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Evaluation of the Utility of Using Classification Algorithms when Designing New Polymer Composites

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ABSTRACT

Polymer composites are the materials that can be successfully used in the places where high mechanical strength and chemical resistance as well as low absorbability are required. These unique features of polymer composites are obtained mainly due to a suitably selected binder, i.e. a synthetic resin. At the same time, this component accounts for the high production costs of these materials. Partial substitution of the resin with glycolisates obtained using poly(ethylene terephthalate) waste (PET), helps reduce the price of polymeric mortars, while maintaining favourable physicomechanical properties. This modification method also has a beneficial effect on the environment, as it allows the utilisation of a very common waste, which is difficult to dispose of. The article concerns three types of resin mortars, i.e. epoxy, polyester and polyester with the addition of colloidal silica, modified with PET glycolisate. On the basis of the obtained data set and database knowledge mining techniques, such as discriminant analysis and decision trees, it was shown to what extent the type of resin and the presence of an added modifier differentiate the mortar properties. The results obtained with both methods were compared. It was confirmed that these techniques are effective both in the classification and prediction of the type (selection) of mortar in the process of designing new composites.

Keywords: polymer mortars, waste materials, waste poly(ethylene terephthalate), discriminant analysis, decision trees

INTRODUCTION

In recent years, a dynamic development of the companies producing polymer precast concrete has been observed, including the systems for specialized applications, such as: bridge elements (ledges, curbs, grooves), elements for municipal wastewater drainage (wells, channels, tanks), tanks for aggressive media used in industry, modern railway sleepers. The direction of application of this type of composites results from, among others, excellent chemical resistance, low water absorption, and at the same time the high strength parameters of resin concretes [1–3]. These features, in turn, are conditioned by the type of synthetic resin used as a binder. It is the resin that first and foremost determines the properties of such a composite, especially its chemical resistance. The use of a given type of resin causes the obtained composite to have different properties. Therefore, it is extremely important to judiciously select the type of binder for the anticipated conditions of the process of manufacturing and using the products made of resin concrete. Since the cost of producing this type of composites is higher than that of cement concrete, the glycolysis products based on poly(ethylene terephthalate) (PET) waste are used as a partial replacement for the resin, which leads to a significant reduction in the production costs of the finished goods. This approach allows us to obtain a less expensive material that also has very good physical and mechanical parameters. In addition, this solution fits into the idea of sustainable development in the construction industry, as the waste materials that constitute a major environmental problem, are used during the production of polymer prefabricates. A method of obtaining the composites modified with glycolisates obtained on the basis of PET waste, and their effect on selected properties of epoxy mortars, is described in detail in the article [4]. The experiments conducted formed the basis for the construction of a laboratory database which brings together, among others, the data on the type and composition of raw materials used for the production of composites and the corresponding properties of the polymer concretes obtained. Such datasets can be used to search for useful regularities hidden within them. For example, while designing construction elements, we want to find an answer to the question: which resin should be used for the production of polymer precast concrete so that the construction meets the required mechanical properties. In order to demonstrate the extent to which the type of resin and the presence of an added modifier differentiate the properties of resin mortars, this article uses two selected database knowledge mining techniques, i.e. discriminant analysis and classification trees. In both cases, the database is searched for a dependency of the form:

properties of the composite → type of resin.

The properties of the composite serve here as input variables (features of the examined objects, attributes of the analysed cases). The type of resin is sought in the population (group, label) to which the composite belongs. Discriminant analysis is used to decide which variables distinguish (discriminate between) two or more naturally emerging groups. It searches for the rules of conduct aimed at assigning multivariate objects to one of many populations with known parameters with possibly minimal classification errors. The discriminant analysis techniques are based on a rather simple mathematical model, the core of which is a linear combination of independent variables (also called discriminating variables). It allows classification of observations (e.g. test mortars) into one of the groups that are of interest to the researcher [5].

Two main stages can be distinguished in discriminant analysis:

1. Training stage (model construction), in which the classification rules are created based on the research results (training set) gathered in the database.

The canonical discriminant functions separating the studied groups were determined. In the case of differences between groups, each of them can be treated as a cloud of points in space with axes that are discriminating variables. These point clouds may overlap slightly, but most of the points are concentrated in centroids spaced apart, i.e. fictitious points the coordinates of which are equal to the group mean of each discriminating variable. It is accepted that the centroids are typical representatives of each group. All classification procedures use a case-by-case comparison with each calculated centroid to find the closest one. The classification process is associated with the creation of one or more functions, classifying the analysed cases to the appropriate groups. It is conducted on the basis of Ronald Fisher's linear combination in the form (1):

$$K_i = a_{i0} + a_{i1} * x_1 + \cdots + a_{ij} * x_j \quad (1)$$

where: a_{ij}, $j = 0, 1, \dots$, n are the coefficients calculated from discriminant variables for each classification function.

There are as many of these functions as there are groups and they are used to decide which group most likely belongs to the given case. With the functions so defined, the case is classified in the group for which K_i assumes the highest value.

2. Classification stage (using the model), in which classification is carried out of a set of objects whose membership is unknown, based on the class characteristics found earlier.

If the database (sample) is large, the data set can be divided into two subsets: the training and test, in order to assess the usefulness of the designated classification equations. Otherwise, new data should be collected to confirm the accuracy of the classification. In practical use, the database is constantly expanded with new objects (data collected during the conduction of new laboratory experiments), which usually increases the correctness of the results of the classification stage (class prediction effectiveness).

