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Prediction of the mechanical behavior of mortars incorporating phase change materials using data mining techniques

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ABSTRACT: Nowadays, it is imperative to reduce the energy bill in order to contribute to a more sustainable planet. In this sense, the use of materials that contribute to the energy efficiency of buildings is a very important contribution to achieve this goal. Mortars incorporating phase change materials (PCM) can make an important contribution to this end, due to its thermal storage capacity, increasing the energy efficiency of buildings. In this work several mortars with different PCM contents were developed, using different binders (cement, aerial lime, hydraulic lime and gypsum). The aim of this study was to apply data mining techniques such as artificial neural networks (ANN), support vector machines (SVM) and multiple linear regressions (MLR) to forecast the compressive and flexural strengths of these mortars at different exposure temperatures. It was concluded that ANN models have the best predictive capacity both for compressive strength and flexural strength. However, the SVM models have a flexural strength forecasting capacity very close to ANN models.

KEY WORDS: Mortars; Phase change materials (PCM); Data mining techniques; Artificial neural networks; Support vector machines.

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RESUMEN: *Predicción del comportamiento mecánico de morteros que incorporan materiales de cambio de fase mediante técnicas de minería de datos.* Hoy en día es imperativo reducir la factura energética para contribuir a un planeta más sostenible. El uso de materiales que contribuyan a la eficiencia energética de los edificios es muy importante para conseguir este objetivo. Los morteros con materiales de cambio de fase (PCM), por su capacidad de almacenamiento térmico, pueden contribuir de forma importante a este fin aumentando la eficiencia energética de los edificios. En este trabajo se desarrollaron morteros con diferentes contenidos de PCM, utilizando diferentes conglomerantes (cemento, cal aérea, cal hidráulica y yeso). El objetivo de este estudio es aplicar técnicas de minería de datos como redes neuronales artificiales (ANN), máquinas de vectores de soporte (SVM) y regresiones lineales múltiples (MLR) para pronosticar las resistencias a la compresión y flexión de morteros a diferentes temperaturas de exposición. Se concluyó que los modelos ANN tienen la mejor capacidad predictiva para la resistencia a la compresión y flexión. Los modelos SVM tienen una capacidad de predicción de la resistencia a flexión semejante a los modelos ANN.

PALABRAS CLAVE: Morteros; Materiales de cambio de fase (PCM); Técnicas de minería de datos; Redes neuronales artificiales; Máquinas de vectores soporte.

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1. INTRODUCTION

Currently, the huge energy crisis and the increase in energy demand in the construction sector result in challenges for the prosperity and sustainable development of society and the environment. Thus, the incorporation of materials with thermal storage capability is gaining in popularity (1, 2). The phase change materials (PCM) have the ability to decrease the temperature fluctuations inside buildings, only using solar energy, a widely available, clean and accessible energy source for everyone across the planet (3-7). Thus, the use of construction materials doped with PCM becomes increasingly interesting from a thermal and sustainability point of view.

The PCM incorporation in construction materials applied to buildings can be described as a thermal energy storage system, increasing the thermal mass and improving the thermal performance of building elements (8-9).

Over the last years, several investigations have been published reporting the benefits from the thermal performance point of view of using PCM in different construction materials, such as mortars (2-3), gypsum plasterboards (10-15), bricks (16-19), concrete (20-25) and panels (26-31). The PCM presence in the construction material contribute to improve the energetic efficiency of buildings (7). However, the incorporation of this type of materials in construction products also alters their properties from a physical and mechanical point of view, especially the compressive and flexural strengths (32-35). The performance of construction materials incorporating PCM depends on parameters such as the raw materials used, the binder dosage, the PCM content, as well as the thermophysical properties of the PCM.

The experimental studies to evaluate the behavior of construction materials doped with phase change materials is challenging and time-consuming. Thus, optimization studies for the PCM integrated construction materials are needed to improve their behavior and efficiency.

Data mining (DM) is a process of extracting information or knowledge from data sets for decision-making purposes (36). The success of data mining approach is well documented in civil engineering literature, particularly in domain of the mortars. In the last decades, with the advance of the artificial intelligent, many models for predicting the mechanical properties of mortars such as compressive strength and tensile strength have been developed. In this way, many compositions of mortars have been tested with different kind of reinforcements and additives. Most of the forecasting models both for compressive strength and flexural strength are based on artificial neural networks (ANN) (37-43). However, there are also models based on adaptive neuro-fuzzy inference systems (ANFIS) (37, 43), fuzzy logic methods (38), genetic programming (41), support vector machine (SVM) (44), random forest (44), decision tree (44), and k-nearest neighbors (44). ANN models have also been used to predict the effect of elevated temperature both on mortar compressive strength (45-46) and on mortar flexural strength (46). However, none has incorporate phase change materials.

Selimefendigil and Öztop (47), studied an artificial neural network modeling approach in order to estimate the required time for a complete phase change with respect to changes in the input variables of magnetic field strength in each domain and solid volume fraction. The authors revealed that the technique used provides fast and accurate results.

Bhamare et al. (48) used an artificial neural network as a deep learning approach for predicting the Measure of Key Response index (MKR index). The MKR index is a comparative assessment indicator that provide to select a system that offers better thermal behavior compared with others. The ANN-based model shows a good performance and proved its efficacy in training, testing, and sensitivity analysis with the independent dataset.

Marani and Nehdi (49) claimed to use machine learning for the first time to predict the compressive strength of PCM-integrated cementitious composites. In fact, they modeled this mechanical property using different machine learning algorithms such as random forest, extra trees, gradient boosting and extreme gradient boosting. All of these algorithms are based on decision trees. Later, these authors presented a similar work, but based on ANN (50).

We did not find in literature any work similar to those developed by Marani and Nehdi (49-50). Furthermore, according our best knowledge, DM techniques has not yet been applied to predict the flexural strength of mortar incorporating PCM.

