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Neural network prediction of unconfined compressive strength of coal fly ash–cement mixtures

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Abstract

Addition of coal fly ash is a common practice in cement and concrete; an important amount of information can be found in the literature of the unconfined compressive strength (UCS) of these products. Prediction of mechanical properties such as UCS of cement-based pastes, mortars and concrete containing coal fly ash has been done using neural network analysis (NNA) based on the Trajan Neural Network Simulator. The application of NNA has been able to identify the main variables showing an influence on UCS, and the best model to describe UCS with a root mean squared error of 6 MPa for all formulations and 5.5 MPa when formulations are restricted to the maximum addition of coal fly ash established in the European Standards (35% for cement and 55% for concrete). These results allow a good description of the experimental data for the European limits based on cement and concrete, where UCS ranges between 32.5–52.5 MPa and 12–60 MPa, respectively.

Keywords: Cement; Concrete; Fly ash; Compressive strength; Neural network analysis

1. Introduction

Cement-based pastes, mortars and concrete are a complex mix of hydraulic, pozzolanic, reactive and inert materials with water. The influence of the types and dosage of components in the mechanical properties of the hardened products has been extensively reported in the literature [1–4]. The water-to-cement ratio, the types, dosage and particle size of coarse and fine aggregates, the types and dosage of additives, and the partial replacement of cement by mineral admixtures affect the unconfined compressive strength (UCS) at a given sample age.

Examples of mineral admixtures are natural pozzolans, coal fly ash and silica fume. Coal fly ash is the most common pozzolan in cement and concrete. Coal fly ash is encoded in the European Waste Catalogue as 10 01 02 (10 01 Power stations and other combustion plants; 02 coal fly ash) [5], but commercially available fly ash can be obtained from thermal power plants [6].

The present use of coal fly ash is mainly based on its pozzolanic properties, meaning that it will form cementitious compounds when in a finely divided form and in the presence of water, it combines with calcium hydroxide. In practice, it also can be used as aggregate in cement and concrete making them stronger, more durable and easier to work with. In addition, the utilisation of fly ash avoids the disposal of large amounts of material simplifying the environmental waste management [7]. At early ages, the strength of concrete with fly ash is lower than the strength for ordinary concrete, however, for larger ages, concrete with fly ash shows higher strengths [8].

According to ASTM [8], there are two main types of coal fly ash:

- Class F: fly ash that is produced from the burning of anthracite or bituminous coal, it is typically pozzolanic and has low lime content.

Table 1
Properties of coal fly ash for cement addition [9]

Properties	Siliceous coal fly ash (V)	Calcareous coal fly ash (W)
Loss of ignition (wt.%)	< 5.0	< 5
Reactive CaO (wt.%)	< 10.0	> 10.0
Free CaO (wt.%)	< 1.0	–
Reactive SiO_2 (wt.%)	> 25	–
Stability (mm)	< 10	< 10

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Table 2
Properties of coal fly ash for concrete addition [10]

Properties	Values
Loss of ignition (wt.%)	< 5.0
Chloride (wt.%)	< 0.10
Free CaO (wt.%)	< 1.0
SO_3 (wt.%)	< 3.0
Stability (mm)	+ 1.0
Activity rate (%)	
28 days	>75
90 days	>85

- Class C: fly ash that is produced from the burning of lignite or subbituminous coal. In addition to having pozzolanic properties, it also has some self-cementing properties. It presents high lime content.

A classification of coal fly ash is also made by the European Standards: siliceous coal fly ash (V), equivalent to type F, and calcareous (W), equivalent to type C. The addition of coal fly ash to cement and concrete is regulated in Europe according to Norms. Table 1 shows the properties that fly ash must have to be a component of cement according to EN 197-1:2000 [9]. On the other hand, the dosage of fly ash to cement may be between 6% and 55% weight (EN 197-1:2000) [9].