The discovery in the historical data (database) of a method for allocating the objects to classes can also be implemented using the algorithms representing the classification system in the form of a binary tree. Classification trees are data mining tools used to build predictive models the task of which is qualitative or quantitative prediction of the results pertaining to the studied phenomenon.

The tree is a graphical model created as a result of a recursive division of the set of observations A into n disjoint subsets A_1, A_2, A_3, ... A_n. The goal of building a model is to obtain subsets of maximum homogeneity from the point of view of the value of a dependent variable. It is a multi-stage process that can use another independent variable in each step. At each stage, all of the predictors are analysed, and the one that ensures the best node division, i.e. it separates the most homogeneous subsets, is chosen.

An example of a classification tree is shown in Fig. 1. The beginning of each tree is the whole set of observations (the root of the decision tree), which is divided into 2 or more subsets. The first case concerns binary trees, and the second case any trees. The divided collection is called the parent node, while the separated subsets are called the child nodes. In the stage of division, the child node, which is further subdivided, becomes the parent node for the 2nd stage, and the node that remains unchanged becomes the terminal node, referred to as the leaf. The size of the tree is the number of leaves, and the depth of the tree is the number of edges between the top and the most distant leaf. The graphical representation of the knowledge on the studied process in the form of a tree makes the interpretation of results easier than in the case of purely numerical results [6, 7].

The aim of the analysis based on classification trees is to predict or explain the response (reaction) encoded in the qualitative dependent variable, and therefore the techniques used in this module have much in common with the techniques used in more traditional statistical methods, such as discriminant analysis, discussed above. Therefore, both methods were used in this study, and the results obtained were compared. For this purpose, the STATISTICA software was used, in which both discriminant methods and classification trees are implemented. The STATISTICA software enables to build trees by an exhaustive search for division of cases into classes. This algorithm is a complete implementation of techniques for calculating binary classification trees based on univariate divisions.

M. R Feldesman [8] presented the circumstances that limit the possibilities of applying both of the methods mentioned above. In many situations, similar results are obtained, but sometimes one method can be an alternative to the other. The data mining methods are widely used in many fields of science, including psychology, sociology, economics, and medicine. However, their use in materials science is much more modest. Y. Li [9] demonstrated the possibilities of applying the decision tree method to the classification of stainless steel. Article [10] describes the use of the decision tree method to the classification of beer samples. M. Hajigholizadeh and A.M. Melesse used the methods of discriminant analysis to assess water quality and to evaluate its spatial and temporal changes [11]. S.R. Oro et al. described a multivariate statistical analysis of displacements of a concrete dam in relation to the environmental conditions, using various statistical methods, including discriminant analysis [12]. Gabriela Vítková et al. used this method to classify bricks [13]. In another article [14], B. Dębska showed the possibility of using the discriminant analysis method for testing the mortars obtained using three different types of aggregates, i.e. perlite, expanded clay and granulated waste rubber, which are a partial substitute for quartz sand.

This article describes a study on the impact of the binder type on the change of mechanical properties of polymer mortars. The methods used were discriminant analysis and decision trees for the classification of mortars. The results obtained with both methods were compared.

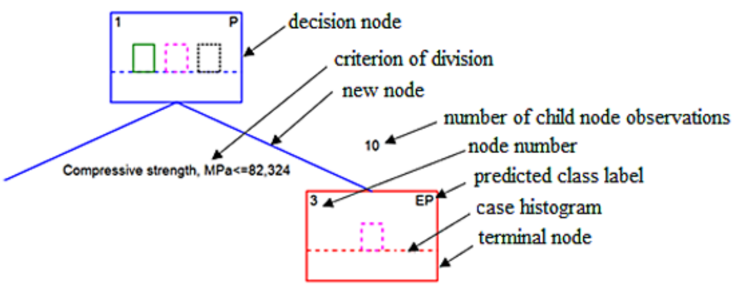


Fig. 1. Example of a decision tree created in the STATISTICA software package.

MATERIALS AND METHODS

Three types of resin mortars were prepared:

A. Epoxy mortar modified with PET degradation product – (EP), of the following composition:

- epoxy resin (EP) – 20% of the total composition
- poly(ethylene terephthalate) (PET) glycolisate – 0%, 5%, 10% or 15% by weight relative to the amount of resin
- Z-1 (triethylenetetramine) hardener – 10% by weight relative to the amount of resin
- quartz sand with a grain size of 0–2 mm, conforming to the requirements of standard PN EN 196–1 – 80% of the total composition

B. Polyester mortar I modified with PET degradation product – (P), of the following composition:

- unsaturated polyester resin Polimal 103 – 20% of the total composition
- poly(ethylene terephthalate) (PET) glycolisate – 0%, 5%, 10% or 15% by weight relative to the amount of resin
- K-1 hardener – 2 g per 100 g of resin
- Co accelerator 1% – 0.4 g per 100 g resin
- quartz sand with a grain size of 0–2 mm, conforming to the requirements of standard PN EN 196–1 – 80% of the total composition

C. Polyester mortar II modified with PET degradation product – (P-HDK), of the following composition:

- unsaturated polyester resin Polimal 103 – 20% of the total composition
- poly(ethylene terephthalate) (PET) glycolisate – 0%, 5%, 10% or 15% by weight relative to the amount of resin
- K-1 hardener – 2 g per 100 g of resin
- Co accelerator 1% – 0.4 g per 100g of resin
- Colloidal silica HDK H 20 – 1% by weight in relation to the amount of resin, used to eliminate the phenomenon of sedimentation of aggregate in polyester mortars
- quartz sand with a grain size of 0–2 mm, conforming to the requirements of standard PN EN 196–1 – 80% of the total composition

Selected physicochemical properties of resins and glycolisate, respectively, are presented in tables 1–3.

