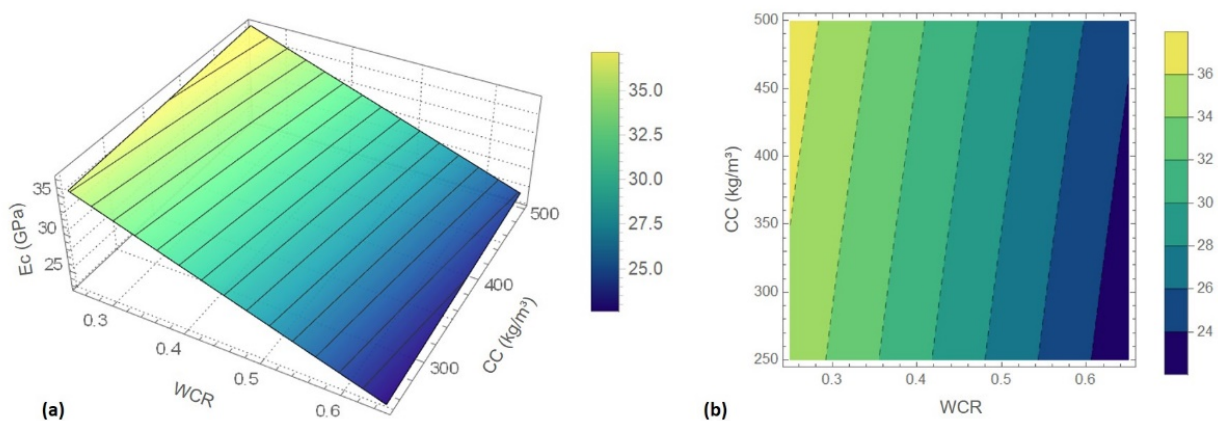

Figure 12. Effect of WCR and CC in the elastic modulus in (**a**) 3D and (**b**) isoline.

Results obtained with the proposed analytical model show a reduction of 22% in the elastic modulus for concretes made with 100% recycled aggregate compared with concrete made only with natural aggregate (see Figure 13). These results are consistent with those obtained by Etxeberria et al. [80], where the authors evaluated the influence of the RCA in concrete properties and verified that the stiffness of concretes made with recycled aggregate increases with increments of the CC, which resulted from a more compact matrix. The authors also observed that, for a WCR of 0.5 and a CC of 325 kg/m^3, concretes made with 100% of RCA had a decrease of 20–25% in the elastic modulus.
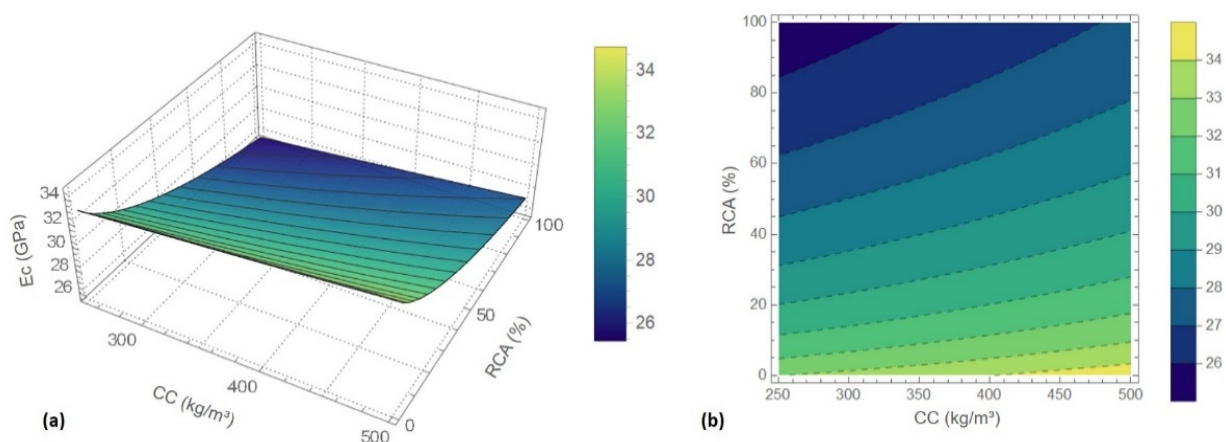

Figure 13. Effect of CC and RCA in the elastic modulus in (**a**) 3D and (**b**) isoline.