Table 3
Summary of variables and data

Variable	No. data	Range of the variable (%)
Cements		
Blended cement	57	8.7–80
Calcium aluminate cement	29	16–90
Ordinary Portland cement	541	2.86–90
Other cement	22	20–69.2
Rapid hardening Portland cement	27	13.7–90
Sulphate resisting Portland cement	36	15.3–90
Fly ashes		
Coal fly ash—ASTM C618 Class C	107	2.45–92.3
Coal fly ash—ASTM C618 Class F	112	2.9–92.3
Coal fly ash—Unspecified type	493	1.3–95
Water		
Added water	609	0.5–70
Total water	103	5.17–81.8
Additives		
Air-entraining agent	14	0.012–0.06
Clay	27	1–22
Coal bottom ash	17	30–51.4
Gypsum/hemihydrate	19	0.4–36
Hydrated lime—$Ca(OH)_2$	11	9–14.5
Plasticizer/superplasticizer/ water reducer	105	0.04–2
Silica fume	22	0.7–6.3
Aggregates		
Coarse aggregate	175	30–54.5
Fine aggregate	380	24.4–77.8

Table 4
Lumped variables for 10 input variables

Input variable	Sum of	No. of cases
1. Ordinary Portland cement		541
2. Other cements	Blended cement Calcium aluminate cement Other cement Rapid hardening Portland cement Sulphate resisting Portland cement	171
3. Coal fly ash—ASTM C618 Class C		107
4. Coal fly ash—ASTM C618 Class F		112
5. Coal fly ash—Unspecified class		493
6. Added water		609
7. Total water		103
8. Additives	Air-entraining agent Clay Coal bottom ash Gypsum/hemihydrate Hydrated lime—$Ca(OH)_2$ Plasticizer/superplasticizer/ water reducer Silica fume	215
9. Coarse aggregate		175
10. Fine aggregate		380

For concrete composition, fly ash characteristics are given in Table 2 (EN 450) [10]. The amount of fly ash used to replace cement in concrete may be between 15% and 35% of the total cementitious material. (EU Directive 98/34/CE) [11]. In some cases, the dosage of different additives to cement and concrete is due to strength requirements. According to the European Norm EN 196-1:1995 [12], the cement–concrete normal strength is defined as the UCS measured at 28 days. The UCS is regulated depending on the mixture (cement or concrete). For cementitious mixtures, the UCS ranges between 32.5 and 52.5 MPa (EN 196-1:1995) [12]. In the case of concrete, the specified strength may be between 12 and 60 MPa (ENV 206:1990) [13].

Different methods can be used to model the UCS of cements and concretes as a function of the mixture composition. There are semi-empirical models to predict

Table 5
Lumped variables for five input variables

Variable	No. data	Range of the variable (%)
Cement	712	2.86–90
Fly ashes	712	1.3–95
Water	712	0.5–81.8
Additives	181	0.012–51.4
Aggregate	397	30–77.8

Table 6
Statistics for prediction of 28-day UCS

Regression coefficients	Linear model	Neural network					
		Root mean squared error			Correlation coefficient		
		Training	Verification	Test	Training	Verification	Test
20 Input	0.77	5902.8	6948.7	7067.9	.962	.952	.944
10 Input	0.57	6895	8038.5	8001.3	.948	.935	.934
5 Input	0.47	12,275.2	14,343.1	9995	.820	.789	.890

cement or concrete UCS depending on the age [8,14] when the composition of the mixtures includes few components. However, when the number of components increases, the relationship between variables is complex and the use of a nonlinear modeling approach is required. Neural network analysis (NNA) has been shown to be a useful technique for modeling complex nonlinear systems, and it has been used with some success in predicting setting, strength and leachate pH of S/S products. This technique has been also applied to the prediction of cement and concrete strength. Lai and Serra [15] develop a neural network model for predicting the strength of concrete using seven quantitative variables of composition (amount of fine and coarse sand, fine and coarse aggregate, cement, water and superplasticizer), and the type of cement as qualitative variable. The strength prediction performance was within 5%. More recently, Stegemann and Buenfeld [16] used NNA for constructing models of UCS of cement pastes containing metal species. The root mean squared error in the prediction of UCS was 7.6 MPa, which is within the interlaboratory error.

This work uses available data from the literature to test neural network models in order to predict the UCS in fly ash-based cement and concrete.

2. Neural network analysis

There are many different neural networks. In this work, the multilayer perceptron architecture, which is the most common for engineering applications, was used. Neural network models were constructed using Version 4.0 of the Trajan Neural Network Simulator [17].