This work aims to build models to estimate the compressive and flexural strengths of mortars incorporating PCMs. The large number of parameters involved in the formulations of these materials, as well as the complex non-linear relationships between them, point out to the use of artificial intelligence tools, in particular data mining techniques, which have a great potential to obtain such models.

This paper is structured in the following way. After this introduction, chapter 2.1 presents the research methodology. Chapter 2.2 describes the selection of materials regarding the mortar formulations. Chapter 2.3 describes the experimental tests to obtain compressive and flexural strengths. Chapter 2.4 briefly describes the data mining process and DM techniques. Chapter 3 presents and discuss the results obtained through developed data mining models the allow to forecast the compressive and flexural strength of mortars incorporating phase change materials. Finally, conclusions are drawn in Chapter 4.

2. MATERIALS, FORMULATIONS AND TEST METHODS

2.1. Research methodology

Figure 1 outlines the steps and methodology adopted for the development of this work.

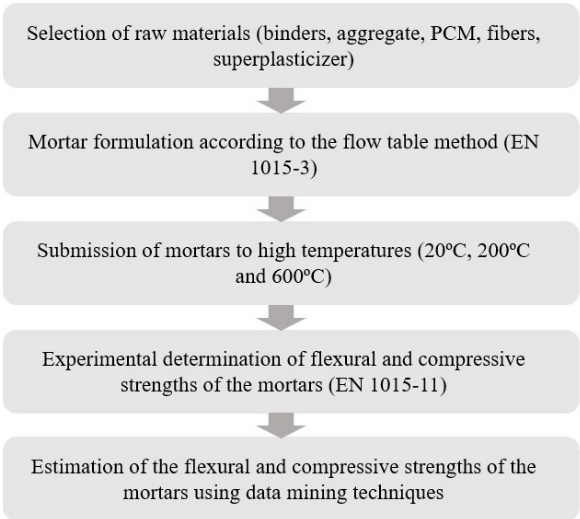

Figure 1. Research methodology.

2.2. Materials and formulations

The raw materials selected for this work were based in previous research works developed by the authors regarding to the mortars formulation, physical, mechanical and severe temperature exposure behavior (32-33, 51-52).

The selected materials were Portland cement (CEM), aerial lime (AL), natural hydraulic lime (HL), gypsum (G), superplasticizer (SP), fibers, sand and phase change material (PCM). The materials densities are presented in Table 1.

The used aerial lime had a purity of 90%. The gypsum corresponds to a traditional one, with high fineness. The hydraulic lime was a natural one (NHL5) and the cement is a CEM II B-L 32.5N. The used sand has an average particle size of 439. 9 µm. The fibers used are synthetic polyamide fibers, with a length of 6 mm and 22.3 µm of thickness.

The PCM selected for this work is a microencapsulated solution commercialized by the Devan Chemicals (Mikathermic D24). The PCM microcapsules consist of a melamine-formaldehyde capsule and a core in paraffin, with the characteristics present in Table 2. The selection of this PCM was based on its transition temperature, so that it was ideal to operate in the range of comfort temperatures inside buildings (53-55).

Table 1. Materials densities.

Material	Density (kg/m^3)
Portland Cement	3030
Aerial Lime	2450
Hydraulic Lime	2550
Gypsum	2740
Superplasticizer	1050
Fibers	1380
Sand	2600
Phase Change Material	880

In this work, twelve different compositions were studied and simulated (Table 3 and Figure 2). The mortars formulation was based on the flow table method, according to the European standard EN 1015-3 (56). The resulting value from the test was only considered when between 200-220 mm.

The selected compositions possess different PCM contents (0% and 40% of aggregate mass) and different type of binders (AL, HL, G and CEM). The use of different PCM contents and different binder types allow to obtain a broader study of the PCM influence in mortars for interior coating with capacity for application in different buildings, since mortars can be obtained with greater propensity for application in new buildings or in rehabilitation operations.

Table 2. Phase Change Material properties.

Property	
Temperature transition	22.5ºC
Enthalpy	147.9 kJ/kg
Minimum microcapsule dimension	5.8 µm
Maximum microcapsule dimension	55.2 µm
Average particle size	43.91 µm

2.3. Experimental tests

The obtainment of experimental data for this study was based on the performance in flexural and compression of mortars with PCM, when submitted to different temperatures (20ºC, 200ºC and 600ºC).

The mechanical performance of the mortars was based in the European standard EN 1015-11 (57). The flexural and compression tests were performed with load control at a speed of 50 N/s and 150 N/s, respectively. Three specimens with dimensions of 40×40×160 mm^3 were used for the flexural tests. Regarding the compression tests the 6 half parts resulting from the flexural test were used with approximate dimensions of 40×40×80 mm^3. However, the load was applied uniformly distributed over a section of 40×40 mm^2.

Table 3. Mortars formulation (kg/m³).

Formulation	Binder		Sand	PCM	Superplasticizer	Fibers	Water/Binder
AL0PCM	AL	500	1447.2	0	15	0	0.45
AL40PCM	AL	800	451.2	180.5	24	0	0.34
AL40PCM-F	AL	800	425.2	170.1	24	8	0.36
HL0PCM	HL	500	1351.1	0	15	0	0.54
HL40PCM	HL	500	571.6	228.6	15	0	0.62
HL40PCM-F	HL	500	567.2	226.9	15	5	0.62
CEM0PCM	CEM	500	1418.8	0	15	0	0.55
CEM40PCM	CEM	500	644.3	257.7	15	0	0.56
CEM40PCM-F	CEM	500	622.2	248.8	15	5	0.59
G0PCM	G	500	1360.4	0	15	0	0.56
G40PCM	G	500	540.1	216.0	15	0	0.70
G40PCM-F	G	500	535.8	214.3	15	5	0.70