Obtaining of epoxy and polyester compositions modified with PET glycolisate

The epoxy compositions modified with PET glycolisate were obtained on the basis of Epidian 5 epoxy resin and a PET degradation product. Appropriate amounts of epoxy resin and modifier were weighed in a beaker using technical scales with an accuracy of ± 0.01 g and mixed with a rod to make them uniform.

After mixing, the ingredients were baked for 60 minutes at 353 K to enable the functional groups of the two components to react.

Table 1. The physicochemical properties of Epidian 5

Type of resin	Density, g/cm^3	Viscosity 25°C, mPa s	Molecular weight, g/mol	Epoxy count LE, mol/100 g
Epidian 5	1.17	30000	450	0.49

Table 2. The physicochemical properties of Polimal 103

Type of resin	Density, g/cm^3	Viscosity 25°C, mPa s	Gelation time 25°C, min	Acid numer LK, mg KOH/g
Polimal 103	1.10 ÷ 1.16	350	30	32

Table 3. The physicochemical properties of PET glycolisate

Type of glycolisate	Density 23°C, g/cm^3	Melting temperature, °C	Form	Hydroxyl number, mgKOH/g	Molecular weight	
					$\overline{M_n}$ g/mol	$\overline{M_w}$ g/mol
PET	1.30	78 ÷ 82	Semi-solid wax	515	404	849

Obtaining polyester compositions modified with PET glycolisate

The polyester compositions modified with PET glycolisate were obtained on the basis of Polimal 103 polyester resin and a PET degradation product. Appropriate amounts of polyester resin and modifier were weighed in a beaker using technical scales with an accuracy of ± 0.01 g and mixed with a rod make them uniform.

Production and curing of mortars

Curing of epoxy compositions

After reaching room temperature, the prepared PET glycolisate modified epoxy composition was mixed with the appropriate amount of Z-1 hardener (10 parts/100 g resin). The ingredients were mixed thoroughly with a glass rod until a homogeneous mixture was obtained.

Curing of polyester compositions

The prepared compositions were combined with the K-1 hardener in an amount of 2% in relation to the amount of resin and mixed thoroughly. The cobalt accelerator was then added in an amount of 0.4 g per 100 g resin and mixed thoroughly again.

Production of epoxy and polyester mortars

The mortar samples were prepared using a laboratory mixer. The previously prepared resin compositions were transferred to the mixer bowl and mixed with standard sand while maintaining the same mixing time and mixer speed. For each composition differing in ingredients, three mortar samples of 40x40x160 mm were made for the flexural and compressive strength tests as well as hardness tests. The samples thus prepared were left to cure for 7 days at room temperature.

Mortar testing

For hardened mortars, the following properties were determined:

a) Strength: flexural f_f and compressive strength f_c.

These tests were carried out in a strength testing machine equipped with appropriate inserts, on standard bars according to the PN-EN 196–1:2016 standard.

b) HB hardness

The determination was performed based on PN-EN ISO 2039–1: 2004. This standard applies to the determination of hardness by ball pressing and is intended for testing of plastics. This test method was chosen due to the fact that the matrix in the tested mortars was an epoxy resin. The test method consists in pressing balls, under a given load, into the surface of the test piece. The depth of the impression under the load is measured and the ball surface impression area is calculated on this basis. Using the ball pressing method (HB) hardness can be calculated from the following relationship:

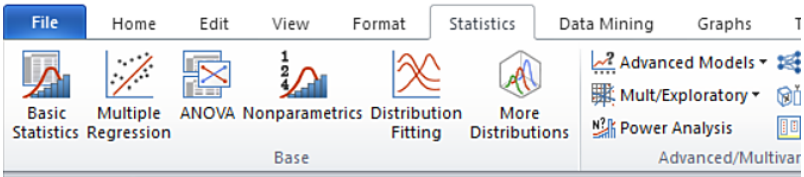
$$HB = \frac{Applied\ load}{Impression\ area} \qquad (2)$$

Construction of analytical database

The obtained test results are summarized in a table, which subsequently serves as a data sheet necessary to carry out the analyses using the Statistica 12 software package. A fragment of the table is shown in Figure 2. The data table contained 5 columns. In the first one, the information about the type of resin used to make the mortar is presented. It was, respectively, epoxy (EP), polyester (P) and polyester with the addition of colloidal silica (P-HDK). The mortar also contained, respectively, from 0–15% modifier in the form of a glycolisate obtained on the basis of PET waste. The mortar type here was a grouping variable identifying the type of mortar. The next three columns contain the values of three input variables, i.e. hardness, flexural strength and compressive strength. The final, 5th column lists the labels assigned to the samples at random. This variable has the character of the sample ID. It enables to distinguish between the samples to be analysed (Training) and the sample intended for cross-checking (Test) allowing the assessment of the quality of the classifier.

RESULTS AND DISCUSSION

The following statistical methods were used to develop the results of the conducted research: descriptive statistics, discriminant analysis and classification trees.