A multilayer perceptron may be thought of as consisting of layers of parallel data processing cells. Neurons in the input layer only act as buffers for distributing the input signals to neurons in the hidden layer. Each neuron in the hidden layer sums up its input signals after weighting them with the strengths of the respective connections from the input layer and computes its output as a function of the sum. The differences between the computed output and the target are combined together by an error function to give the network

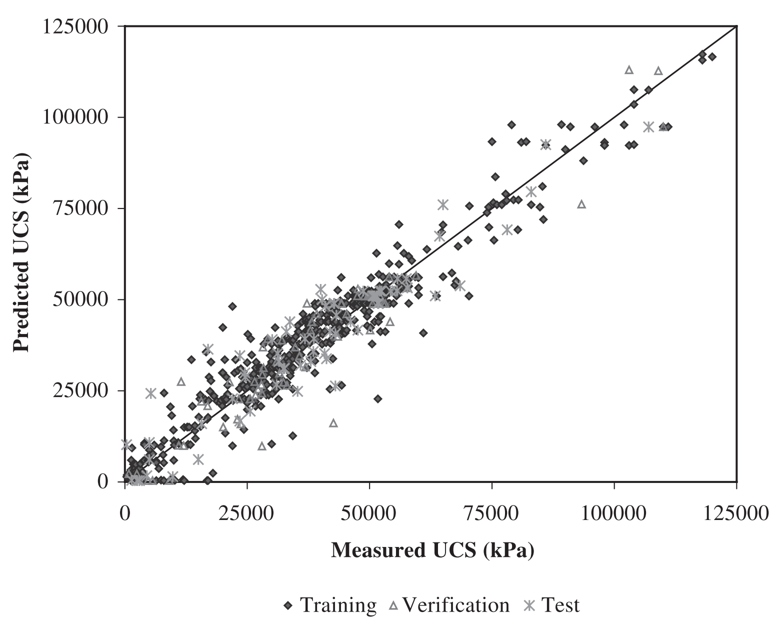

Fig. 1. Parity plot for the UCS prediction with 20 input variables.

Table 7
Sensitivity rank for prediction of 28-day UCS

Sensitivity analysis rank	Number of variables		
	20 variables	10 variables	5 variables
1	Added water	Other cements	Cement
2	Fine aggregate	Fine aggregate	Aggregate
3	Coarse aggregate	OPC	Water
4	OPC	Additives	Additives
5	Total water	Coarse aggregate	Fly ash
6	Coal fly ash Type F	Added water	–
7	Sulphate resisting Portland cement	Total water	–
8	Gypsum	Coal fly ash Type C	–
9	Coal fly ash unspecified type	Coal fly ash Type F	
10	Coal bottom ash	Coal fly ash unspecified type	–
11	Calcium aluminate cement	–	–
12	Rapid hardening Portland cement	–	–
13	Blended cement	–	–
14	Coal fly ash Type C	–	–
15	Plasticizer/superplasticizer	–	–
16	Hydrated lime—$Ca(OH)_2$	–	–
17	Clay	–	–
18	Other cement	–	–
19	Silica fume	–	–
20	Air-entraining agent	–	–

error. The most common error function is the sum of squared errors, where the individual errors of output units on each case are squared and summed together. As a result of training, the neural network will be able to make predictions (e.g., UCS) based on new input data [18].

To avoid overlearning or overfitting of the neural network during training, some of the cases are reserved, comprising the verification set, and used to keep an independent check of the progress of the algorithm. Training of the neural network is stopped when the error for the verification set begins to increase. The most interesting property of a network is its ability to generalize new cases. For this purpose, an independent data set is used to test the neural network and check its performance with data which have not been used in the training and verification. When verification and test errors are reasonably close together, the network is likely to generalize well [17].

NNA was used to construct models of UCS as a function of mix composition using existing data from literature studies [4,6,7,14,19–54] of products containing at least: cement (different types of cement have been taken into account), water (added or total) and coal fly ash (Class C, Class F or unspecified class). The models were able to describe the nonlinear relationship between UCS and the mix composition. UCS data were only considered at 28 days of curing in order to compare them with EN Standards, which state the minimum UCS to be fulfilled at 28 days.

The data set for NNA was obtained from a references list of properties of cement-based formulations. From the 1816 formulations extracted from this list containing coal fly ash and cement, 1345 have been measured for strength at 28 days. In addition to coal fly ash and cement, 453 of these products also contain another waste, being the aim of these formulations the use of coal fly ash as binder in the stabilization/solidification of these wastes; therefore, they have not been considered in this study. Finally, 180 products do not show the water content. According to these restrictions, 712 products from references [4,6,7,14,19–54] were used in the prediction of the UCS as a function of mix composition.