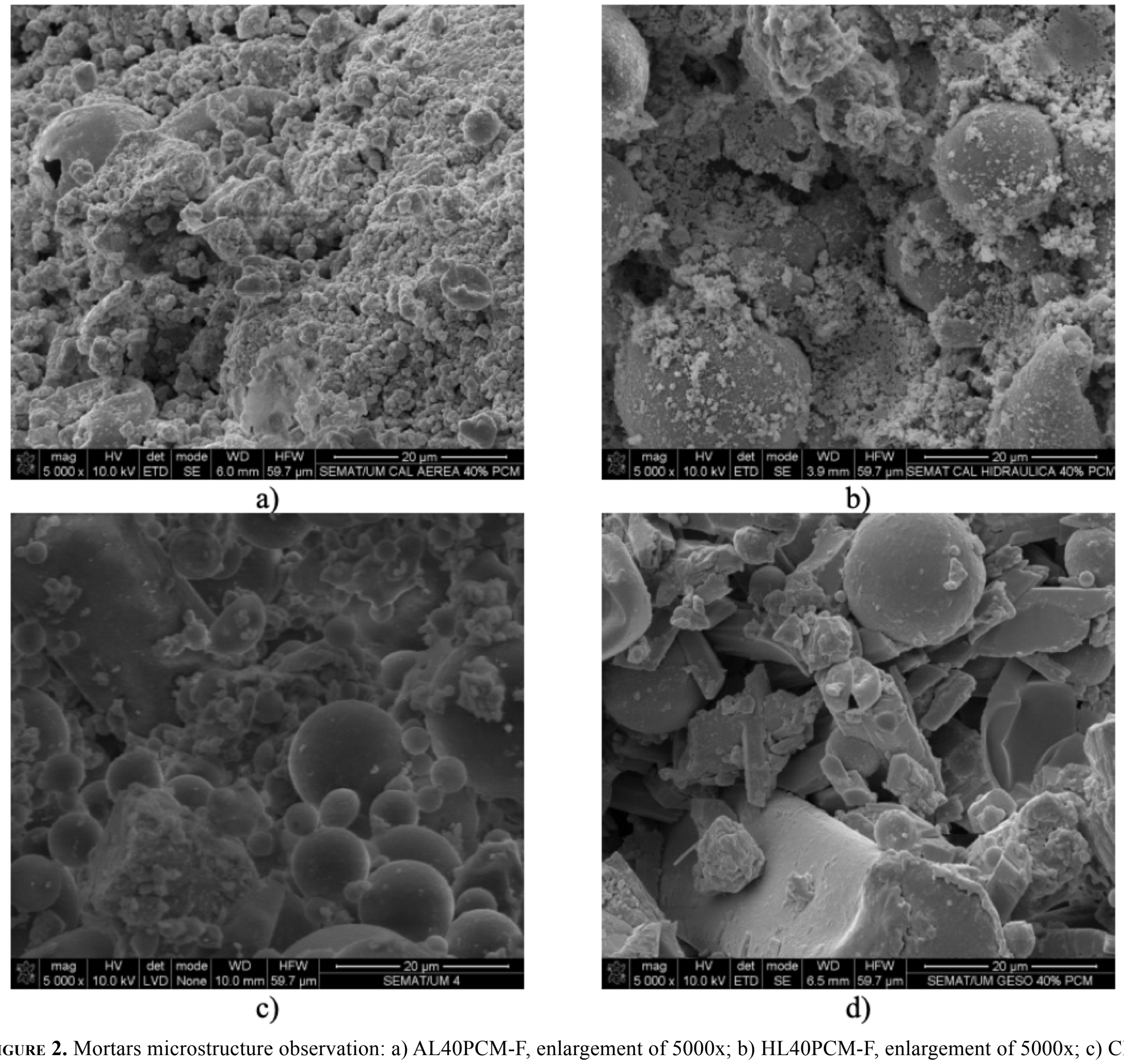

Figure 2. Mortars microstructure observation: a) AL40PCM-F, enlargement of 5000x; b) HL40PCM-F, enlargement of 5000x; c) CEM40PCM-F, enlargement of 5000x; d) G40PCM-F, enlargement of 5000x.

The mortars submission to different temperatures was performed using an oven, after 28 days of curing.

Table 4 shows the compositions, the temperature exposure and experimental results of tests for obtaining the flexural and compressive strengths. Table 5 shows the statistical assessments of the parameters of Table 3 and Table 4.

Table 4 constitutes the database for the DM analyses and the type of binders were labelled as categorical variable: AL, HL, CEM and G.

2.4. Data mining models

The compressive strength and flexural strength of mortars incorporating phase change materials are modeled through three data mining techniques namely multiple linear regression (MLR), artificial neural networks and support vector machines. The overall process was carried out in the R software using the RMiner library (58) which allows the easier use of DM algorithms.

MLR is an expansion of the simple regression that allows the use of more than one independent variable.

Neural networks try to mimic the functioning of the human brain. To do so, they consist of artificial neuron that are interconnected and send signals among them, each one having an associated weight, $w_{i,j}$, where i and j represent neurons. Each neuron has an activation function that allows introducing a non-linear component. This study used the logistic function defined by the expression 1/ (1 + e-x) and the following general Equation [1]:

$$\hat{y} = w_{o,0} + \sum_{j=I+1}^{o-1} f\left(\sum_{i=1}^{I} x_i w_{j,i} + w_{j,0}\right) w_{o,i} \quad [1]$$

where:
x_i – input parameters or nodes;
I – number of input parameters;
o – output parameter.

In this study, a widely used architecture called multilayer perceptron was adopted with one intermediate layer called hidden layer. Therefore, there is one input layer, one hidden layer that has a number of nodes equal to HN (Hidden Nodes) and one output layer. In this study, the search space for HN assumed the values {0, 2, 4, 6, 8, 10} (59).