	1 Type of mortar	2 Hardness, MPa	3 Flexural strength, MPa	4 Compressive strength, MPa	5 Stage
1	EP	100,70	25,55	86,75	Training
2	EP	95,70	24,61	85,65	Training
3	EP	103,50	23,91	82,75	Training
4	EP	180,30	30,00	95,80	Test
5	EP	177,20	31,41	93,55	Training
6	EP	193,30	33,75	93,20	Training
7	EP	174,20	35,16	102,60	Training
8	EP	174,20	34,69	94,45	Training
9	EP	177,20	40,31	98,85	Test
10	EP	165,90	30,70	93,65	Training
...					
15	P	119,60	20,86	77,70	Training
16	P	112,60	22,97	74,40	Training
17	P	119,60	22,50	76,45	Training
18	P	112,60	22,73	77,30	Training
19	P	75,10	23,20	67,75	Test
20	P	76.60	22,27	70,25	Training
...					
30	P-HDK	76,60	20,63	66,30	Training
31	P-HDK	76,60	20,86	65,05	Training
32	P-HDK	116,00	20,39	60,35	Training
33	P-HDK	87,00	21,09	61,40	Training
34	P-HDK	112,60	18,98	56,00	Training
35	P-HDK	106,30	18,98	55,25	Training
36	P-HDK	119,60	18,98	54,00	Training

Fig. 2. Fragment of the database describing selected parameters of the analysed mortars.

Descriptive statistics

For the purpose of graphical assessment of laboratory data sets, a box and whisker plot was produced, showing the ranges of the described variables marked in the studies (Figure 3). On the basis of Figure 3, it can be concluded that the variables are significantly different in terms of the average value of variables. This forces the application of the standardization procedures during the construction of the classification model by means of discriminant analysis. The basic measures for the marked variables are included in the table shown in Figure 4. For all three variables, histograms were also produced, and the Shapiro-Wilk normality test was carried out. The obtained results are presented in Fig. 5.

Discriminant analysis

Discriminant analysis was carried out using the Multivariate exploration techniques module available in the Statistica 12 software package. Two stages of building the model were distinguished:

1. ***Learning stage.*** Building a classifier using cases that make up the training set, marked in the table as **Training** – a total of 30 cases. At this stage, the discriminant function analysis is used to decide which variables allow the best way to divide a given set of cases into naturally occurring groups.
2. ***Test stage.*** Classifier validation using the cases labelled **Test**. For this purpose, 2 cases for each type of mortar, previously selected from the entire data set, were used, which created a 6-piece test set allowing for the assessment of prognostic correctness of the designated discriminant functions with the cross-analysis method.

In the first stage of the analysis, the use of discriminant analysis methods allows to search for an answer to the question whether the three groups of classified mortars differ significantly in the average values of variables describing the

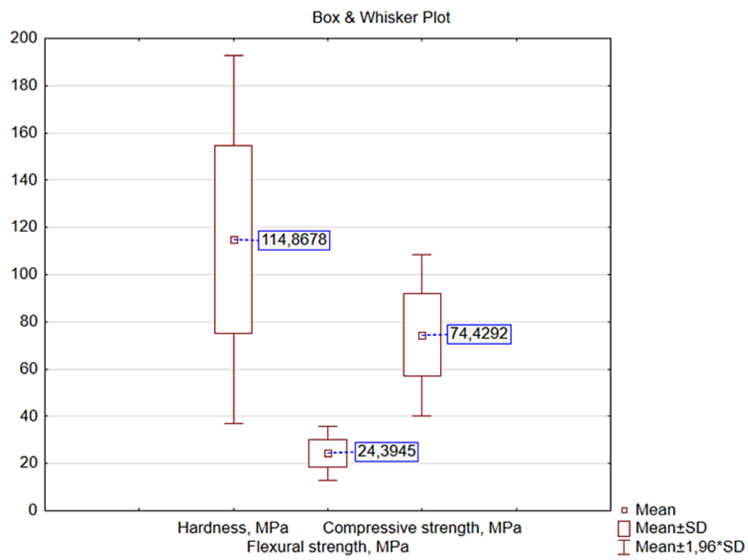


Fig. 3. Ranges of variables tested.

Variable	Descriptive Statistics (2019-01-18-data-EP-P-HDK)				
	Valid N	Mean	Minimum	Maximum	Std.Dev.
Hardness, MPa	36	114,8678	50,56000	193,3000	39,71282
Flexural strength, MPa	36	24,3945	17,10938	40,3125	5,85773
Compressive strength, MPa	36	74,4292	44,60000	113,1000	17,44981

Fig. 4. Results of calculations of strength and hardness parameters for the tested mortars.

samples produced, i.e.: hardness, flexural strength and compressive strength. Thus, it can be determined if these variables can be used to test whether the tested mortars belong to these three groups. One of the basic assumptions of the possibility of applying the discriminant analysis is the origin of data from a population with a multivariate normal distribution. In the case of the analysed mortars this assumption is violated, as evidenced by the results of the Shapiro-Wilk normality test shown in Figure 5. Only in the case of the compressive strength variable is the normality condition met. Despite this, an attempt was made to apply the discriminant analysis to the classification of mortar types. The simulation studies carried out in recent years using the Monte Carlo methods have shown empirically that the impact on the obtained results of non-compliance with the assumption of normality is negligible [15]. The results of the discriminant analysis carried out are presented in Figures 6–8. They show that among the three predictors used, only the compressive strength parameter plays a significant role in discrimination ($p < 0.05$). The fractional Wilks' Lambda values (Fig. 7) indicate the contribution of individual variables in the predictive model. On this basis, it can be concluded that after compressive strength, the largest share in the model is played by the flexural strength variable and the smallest by hardness. The results of the chi-square test carried out in the canonical analysis indicate the high significance of the generated discriminant function (Figure 8). On the basis of this test, it can be concluded that only one discriminant function can be interpreted (only the first function is statistically significant, $p < 0.05$).