The studied component are summarised in column 2 of Table 3 with the number of products containing the com-

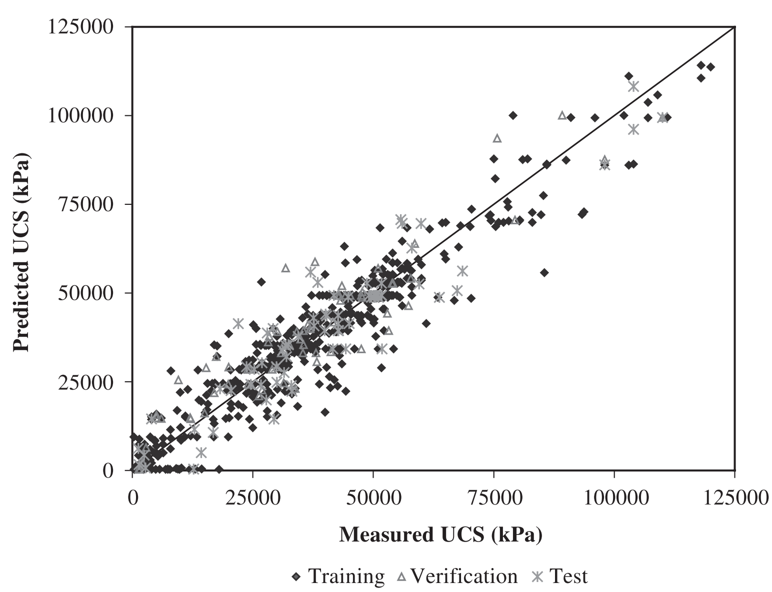

Fig. 2. Parity plot for the UCS prediction with 10 input variables.

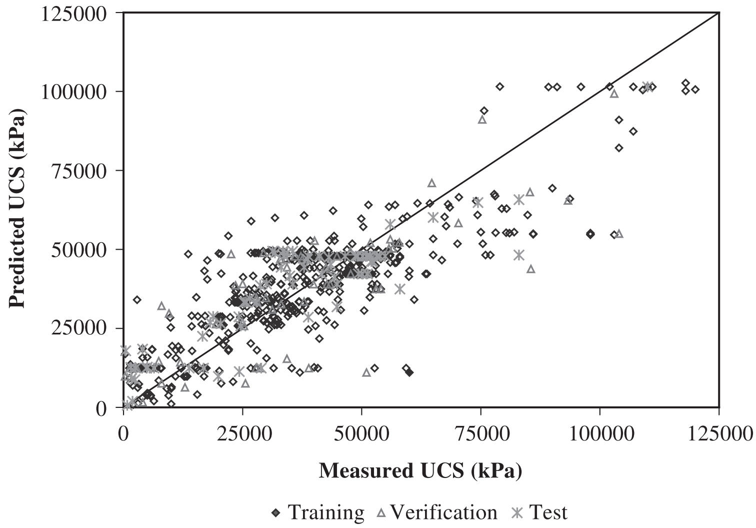

Fig. 3. Parity plot for UCS prediction with five input variables.

ponent in column 3 and the maximum and minimum value of the variable when it is different than zero in column 4. The product formulation must sum 100% dry wt. The output variable, UCS, ranges from 0.327 to 120 MPa.

Once the input and output variables were defined, the next step was the introduction of values of the selected variables in the commercial software. The training objective was the prediction of the UCS of the products at 28 days of curing as a function of the mix composition. Due to the difficulties to fit the curing conditions from the literature data, it has not been possible to introduce this variable into the neural network models. To reach this objective, three different neural networks were developed.

2.1. Selection of input variables: lumping of variables

The first neural network model was built using the 20 variables of composition given in Table 3 as input variables. Simpler neural networks were also constructed lumping some input variables after consideration of:

- *Sensitivity analysis*: the variables which had less influence in the training of 20 inputs developed before were grouped.
- *Number of cases*: the input variables included in few products were grouped with similar variables in such a way that the new lumped input variables were included in at least 100 formulations.