Support vector machines were initially designed for classification tasks and later adapted to regression tasks with the introduction of the ε-insensitive loss function (60-61). The main idea of SVM is to transform the input data into a multidimensional feature space using a nonlinear mapping and find the best hyperplane of linear separation within the characteristic space. The nonlinear mapping requires a kernel function k(x,x') that in this study was adopted the Equation [2]:

$$k(x, x') = e^{(-y \cdot \|x - x'\|^2)}, y > 0 \quad [2]$$

Table 4. Compositions and experimental results of tests for determining compressive strength (σc) and flexural strength (σf).

Composition	Binder Type (BT)	Temperature (ºC)	Compressive strength - σ_c (MPa)	Flexural strength - σ_f (MPa)
AL0PCM	AL	20	1.61	0.76
AL0PCM	AL	200	2.79	0.79
AL0PCM	AL	600	1.86	0.19
AL40PCM	AL	20	1.5	0.71
AL40PCM	AL	200	0	0
AL40PCM	AL	600	0	0
AL40PCM-F	AL	20	3.26	1.24
AL40PCM-F	AL	200	3.06	0.93
AL40PCM-F	AL	600	0	0
HL0PCM	HL	20	5.37	1.64
HL0PCM	HL	200	6	1.77
HL0PCM	HL	600	1.81	0.21
HL40PCM	HL	20	2.58	1.09
HL40PCM	HL	200	1.59	0.83
HL40PCM	HL	600	0	0
HL40PCM-F	HL	20	3.27	1.18
HL40PCM-F	HL	200	1.85	0.87
HL40PCM-F	HL	600	0	0
CEM0PCM	CEM	20	28.1	6.78
CEM0PCM	CEM	200	24.6	6.58
CEM0PCM	CEM	600	12.9	1.69
CEM40PCM	CEM	20	8.53	3.03
CEM40PCM	CEM	200	3.83	1.32
CEM40PCM	CEM	600	0.64	0.11
CEM40PCM-F	CEM	20	10.8	3.24
CEM40PCM-F	CEM	200	5.49	1.71
CEM40PCM-F	CEM	600	0.91	0.19
G0PCM	G	20	9.59	3.63
G0PCM	G	200	7.7	2.5
G0PCM	G	600	3.05	0.74
G40PCM	G	20	3.45	1.57
G40PCM	G	200	1.47	0.77
G40PCM	G	600	0.41	0.16
G40PCM-F	G	20	2.7	1.26
G40PCM-F	G	200	0.98	0.51
G40PCM-F	G	600	0.12	0.07

In addition to the kernel parameter, γ, and ε-insensitive zone width, the regression performance is also affected by a penalty parameter, C. The high number of possible combinations of ε and C would require a huge computational cost. To avoid this, the heuris-

Table 5. Basic descriptive statistics of the parameters used in database.

Parameters	Min.	Mean	Max.	Standard Deviation	Coef. Var. (%)
Binder - ρ (kg/m^3)	500	550	800	113.39	20.62
Fibers (kg/m^3)	0.00	1.917	8.00	2.85	148.82
PCM (kg/m^3)	0.00	145.20	257.7	106.77	73.51
Sand (kg/m^3)	425.20	827.90	1447.2	245.83	89.94
Superplasticizer (kg/m^3)	15	16.5	24	411.12	49.66
Water (kg/m^3)	225	292.1	350	3.40	20.62
Temperature (ºC)	20.00	273.30	600.00	33.83	11.58
σ_c (MPa)	0.00	4.50	28.14	6.28	139.70
σ_f (MPa)	0.00	1.34	6.48	1.61	120.94

tics developed by Cherkasy and Ma (62) was used to evaluate these parameters. Therefore, the search space was limited to γ by using the following values: {2-15, 2-13, 2-11, 2-9, 2-7, 2-6, 2-5, 2-4, 2-3, 2-2, 2-1, 20, 21, 22, 23}.

To evaluate the performance of the models, mean absolute deviation (MAD), root mean squared error (RMSE) and coefficient of determination (R^2) given by Equations [3], [4] and [5] were used:

$$MAD = \frac{1}{N} \times \sum_{i=1}^{N} |y_i - \hat{y}_i| \quad [3]$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{N}} \quad [4]$$

$$R^2 = \left(\frac{\sum_{i=1}^{N}(y_i - \bar{y}) \times (\hat{y}_i - \bar{\hat{y}})}{\sqrt{\sum_{i=1}^{N}(y_i - \bar{y})^2} \times \sqrt{\sum_{i=1}^{N}(\hat{y}_i - \bar{\hat{y}})^2}} \right)^2 \quad [5]$$

where:
N – number of examples;
y_i – real value;
$\hat{y}_i$ – value estimated by the model;
$\bar{y}$ – mean of the real values;
$\hat{y}$ – mean of the estimated values.

The higher the MAD and RMSE are, the better the performance of the models. The opposite is valid for R.

In the data mining learning process, an algorithm is applied to the database to develop a model applicable to new cases. The performance of data mining algorithms can be evaluated using several methods. In this study, the cross-validation method was used, which allows using all available data (63). The database was divided into five parts each containing roughly the same number of data. Ten runs were performed using four parts of the data for training and one part for testing. This allowed obtaining ten validation metrics whose average allowed establishing the final validation metrics.

To assess the importance of each of the input parameters in the models, a sensitivity analysis was performed. In this context, the average values of all input parameters were maintained except the parameter whose sensitivity was being analyzed. Then, the value of that parameter was varied from its minimum value to its maximum value. In the end, the most important parameter in the model is the one that causes the greatest variance in the model output.

To carry out the DM process, firstly all the input parameters (binder, fibers, PCM, binder type, Temperature, Sand, Superplasticizer and water) (Tables 3 and 4) were used and based on the sensitivity analysis, the number of input parameters was reduced bearing in mind their importance. This approach was applied to develop models to predict the output parameter: compressive strength in chapter 3.1 and flexural strength in chapter 3.2.