Determination of canonical discriminant functions was performed by calculating their coefficients (Figure 9).

These coefficients relate to the standardized variables and refer to comparable ranges of attribute variability. Therefore, they may be used to interpret the variables that vary considerably in size, as is the case with the tested mortars (Figure 3). In the last two lines of the table presented in Figure 9, there are eigenvalues (roots) and the cumulative ratio of the explained variance corresponding to each function. These parameters allow us to conclude that the first function is responsible for almost 99% of the explained variance, i.e. almost 99% of the discriminative power is explained by this function. On the basis

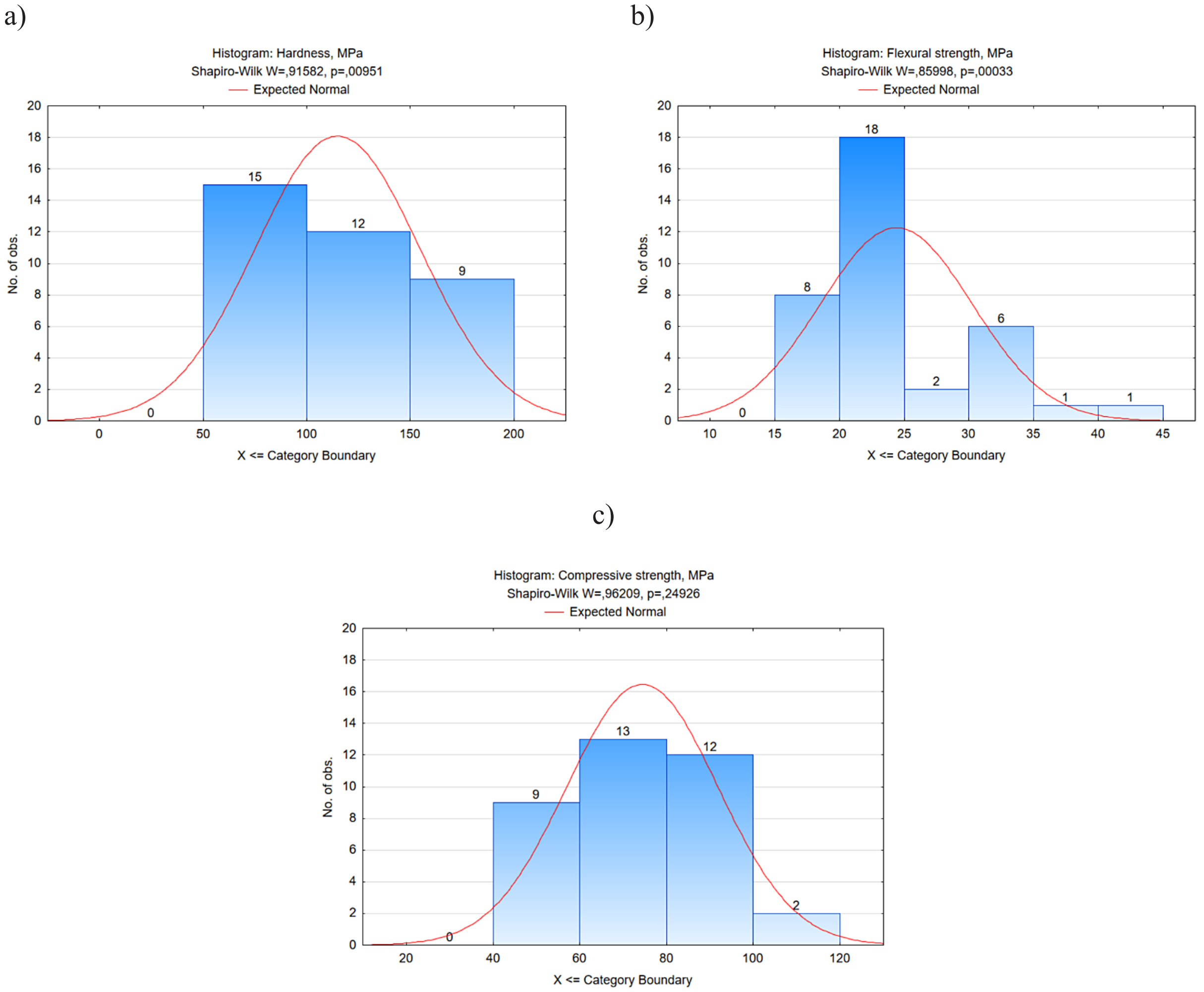


Fig. 5. Histograms of the variable distribution: (a) hardness, (b) flexural strength, (c) compressive strength.

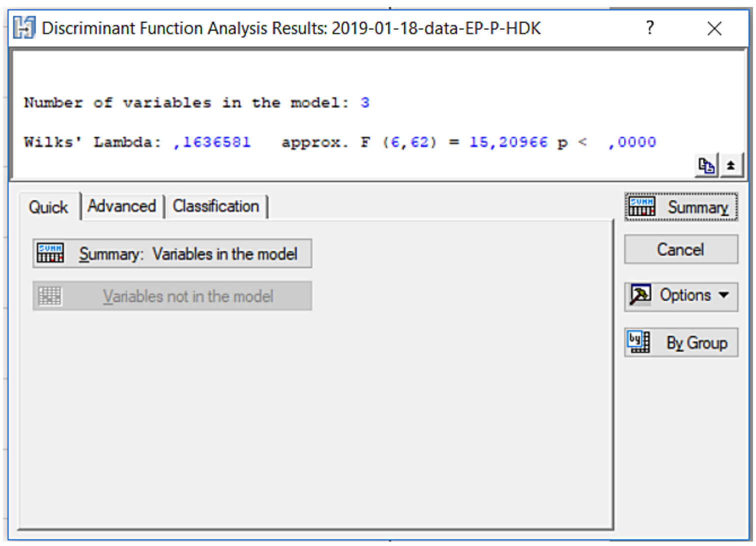


Fig. 6. Results of discriminant analysis.

of the table containing mean canonical variables (Figure 10), it can be concluded that the considered discriminant function mainly differentiates the mortars obtained on the basis of epoxy resin.