The input variables used for this training are reported in Table 4. Column 2 indicates the variables grouped to form the input variable given in column 1. As it can be observed, in this case 10 input variables were used to predict UCS.

An even simpler analysis was done where the input variables were taken in five groups indicated in column 1 of Table 3. These groups describe the usual components of cement and concrete without the specification of additives or aggregates. The characteristics of these groups are shown in Table 5. For the UCS prediction in the three models, the data set was divided to develop the training as follows: 572 cases for training, 70 cases for verification and 70 cases for test.

The training performance was evaluated according to the regression coefficient, *r*, and examination of the predicted versus target UCS (parity graph). Linear regression analysis was also applied to the data to obtain a linear approach to UCS, for comparison with the nonlinear neural network models.

Sensitivity analysis of the models was performed using the Trajan Neural Network Simulator, which studies the error of the model after removing the input variable, which

Table 8
Statistics for prediction of 28-day UCS products restricted to the EN Norms

Regression coefficients	Linear model	Neural network					
		Root mean squared error			Correlation coefficient		
		Training	Verification	Test	Training	Verification	Test
15 Input	0.75	5364	5782	5847	.957	.955	.965
9 Input	0.56	6233	6806	4957	.945	.930	.974
5 Input	0.42	9659	9996	12,760	.862	.867	.815

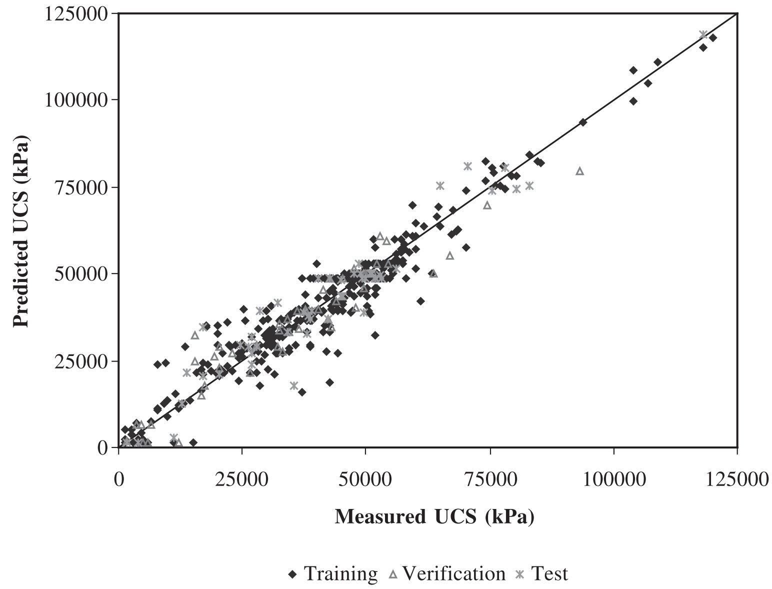

Fig. 4. Parity plot for UCS prediction with 15 input variables (products restricted to EN Norms).

sensitivity is intended to check, and the error of the model using all the input variables.

3. Results

The fitting of the linear models taken as reference was not as good as those obtained with the nonlinear neural network, as it is shown in Table 6. The root mean squared error of the best neural network model is around 6 MPa for a training developed using 20 input variables, as it is shown in Fig. 1 and the statistics for the corresponding neural network are given in Table 6. From this figure important discrepancies between measured and predicted values can be observed for products with low UCS values. The root mean squared error of 6 MPa is important at low UCS, but may be considered in the range of experimental error for high UCS.

Sensitivity analysis of this model shows the following influence of the variables: added water>fine aggregate ≈ coarse aggregate>OPC>total water>coal fly ash type F>sulphate resisting Portland cement>gypsum>coal fly ash unspecified type>coal bottom ash. According to the sensitivity analysis (see Table 7), it can be observed that the variables which have less influence in the prediction of the UCS are the additives, being water, aggregates and OPC as the main variables.

The number of variables has been lumped to 10 in order to have the new lumped input variables contained in at least 100 formulations; the results of these models are shown in Fig. 2 and the statistics in Table 6. The regression coefficients are compared with the 20 input variables training; it can be observed that they are in the same range and the lumping of variables was not a big influence on the statistics. However, the regression coefficient using linear analysis was only .57, a value much lower than that obtained for 20 inputs.