3. RESULTS AND DISCUSSION

3.1. Compressive strength

As it was mentioned before, the data mining process was started using all input parameters given in Tables 3 and 4. Through a cross-validation scheme using the eight parameters, the metrics shown in Table 6 were obtained. Table 6 allows to conclude that all the determination coefficients are above 0.64, that, according Johnson (64) may be an indication of a good forecasting capacity of these models. Table 6 also shows that the ANN model has the best predictive capacity, given that this model has the highest R^2 and the lowest errors.

Table 6. Mean values of the metrics obtained in the cross-validation scheme for compressive strength.

	MLR	ANN	SVM
R^2	0.712	0.800	0.716
MAD	2.655	2.022	2.164
RMSE	3.321	3.094	3.854

Figures 3 to 5 show the performances of the three DM models for compressive strength. Analyzing these figures, it is possible to confirm that artificial neural networks have the best predictive capacity. Furthermore, Figure 3 shows that up about 10 MPa the SVM model has a good forecasting capacity.

To assess the relative importance of each one of the input parameters a sensitivity analysis was performed. Results for all used techniques are presented in Table 7 and shown graphically in Figure 6. It should be underlined the strong importance of the binder type in all the models. It should be noted that the sum of the three most important parameters (binder type, temperature and sand) is around 72% in the ANN model and 76% in the SVM model. The importance of binder type and temperature in compressive strength translates the experimental results. However, an experimental study carried out by Pilehvar et al. (65) showed that the compressive strength is only slightly affected by temperature of the specimen at the testing time and models developed by Marani and Nehdi (49) yielded low importance values for this temperature. Maybe the high temperatures applied in this study can justify this difference of importances. As for the importance of sand, once its packing is altered by its replacement by softer PCM, the porosity and microstructure of the mortar are also altered and, consequently, its compressive strength. This importance was demonstrated by experimental studies (65-66), and confirmed by the developed models of Marani and Nehdi (49). The superplasticizer dosage is of residual importance in the MLR and SVM models which is in accordance with the models prediction of Marani and Nehdi (49). Conversely, superplasticizer content is the fourth most important feature in the ANN model. The models developed by Marani and Nehdi (49) attribute a great importance to PCM dosage and it was demonstrated in previous studies that (66-68) the strength of the paste mixtures reduce with the increase of PCM percentage. In this study PCM is the most important feature proposed by the MLR model, the seventh in the ANN model and the fifth in the SVM model.

To reduce the number of input parameters, binder, fibers and SP were extracted from the database. This is because they present the worst averages of the amounts obtained in all models. In this way, another analysis was done using only five input parameters (PCM, binder type, Temperature, sand, superplasticizer and water).

Table 8 shows the performance of the different models through the mean values of the three used metrics obtained using the cross-validation scheme. Once again it is verified that a correlation coefficient greater than 0.64 is obtained for all models. This result is indicative of the good predictive capacity of all models. It should be stressed the great improvement of the ANN and SVM models in relation to the models based on eight input parameters. Figure 7 to 9 show the comparison between the measured and estimated compressive strength using only five input

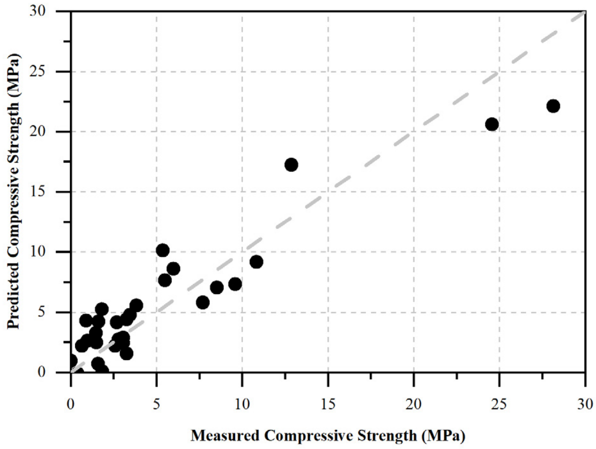

Figure 3. Predicted versus measured compressive strength using MLR model.

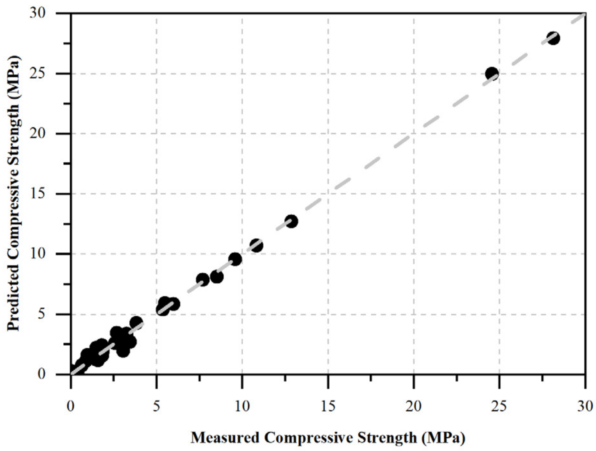

Figure 4. Predicted versus measured compressive strength using ANN model.

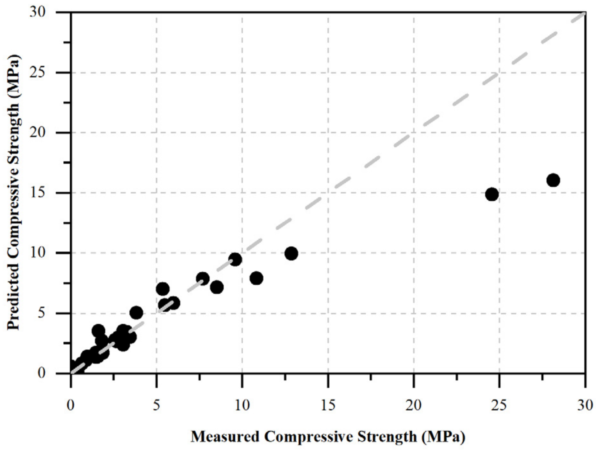

Figure 5. Predicted versus measured compressive strength using SVM model.