This interpretation is also confirmed by the analysis of the scatterplot of non-standardized values of the first function with respect to the value of the second function presented in Figure 11.

N=36	Discriminant Function Analysis Summary (2019-01-18-data-EP-P-HDK) No. of vars in model: 3; Grouping: Type of mortar (3 grps) Wilks' Lambda: ,16366 approx. F (6,62)=15,210 p< ,0000					
	Wilks' Lambda	Partial Lambda	F-remove (2,31)	p-value	Toler.	1-Toler. (R-Sqr.)
Hardness, MPa	0,167695	0,975925	0,382370	0,685415	0,536736	0,463264
Flexural strength, MPa	0,189685	0,862790	2,464985	0,101514	0,498275	0,501725
Compressive strength, MPa	0,234021	0,699331	6,664048	0,003914	0,646716	0,353284

Fig. 7. Evaluation of the suitability of variables in the discriminant analysis.

Removed	Chi-Square Tests with Successive Roots Removed (2019-01-18-data-EP-P-H Sigma-restricted parameterization					
	Eigen-value	Canonicl R	Wilk's Lambda	Chi-Sqr.	df	p-value
0	4,771050	0,909242	0,163658	57,91923	6,000000	0,000000
1	0,058785	0,235629	0,944479	1,82791	2,000000	0,400936

Fig. 8. The results of chi-square test with successive canonical roots.

Variable	Standardized Coefficients (2019-01-18-data-EP-P-HDK) for Canonical Variables	
	Root 1	Root 2
Hardness, MPa	0,178795	0,576091
Flexural strength, MPa	-0,545288	0,729594
Compressive strength, MPa	-0,704308	-0,993681
Eigenval	4,771050	0,058785
Cum.Prop	0,987829	1,000000

Fig. 9. Standardized discriminant function coefficients.

Group	Means of Canonical Variables (2019-01-18-data-EP-P-HDK)	
	Root 1	Root 2
P	0,60458	-0,321355
EP	-2,80949	0,102560
P-HDK	2,20491	0,218795

Fig. 10. Average values of discriminant function.

The points corresponding to the epoxy mortars are placed much more to the left in the figure (they take negative values for the first function), so this discriminant function mainly distinguishes this type of mortar.

The classification functions assume a linear model of the general form described by formula (1). The coefficients of these functions enabling the classification of cases are presented in the table shown in Figure 12.

The values of the calculated coefficients were used to create linear classification functions K1, K2 and K3 in the form (3)-(5):

$$K_1 = -49.6562 - 0.151 * Hardness + 2.0837 * \\ * Flexuralstrength + 0.9296 * Compressivestrength \tag{3}$$

$$K_2 = -88.326 - 0.1649 * Hardness + 2.8263 * \\ * Flexuralstrength + 1.1773 * Compressivestrength \tag{4}$$

$$K_3 = -35.0257 - 0.1282 * Hardness + 1.92 * \\ * Flexuralstrength + 0.7218 * Compressivestrength \tag{5}$$

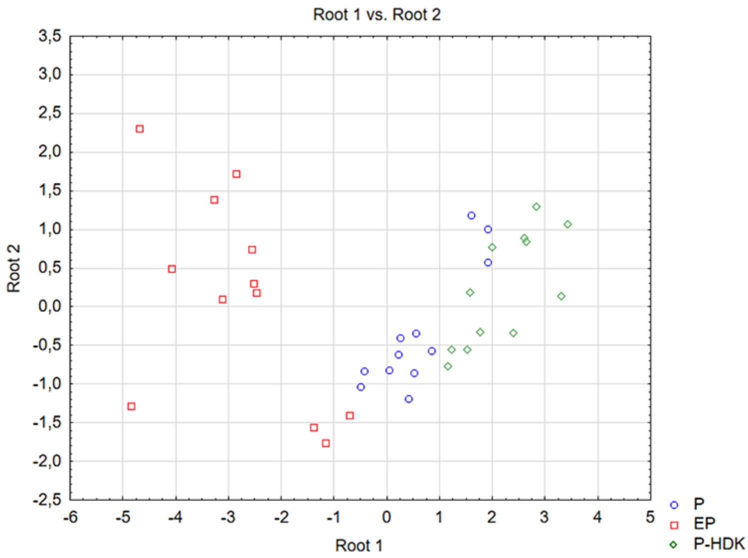


Fig. 11. Scatterplot for the first two discriminant functions.

The table shown in Figure 13 contains the results pertaining to the correctness of the classification process carried out for the training set (30 cases). It can be concluded that 77.78% of cases were classified correctly. The designated classification functions (K1, K2, K3) enable to classify new cases. A mortar obtained on the basis of a given resin is included in the group for which the value of the classification function is the highest.

In the second stage, the model created was used to predict the type of mortar. The correctness of the operation of the designated classification functions was checked by classifying the cases from the drawn test set (column 5, Fig. 2), i.e. those that had not been previously used to calculate the function coefficients K1, K2 and K3 (cross-evaluation). The obtained results are presented in the table shown in Fig. 14.