The sensitivity analysis in this case is given by the next series of variables: other cements>fine aggregate>ordinary Portland cement>additives>coarse aggregate>added water>total water>coal fly ash type C>coal fly ash type F>coal fly ash unspecified type. The cements are still the main variables, however, for this case, additives present a higher rank in the sensitivity analysis. This fact could be due to the lumping of these variables, which increases the number of cases and is added to the influence of these variables.

Finally, the input variables were lumped in five types as it is shown in Table 5. The results for the UCS prediction are given in Table 6 and Fig. 3. For this training, the regression coefficients are lower than that found for the previous neural

Table 9
Sensitivity rank for prediction of 28-day UCS products restricted to the EN Norms

Sensitivity analysis rank	Number of variables		
	15 variables	9 variables	5 variables
1	Added water	Fine aggregate	Aggregate
2	Fine aggregate	Added water	OPC
3	Coarse aggregate	Coarse aggregate	Additives
4	OPC	OPC	Water
5	Total water	Additives	Fly ash
6	Coal fly ash Type F	Total water	–
7	Gypsum	Coal fly ash unspecified type	–
8	Plasticizer/ superplasticizer	Coal fly ash Type F	–
9	Coal fly ash unspecified type	–	
10	Coal bottom ash	–	–
11	Coal fly ash Type C	–	–
12	Air-entraining agent	–	–
13	Hydrated lime—$Ca(OH)_2$	–	–
14	Silica fume	–	–
15	Clay	–	–

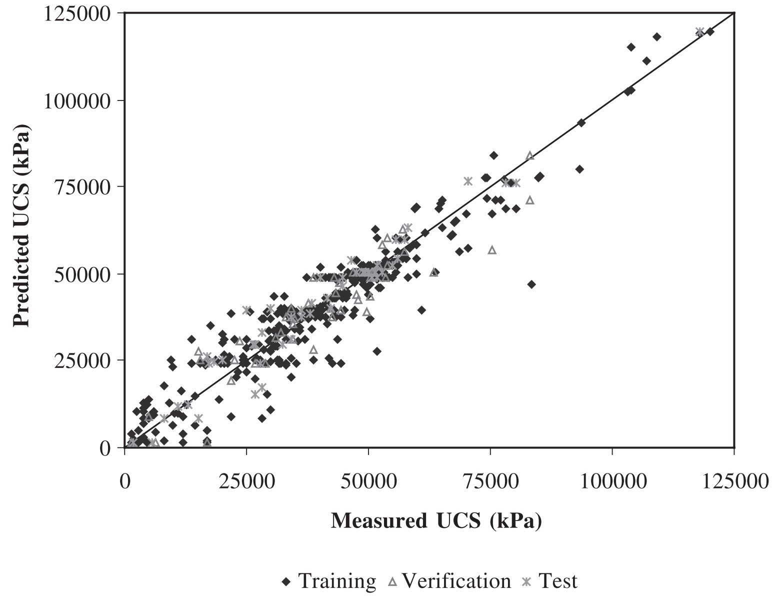

Fig. 5. Parity plot for UCS prediction with nine input variables (products restricted to EN Norms).

networks, the reduction of the input variables to five does not give appropriate results for the prediction of UCS, showing that the complexity of the system cannot be described by five variables.

3.1. Prediction of UCS: mixtures restricted to European Norms

Following the results of the neural network training for the prediction of UCS, it can be observed that the best results are found when the 20 input variables are taken into account or by a 1/2 reduction (10 input variables). However, the results are not good enough when the number of input variables decreases to 5. Another possibility to simplify the system is attending to the maximum content of coal fly ash allowed in the European Norms for common cements and concrete [9,11].

Following these Norms, the products that do not contain Portland cement or with fly ash exceeding the maximum amount specified in the standards (>35% for cements and >55% for concretes) are excluded from the data set. New neural networks models are constructed to predict the UCS of mixtures with fly ash content below 35% for cements and 55% for concretes. Now, the data set is based on 489