Table 7. Importance of the parameters used in database for compressive strength (%).

Parameters	MLR	ANN	SVM
Binder	2.42	9.37	0.42
Fibers	0.13	0.57	0.20
PCM	44.57	2.33	10.51
Binder Type	23.41	29.99	42.17
Temperature	1.60	16.94	19.16
Sand	11.84	24.45	14.61
Superplasticizer	0.93	11.07	0.42
Water	15.1	5.27	12.50

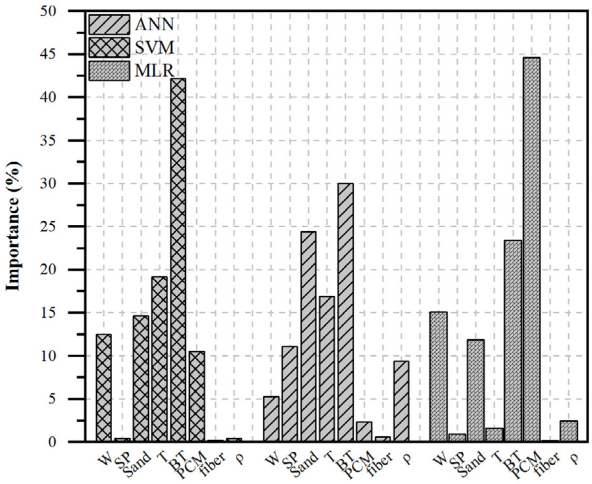

Figure 6. Importance of each parameter in all DM models – Compressive strength.

parameters (PCM, binder type, Temperature, sand and water). Looking at these figures, it is possible to confirm the better predictive capacity of the ANN model. Regarding the SVM model, it is found a good predictive capacity up to about 15 MPa (Figure 9).

Table 8. Mean values of the metrics obtained in the cross-validation scheme for compressive strength using PCM, binder type, T, Sand and water as input parameters.

	MLR	ANN	SVM
R^2	0.699	0.858	0.714
MAD	2.610	1.624	2.001
RMSE	3.417	2.407	3.753

3.2. Flexural strength

In this analysis, steps similar to those carried out in the analysis of compressive strength were followed. Therefore, initially all parameters were used for data mining analysis. Table 9 presents the results obtained in the cross-validation scheme.

It is possible to see in Table 9 that both MLR and SVM models have R^2 lower than 0.64. Furthermore, the ANN model has higher R^2 and lower RMSE but SVM has the lower MAD. Therefore, ANN model has the best performance. Figure 10 to 12 allow to see the performance of the three models. Both ANN and SVM models have a very good forecasting capacity whereas MLR has a poor forecasting capacity.

Table 10 and Figure 13 present the importance of each input parameter obtained through a sensitive analysis. It should be stressed the great importance of temperature and binder type both for ANN and SVM models. The sum of the importances of these two input parameters is about 68% for ANN model and 75% for SVM model. The third most important feature is the water for ANN model and sand for SVM model. It should be stressed that three of the four models developed by Marani and Nedhi (49) to predict compressive strength, not flexural strength, considered the water-to-cement ratio as the fourth most important feature. PCM dosage has the fourth position of importance given by ANN and SVM models. In fact, experimental studies showed that flexural strength of a cement mortar incorporating phase change material decreases with increasing amount of PCM (69-70). In relation to compressive strength for ANN model only one feature of the three most important was changed: sand was replaced by water. SVM model maintained the same top three important features.

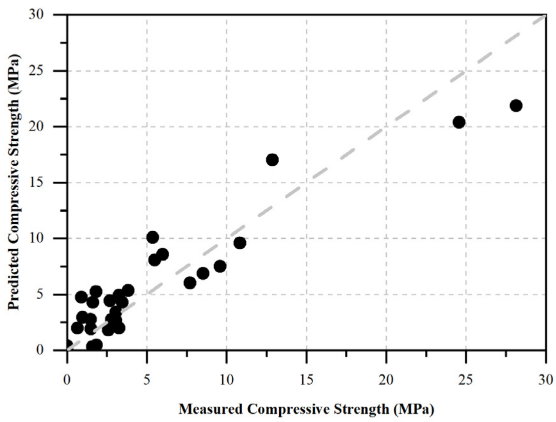

Figure 7. Predicted versus measured compressive strength using MR model using PCM, binder type, temperature, sand and water as input parameters.

To reduce the number of input parameters, binder content, fibers and superplasticizer content were extracted from the database. This is because they present the worst importance obtained in ANN and SVM models. Therefore, taking this into account, the analyses with only five parameters include the same input parameters as those used in the analysis performed with the compressive strength (PCM, binder type, temperature, sand, superplasticizer and water).

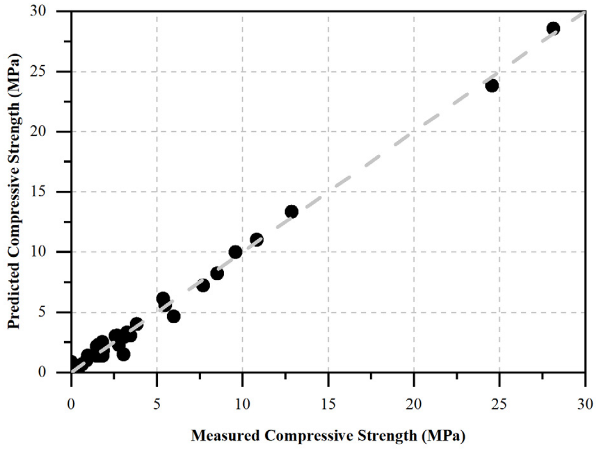

Figure 8. Predicted versus measured compressive strength using ANN model using PCM, binder type, temperature, sand and water as input parameters.