Comparing the results from both tables (Figures 13 and 14), it can be concluded that the average percentage of the correctly classified mortars for the test sample is slightly larger (83.3%) than the result obtained for the training set (77.78%). This is probably related to the fact that the predictive capability of the classification functions generated is assessed only on the set of 6 data points drawn from the studied sample (the remaining data were the test sample), and not, for example, on the new data obtained as a result of planning and implementing a similar research experiment.

Decision trees

The second of the suggested algorithms for searching for patterns characterizing the relationships occurring between the data stored in the database was carried out with a method allowing the presentation of the results in the form of a classification tree. The advantage of this method is the lack of initial assumptions regarding data distributions, which is especially useful in the situations where the correlated data occur. The *Classification Trees* module available in the Statistica 12 software package was used to build a decision tree allowing for the classification of the studied mortars into three groups. The median variability

	Classification Functions for Type of mortar (2019-01-18-data-EP-P-HDK) Sigma-restricted parameterization		
Effect	P p=,3333	EP p=,3333	P-HDK p=,3333
Intercept	-49,6562	-88,3260	-35,0257
Hardness, MPa	-0,1510	-0,1649	-0,1282
Flexural strength, MPa	2,0837	2,8263	1,9200
Compressive strength, MPa	0,9296	1,1773	0,7218

Fig. 12. Parameters defining classification functions K1, K2 and K3.

Class	Classification Matrix (2019-01-18-data-EP-P-HDK) Classifications: Rows(Observed) Columns(Predicted) (Analysis sample)			
	Percent Correct	P p=,3333	EP p=,3333	P-HDK p=,3333
P	75,00000	9,00000	0,00000	3,00000
EP	83,33333	2,00000	10,00000	0,00000
P-HDK	75,00000	3,00000	0,00000	9,00000
Total	77,77778	14,00000	10,00000	12,00000

Fig. 13. Classification matrix of cases from the training group.

Class	Classification Matrix (2019-01-18-data-EP-P-HDK) Classifications: Rows(Observed) Columns(Predicted) (Validation sample)			
	Percent Correct	P p=,3333	EP p=,3333	P-HDK p=,3333
P	50,0000	1,000000	0,000000	1,000000
EP	100,0000	0,000000	2,000000	0,000000
P-HDK	100,0000	0,000000	0,000000	2,000000
Total	83,3333	1,000000	2,000000	3,000000

Fig. 14. Classification matrix of cases from the test group.

intervals for the values of strength parameters and hardness were used to build the tree. As in the case of the discriminant analysis method, the decision tree was determined based on the input data contained in the table, part of which is shown in Figure 2. Thirty randomly selected mortar samples constituted the training sample used at the tree construction stage, while 6 cases formed a test group, used to evaluate the tree built. The first step assessed the validity of all three variables that were the results of laboratory tests. The results of the ranking are shown in Figure 15.

The analysis of the obtained results shows that the strength parameters are far more important, and much less the mortar hardness. A classification tree was generated, the structure of which is shown in Figure 16. Such a decision tree can be exchanged for three classification rules:

Rule 1: if Compressive strength > 82.734 MPa then EP

Rule 2: if Compressive strength ≤ 82.734 MPa and Flexural strength ≤ 21.137 MPa then P-HDK

Rule 3: if Compressive strength ≤ 82.734 MPa and Flexural strength > 21.137 MPa then P

The number of splits (2) given in the header of Fig. 16 means the number of decision nodes, i.e. the number of questions in the system. The number of terminal nodes was 3. They represent the "leaves" of the decision tree and indicate the type of group identified. The attribute of compressive strength was found in the root of the tree. It proved to be the most important decision attribute (this is confirmed by the results obtained by means of discriminant analysis). The value of flexural strength was then examined. The least important parameter was hardness. We do not ask about the value of this parameter by analysing the decision tree or applying classification rules. This attribute proved to be redundant and, in this case, it does not have to be determined, which significantly speeds up the testing of composite samples in the laboratory.

While analysing the content of leaf nodes, it can be concluded that epoxy mortars form a well-isolated set, as in this case only one decision path leads to a leaf, while for the other groups – two. The tables showed in Figures 17 and 18 present the results of the effectiveness of classifying the generated decision tree for the training and test data sets respectively.

While analysing these results, it can be concluded that among 30 cases forming the teaching set, all of the mortars were classified correctly. However, from a set of 6 mortars forming the test group, one sample was classified incorrectly. Thus, the classification efficiency of the generated decision tree for the training set is 96.67%, and for the test set 83.33%. These results are better than those obtained with the discriminant method.

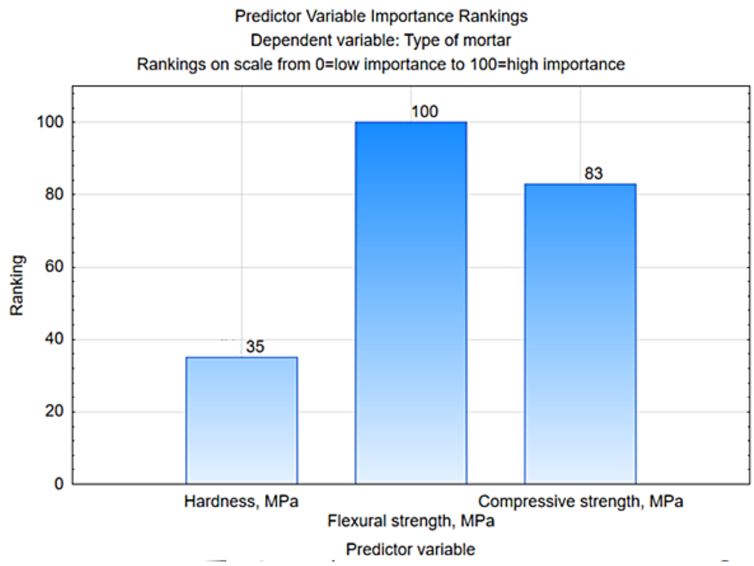


Fig. 15. Evaluation of the validity of predictors for the decision tree method.