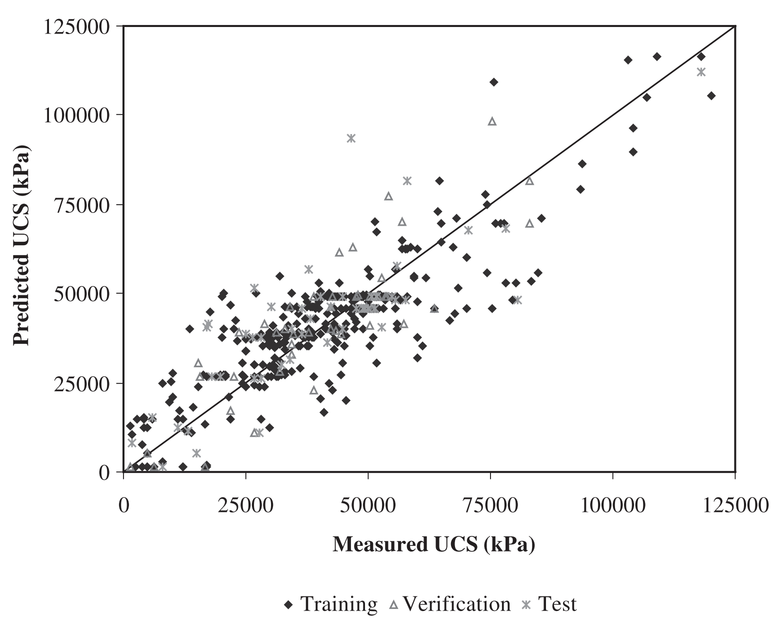

Fig. 6. Parity plot for UCS prediction with five input variables (products restricted to EN Norms).

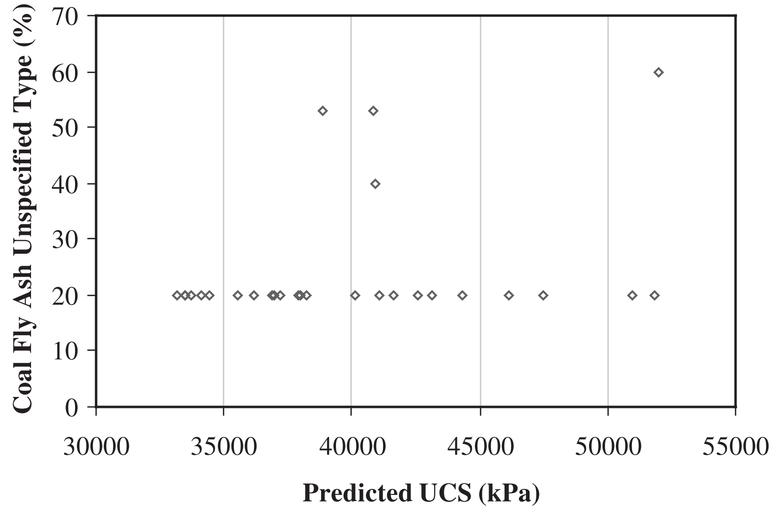

Fig. 7. Influence of fly ash addition on the predicted UCS of cement pastes (coal fly ash unspecified type).

products divided in: 389 cases for training, 50 cases for verification and 50 for testing.

A neural network with 15 input variables was trained after removing the following variables: blended cement, calcium aluminate cement, other cement, rapid hardening Portland cement and sulphate resisting Portland cement (Table 3). The statistical results obtained for this new training are given in Table 8 and Fig. 4 shows the parity graph. As it can be observed, the correlation coefficients are as high as those obtained with 20 input variables (Table 6). However, in this case, the prediction of low values of UCS is better than the prediction with 20 input variables due to the reduction of the root mean squared error to 5.5 MPa, resulting from the removal of mixtures out of regulation. Now, the output variable range is from 1.24 to 120 MPa.

The sensitivity analysis of this model is shown in Table 9; the main 10 variables are: added water>fine aggregate ≈ coarse aggregate>OPC>total water>coal fly ash type F>gypsum>plasticizer/superplasticizer>coal fly ash unspecified type>coal bottom ash. Cements except ordinary Portland cement have been removed from the input variables leading to a new order in the sensitivity analysis, where some additives show an important influence.

A second simplification is made following the same criteria, the nine input variables are the ones referred in Table 4 excluding the group called “Other Cement.” From these nine input variables, different neural networks were built, with the best statistical results given in Table 8; Fig. 5 shows the parity graph. The correlation coefficients for nine variables and the correlation coefficients for 15 inputs are quite similar and the obtained results are not affected by the lumping of variables.