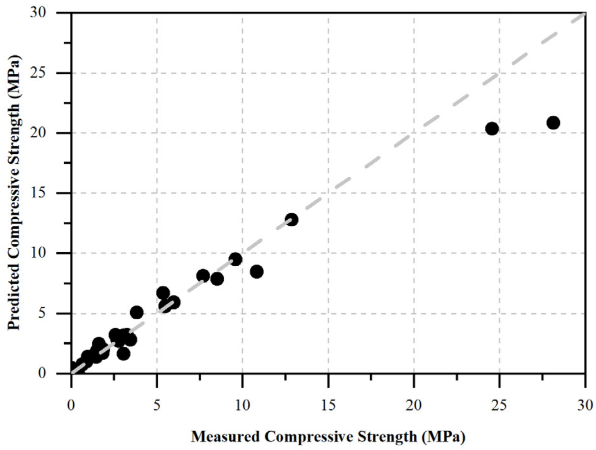

Figure 9. Predicted versus measured compressive strength using SVM model using PCM, binder type, temperature, sand and water as input parameters.

Table 9. Mean values of the metrics obtained in the cross-validation scheme for flexural strength.

	MLR	ANN	SVM
R^2	0.570	0.710	0.629
MAD	0.809	0.684	0.616
RMSE	1.061	0.989	1.027

Table 11 shows the performance of the different models though the mean values of the three used metrics obtained using the cross-validation scheme. In this study the coefficient of determination of MLR is lower than 0.64 and this model has the highest errors. Comparing the ANN and SVM models it can be seen that ANN have higher R^2 and lower RMSE but higher MAD. Figure 14 to 16 show the comparison between the measured and estimated compressive strength

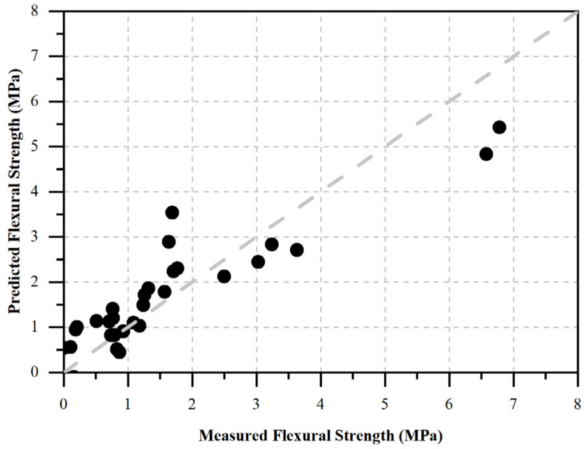

Figure 10. Predicted versus measured flexural strength using MLR model.

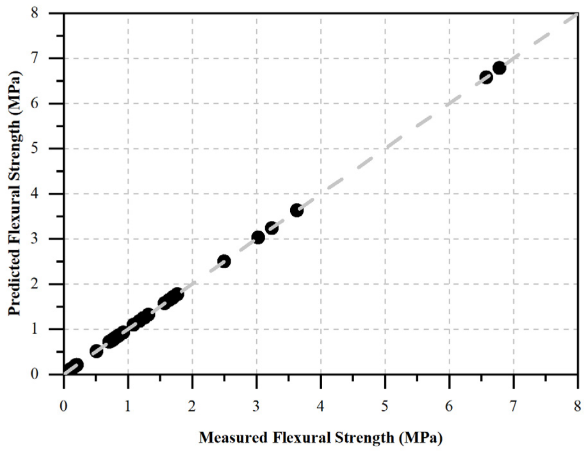

Figure 11. Predicted versus measured flexural strength using ANN model.

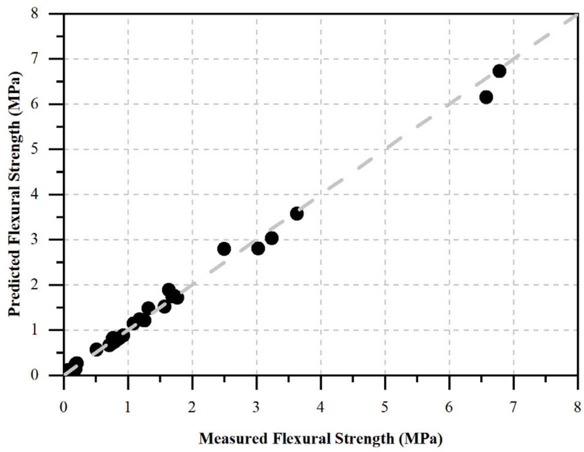

Figure 12. Predicted versus measured flexural strength using SVM model.

Table 10. Importance of the parameters used in database for flexural strength (%).

Parameters	MLR	ANN	SVM
Binder	31.26	1.17	1.34
Fibers	0.02	0.07	0.10
PCM	16.62	7.84	7.96
Binder Type	11.08	27.44	27.53
Temperature	2.67	41.03	47.88
Sand	3.5	6.20	12.45
Superplasticizer	30.88	2.55	1.34
Water	3.97	13.7	1.40

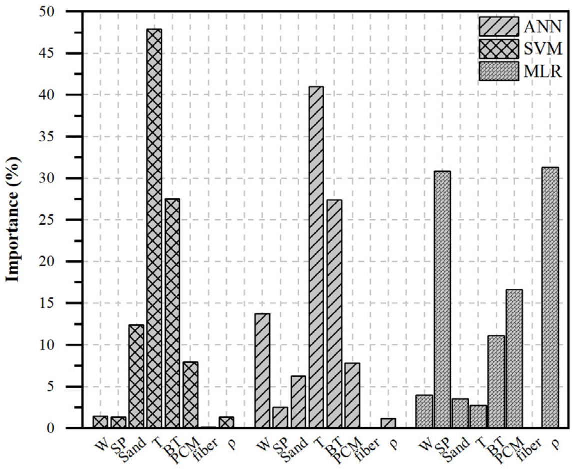

Figure 13. Importance of each parameter in all models – Flexural strength.