Figures 11 and 13 show that concretes made with replacement ratios up to 20% of natural aggregate reach a similar elastic modulus, considering the same CC and WCR. However, concretes made with a replacement ratio above 50% require a reduction of 5–23%

of WCR and an increase of 4–18% of CC to sustain around the same elastic modulus as from concretes made with only natural aggregates.

Figures 14 and 15 show the influence of the replacement ratio of recycled aggregates associated with coarse and fine aggregate/cement ratio, respectively. Smaller ratios of aggregate/cement lead to lower elastic modulus. A minimum value of elastic modulus was found for FACR and CACR close to 2.0 and 100% of RCA.
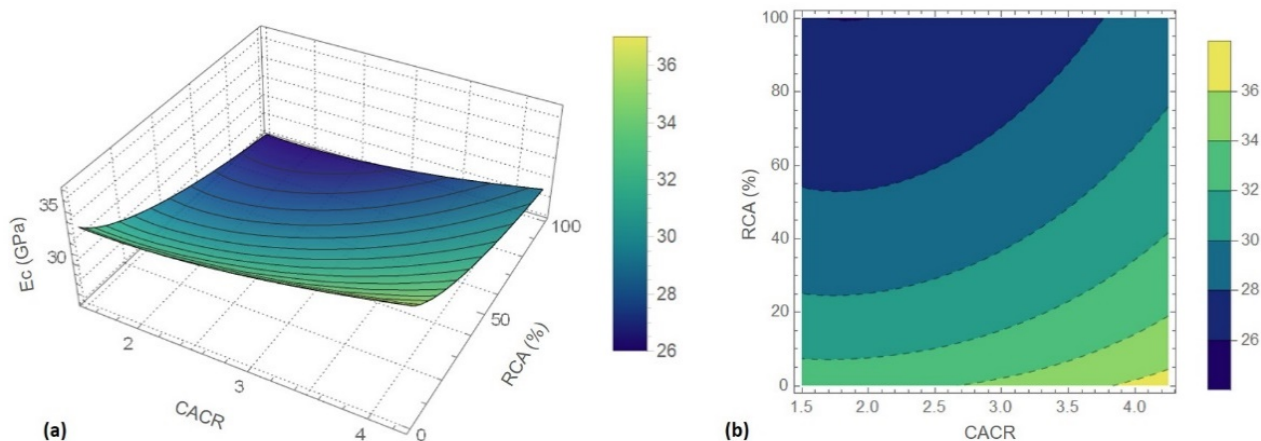

Figure 14. Effect of CACR and RCA in the elastic modulus in (**a**) 3D and (**b**) isoline.
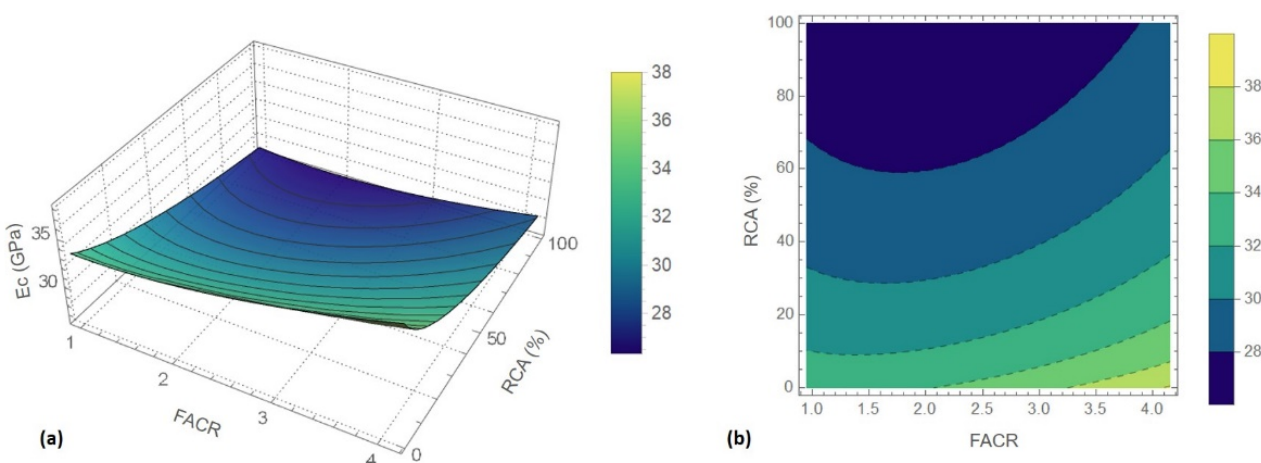