The sensitivity analysis in this case is given by the next series of variables: fine aggregate>added water>coarse

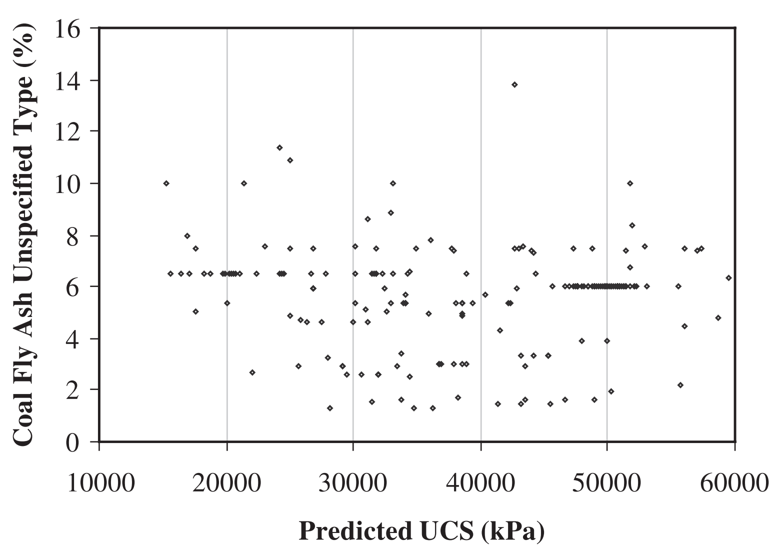

Fig. 8. Influence of fly ash addition on the predicted UCS of concrete (coal fly ash unspecified type).

aggregate>ordinary Portland cement>additives>total water>coal fly ash unspecified type>coal fly ash type F>coal fly ash type C. Following the sensitivity analysis, it should be noted that the variable coal fly ash has usually little influence.

Finally, input variables were lumped in five groups: additives, aggregates, fly ashes, ordinary Portland cement and water, and a new neural network was constructed. Results of this model are given in Table 8 and Fig. 6. As it happens when cements and all fly ash dosages were taken into account, the simplification to five input variables affects statistical results to a great extension, with the correlation coefficients much lower than in the training for 15 and 9 input variables.

However, the influence of the five input variables was similar: aggregate>ordinary Portland cement>additives>water>fly ash. Once again, the aggregates were the most important variable, with fly ash being the least important. The lack of influence of the amount of fly ash in the formulation of cement pastes and concretes on the 28-day UCS is clearly shown in Figs. 7 and 8, where the neural network-based predicted UCS of cements (Fig. 7) and concretes (Fig. 8) containing coal fly ash is plotted. The strength requirements for cement and concrete can be fulfilled by products containing different amounts of coal fly ash, the strength being determined by other compositional variables.

4. Conclusions

Several authors [1–4,7] point out the influence of the composition variables in the UCS of a cement or concrete. NNA was used to model the complex relationship between cement or concrete composition and the UCS of the mixture when the number of composition variables is high. Accurate models have been constructed to predict the UCS of the mixtures at an age of 28 days based on their formulation. Initially, the whole composition variables were introduced separately in the neural network in order to study their influence in the output variable. According to the sensitivity analysis, the variables which have less influence in the prediction of the UCS are the additives being water, aggregates and cements, the main variables of the formulation. However, the number of products containing water and cement is higher than the number of products with specific additives. This fact could have an influence in the sensitivity analysis.

The variables were grouped in order to reduce the input variables which were present only in a few cases. As a result of this lumping, additives reach a higher influence in the sensitivity analysis. However, when the input variables were taken in five groups describing the usual components of cement and concrete, the regression coefficients obtained were lower than for the previous neural networks. Using 20 and 10 variables, the root mean squared error is around 6 MPa.

To simplify the data set, standard criteria of fly ash additions based on EN Norms were taken into account. Then, only products according to some requirements of these Norms were introduced in the neural network training. Using 15 and 9 variables, the root mean squared error is around 5.5 MPa. The statistical results obtained after training the simplified data set were quite similar to the previous fittings. However, in the sensitivity analysis, additives show an important influence.

The obtained models constitute a clear representation for mixes of fly ash addition to cement and concrete. The application of NNA to the prediction of UCS in cementitious mixtures seems to be a useful way to relate composition with UCS, due to the complex relationship between these variables, which does not allow the application of mechanistic models.

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