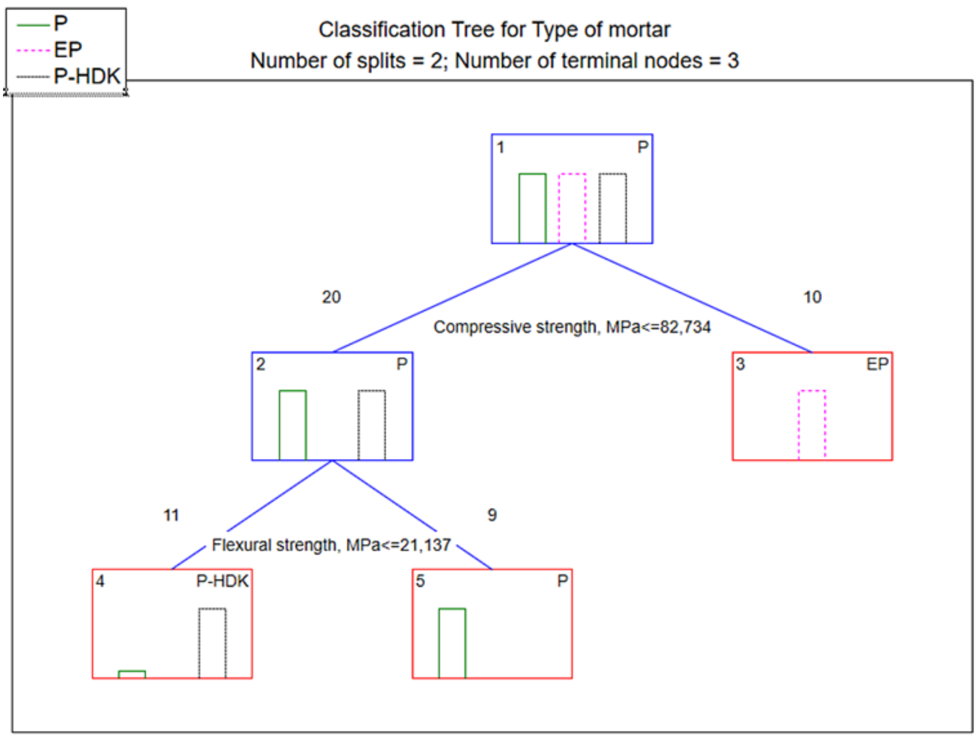


Fig. 16. Classification tree.

Learning Sample Misclassification Matrix (2019-01-18-data-EP-P-HDK)
Predicted (row) x observed (column) matrix
Learning sample N = 30

Class	Class P	Class EP	Class P-HDK
P		0	0
EP	0		0
P-HDK	1	0	

Fig. 17. Results of incorrect classifications for the training sample.

Class	Test Sample Misclassification Matrix (2019-01-18-data-EP-P-HDK) Predicted (row) x observed (column) matrix CV cost = ,16667; s.d. CV cost = ,15215 **Class P**	Class EP	Class P-HDK
P		0	0
EP	0		0
P-HDK	1	0	

Fig. 18. Results of incorrect classifications for the test group sample.

CONCLUSIONS

After application, the following conclusions can be drawn for the classification of the three types of resin mortars, two methods of data mining, i.e. discriminant analysis and decision trees, and a comparison of the obtained results:

- Both of the methods confirmed that the compressive strength is the most important variable that allows the discrimination of mortars with different types of resin.
- In the case of discriminant analysis, one discriminant function can be interpreted (only the first one is statistically significant ($p < 0.05$)), because it explains almost 99% of the entire discriminant power.
- Both methods confirmed that epoxy mortars constitute a well-isolated collection. In the case of the discriminant analysis methods, the elements of this set are placed on the scatterplot much more to the left, so the first discriminant function mainly distinguishes this type of mortar from the other two. However, there is only one decision path in the classification tree chart for epoxy mortars.
- Methods of discriminant analysis and decision trees showed that for the classification of the tested mortars the decisive parameter is compressive strength, flexural strength was less important and the least significant was hardness.
- The K1, K2, K3 functions determined in the discriminant analysis enable the classification of new cases belonging to the test set, which was not used to calculate the function coefficients.
- Classification can also be successfully carried out using decision trees or a set of classification rules. In this case, the classification effectiveness for the training set is significantly better than in the case of discriminant analysis and amounts to 96.67%.
- The predictive capacity of both data mining methods was the same, as the correctness of classification of mortars belonging to the test set amounted to 83.33%. Typically, these results can be improved by extending the database, thus introducing the measurement results of the properties of new polymer composites, obtained in a similar manner, into the data set.
- The conclusion that compressive strength is the most important parameter (when compared with flexural strength and hardness, strictly interrelated), is obvious, at least from the mechanical point of view. In this sense, the results given by the algorithms can be understood as the verification of the correctness also in the mechanics of materials field.

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