Figure 15. Effect of FACR and RCA in the elastic modulus in (**a**) 3D and (**b**) isoline.

Cabral et al. [110] describe that the FACR has a greater influence than the CACR on the elastic modulus, once the concrete elastic modulus is associated with the volume fraction, specific weight, and aggregate elastic modulus. Mehta and Monteiro [8] point out that the aggregate strain is related to its porosity, to the maximum size, its shape, texture, granulometry, and mineralogical composition.

In addition, Figures 11–15 show that the influence of the replacement ratio of natural aggregates by recycled aggregates may decrease the elastic modulus up to 32%. Ajdukiewicz and Kliszczewicz [11], Gómez-Soberón [76], Etxeberria et al. [80], and Cabral et al. [110] point out that 100% RCA generates concretes with an elastic modulus from 25% up to 35% lower than the concretes produced with 100% natural aggregate. Estolano et al. [111] found a decrease of 35.4% of the concrete stiffness due to complete replacement of natural aggregates associated with large increases in void index and water absorption.

5. Conclusions

In this study, we evaluated the possibility of applying machine learning coupled with nonlinear regression to obtain a formulation to estimate the elastic modulus of concretes

made with natural and recycled coarse aggregate. Artificial neural networks, which have the best learning power among various machine learning models, were applied.

The main novelty of this work is the methodology employed in the development of the analytical formulation, which used artificial neural networks coupled with nonlinear regression. The regression modeling considered a dataset generated with an ANN that efficiently mapped the concrete elastic modulus from the following predictor variables: cement consumption, water/cement ratio, replacement ratio of recycled coarse aggregate, fine aggregate/cement ratio, total aggregate/cement ratio, and coarse aggregate/cement ratio. The model was developed considering predictor parameters that are easy to obtain and do not require destructive testing.

Regarding the ANN modeling, it was observed that networks with two hidden layers containing up to six neurons were sufficient to efficiently map the concrete's elastic modulus, reducing the ANN size. In additional, the results show that the replacement ratio of recycled coarse aggregate, fine aggregate/cement ratio, and coarse aggregate/cement ratio are very important parameters to consider as predictors.

Regarding the mathematical expression, the proposed formulation presented a coefficient of determination of 0.88, which indicates its predictive capacity. The error residuals presented a normal distribution with an average close to zero, and 97% of predicted values had errors below the 3.06 GPa, with a maximum error of 3.67 GPa.

In addition to the results, the following conclusions were drawn from the study:

- Concretes made with a ratio of natural aggregates replacement with recycled aggregates of up to 20% reaches almost the same stiffness as concrete made with 100% natural aggregate;
- Concretes made with a replacement ratio above 50% require lower water/cement ratios (about 5–23%) and higher cement consumption (about 4–18%) than concretes made with 100% natural aggregate;
- Results of the analytical model proposed in this work showed a reduction of 7% in elastic modulus for concretes made with 100% recycled aggregate when the WCR increased 25%. On the other hand, when analyzing concrete produced only with natural aggregate, an increase of 25% in the WCR generated a 13% of reduction on the concrete elastic modulus;
- Modeling with a nonlinear regression technique coupled with artificial intelligence provides an alternative and efficient methodology to solve problems related to civil and materials engineering.

Finally, the parametric study of the proposed analytical model demonstrated that it can be used to predict the concrete elastic modulus and that it can indicate better mix proportions for concretes containing natural and/or recycled coarse aggregates, thus enabling its use as a simulation tool in the development of engineering projects focused on durability and sustainability.

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