Table 11. Mean values of the metrics obtained in the cross-validation scheme for flexural strength using PCM, binder type, temperature, sand and water as input parameters.

	MLR	ANN	SVM
R^2	0.608	0.719	0.656
MAD	0.802	0.586	0.575
RMSE	1.026	0.941	0.975

using only five input parameters (PCM, binder type, temperature, Sand and water). Looking at these figures, it is possible to confirm that both ANN and SVM models have very good performances.

4. CONCLUSIONS

The incorporation of PCM microcapsules in mortars leads to a change in their physical and mechanical performance. On the other hand, it is important to note the need for and importance of characterizing the reference mortars and mortars doped with PCM

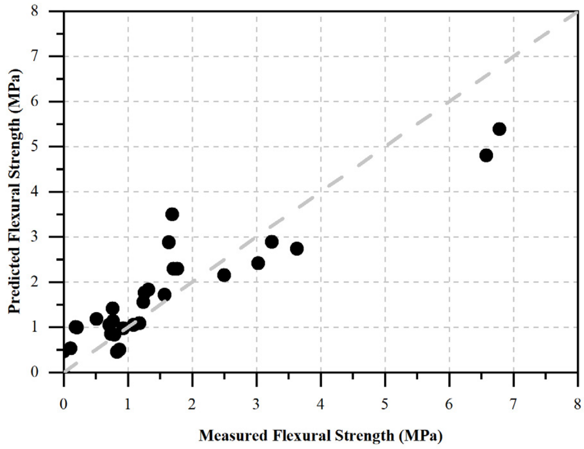

Figure 14. Predicted versus measured flexural strength using MR model using PCM, binder type, temperature, sand and water as input parameters.

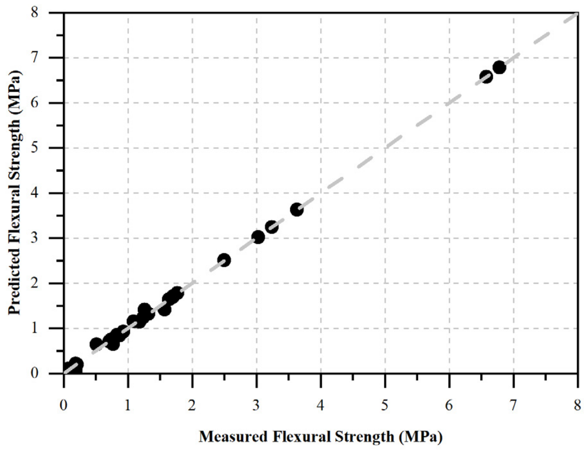

Figure 15. Predicted versus measured flexural strength using ANN model using PCM, binder type, temperature, sand and water as input parameters.

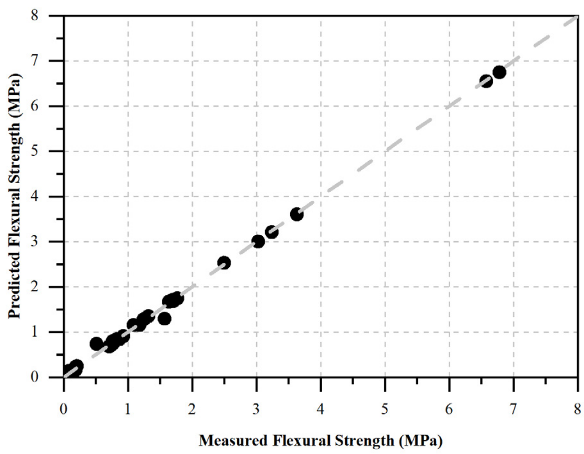

Figure 16. Predicted versus measured flexural strength using SVM model using PCM, binder type, temperature, sand and water as input parameters.

based on experimental tests, however these tasks are quite time-consuming, so the possibility of using DM techniques, based on experimental results, constitutes a possible solution to predict the behavior of mortars.

This work was essentially motivated by the reduced usage of DM techniques on the mechanical behavior of mortars incorporating PCM. Therefore, several samples with different compositions and exposed to different temperatures were submitted to experimental tests to obtain their compressive and flexural strengths. The obtained results allowed to build a database including several parameters. The application of DM techniques allowed the development of predictive models for the strengths mentioned above.

Analyses with eight input parameters (binder dosage, fibers, PCM, type of binder, temperature, sand, superplasticizer and water) were performed and evaluated the relative importance of each parameter in the developed models. Based on the relative importance of the parameters the number of input parameters was reduced to five (PCM, type of binder, temperature, sand and water) and DM techniques were applied.

This study applied the following DM algorithms: Multiple linear regression (MLR), artificial neural networks (ANN) and support vector machines (SVM).

This study allows to extract the following conclusions:

- The ANN algorithm has a very good predictive capacity to assess both compressive strength and flexural strength and has the best performance in all analyses performed whereas the MLR algorithm has the poorest performance. However, SVM algorithms have a great performance to predict the flexural strength.
- The top three important input features attributed by ANN and SVM models to predict the compressive strength are binder type, sand and temperature.
- Concerning the flexural strength prediction, temperature and binder type are the main input features considered by ANN and SVM models. Nevertheless, the third top input feature is the water for ANN model and sand for SVM model. PCM dosage has the fourth position of importance given by ANN and SVM models.
- Bearing in mind the importances attributed to input features by ANN and SVM models, one can say that these models captured, in a way, the expected behaviour of mortars incorporating PCM.
- To improve this study, it is advisable to expand the number of experimental works in order to increase the database and thus better clarify the relative importance of each input parameter in compressive and flexural strengths.

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