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Strength qualities of test specimens of materials for preliminary non-removable prosthetic constructions - Part 2. Principal component analysis

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Prosthetic rehabilitation prior to definitive prosthesis placement is an important stage in dental prosthetic treatment. Fracture of provisional bridge constructions is a common problem in practice, and reinforcement with different materials is an approach for prevention and repair in such cases. Investigating the strength properties of materials for provisional prosthesis through in vitro studies is crucial for making informed choices regarding material and reinforcement in treatment plans. For this purpose, investigation of the physico-mechanical characteristics (maximum force before fracture, flexural strength, and modulus of elasticity) of combinations between six types of polymeric materials and five types of reinforcing fibers was conducted. Comparative analysis of such a large dataset (1260 test specimens) was performed using Principal Component Analysis (PCA). The results are promising for the qualities of provisional non-removable prostheses fabricated using digital methods with or without reinforcement, and they allow for the systematization of the studied materials. The test specimens made of CAD/CAM resin for 3D printing, specifically Temporary CB resin (FormLabs, USA), demonstrated the most optimal strength qualities.

Keywords: Principal component analysis, mechanical characteristics, dental polymers, preliminary non-removable prosthetics, interim dental materials

INTRODUCTION

The theoretical study of the mechanical properties of materials is extremely important for predicting their behavior under applied loads of various types [1] as well as for achieving a better understanding of failure mechanics [2]. This applies to the greatest extent when considering materials that are used in medicine and specifically in dentistry. The mechanical properties of materials for preliminary non-removable prosthetic constructions (PNRPC) are an important factor in determining the clinical application [3] of different materials and methods and are crucial for the long-term success and effectiveness of this mandatory stage prior to final prosthetic treatment, as well as for patient satisfaction and motivation towards the proposed therapeutic approach. In preliminary bridge constructions, the investigation [4] and interpretation of flexural strength, maximum force before fracture, and modulus of elasticity [5] under laboratory in vitro conditions, play a crucial role in clinical approval and selection of materials and reinforcements in treatment plans. In 2004, Kim and Watts [6] examined the influence of glass fiber reinforcement on polymers for PNRPC - three dimethacrylate materials and one monomethacrylate. The effect of water storage on the test specimens was also compared. The study found a significant increase in flexural strength values for the fiber-reinforced groups and lower values for the specimens stored in a water environment, but without statistical significance.

In a similar study, again in 2004, Hamza *et al.* [7] compared the mechanical properties of three types of PNRPC materials (poly(methyl methacrylate) (PMMA), poly(ethyl methacrylate) (PEMA) and composite), reinforced with two types of glass fibers and four types of polyethylene fibers (Kevlar). The authors investigated fracture strength and flexural strength of the test specimens, according to ASTM no. E 399-83 and ISO 14077, respectively, using non-reinforced specimens as a control group.

In a comparative study from 2022, Pantea *et al.* [8] performed testing on polymer materials for the fabrication of preliminary constructions - two using conventional methods and two using digital methods.

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Their results were better for the polymer materials for 3D printing, which they attributed to the homogeneity of the specimens produced using this method.

In data analysis, a contemporary statistical method called principal component analysis (PCA) is used [9]. The capabilities of PCA in processing large volumes of data make it a preferred method in many cases. PCA is performed by transforming the observations of correlated variables into a set of linearly uncorrelated variables through orthogonal transformation. These new transformed variables are called principal components. They are arranged in a way that the preservation of variation in the original variables decreases along the order. Thus, the first principal component retains the maximum variation (maximum possible information) present in the original components, followed by the second principal component retaining the remaining maximum information, and so on.

For the purposes of studying the mechanical characteristics of polymer dental composites for preliminary non-removable prostheses with or without reinforcing fibers, (PCA) was used. Six types of experimental specimens were fabricated according to ISO 10477 standard, employing both laboratory conventional methods and digital methods such as CAD/CAM milling and 3D printing. Some of them were reinforced with five types of fibers - metal (with and without aesthetic coating), glass (with and without polymer coating), and polypropylene fibers. Several mechanical properties of the dental samples were measured, including flexural strength, maximum force before fracturing, and modulus of elasticity. The results obtained for these properties were further analyzed using PCA.

The objective of this study is to evaluate the strength qualities of test specimens made from materials for PNRPC based on in vitro data using PCA analysis.

MATERIALS AND METHODS

The strength properties of experimental specimens made from three types of laboratory dental polymers for PNRPC are studied and compared. The specimens are made from thermopolymerizing material, factory-polymerized material for subtractive fabrication using CAD/CAM, and light-polymerizing material for additive fabrication using CAD/CAM, based on the type of polymerization activation. The specimens were categorized as unreinforced or reinforced with fibers, including dental glass fibers - Fiber Splint One Layer (Polydentia, Switzerland), polyethylene fibers - Ribbond Regular 4.0 mm (Ribbond Inc., USA), braided multi-strand orthodontic wire for splinting - 015" Leone (Leone S.p.a., Italy), esthetically coated chrome-cobalt ligature wire - 012" Leone (Leone S.p.a., Italy), and glass fiber thread coated with light-polymerizing resin for dental use - Interlig 8.5 ×0.2 mm (Angelus, Brazil). The details are presented in Tables 1 and 2.

The specimens were fabricated (Fig. 1) *in vitro* using a device that is registered as a protected subject of industrial property (utility model) in the Patent Office of the Republic of Bulgaria under No. 4383 U1 with the following title: "Device for fabricating specimens from polymer materials for crowns and veneers with reinforcement capability"

For the three-point bending flexural test an universal testing system MultiTest single-column force tester 2.5-i (Mecmesin Ltd., United Kingdom) was used. The testing was conducted following the instructions given in ISO 10477:2021 ‘Dentistry – Polymer-based crown and veneering materials’:

“…Flexural strength test apparatus, appropriately calibrated, to provide a constant cross-head speed of (1,0 ± 0,3) mm/min. The apparatus consists of two rods (2 mm in diameter), mounted parallel with 20 mm between centres, and a third rod (2 mm in diameter) centred between, and parallel to the other two, so that the three rods in combination can be used to give a three-point loading to the specimen...“

All data from specimens tested was collected by the Emperor™ Force software (Mecmesin Ltd., United Kingdom) and exported in table format to Excel (Microsoft, USA).

The obtained statistical data on the physical-mechanical characteristics of the laboratory and clinical experimental specimens, with and without reinforcement, were subjected to a comprehensive analysis using the Principal Component Analysis (PCA) method included in the software package OriginPro 7.5.

The principal components are the eigenvectors of the covariance matrix, and they are orthogonal or perpendicular to each other. The first two principal components have been used to plot the data in two dimensions and visually identify clusters of closely related data points.

The PCA method was performed in several main steps [10]:

Step 1: Data normalization

The PCA method is sensitive to the variations of the initial variables. When the variables vary on different scales with large deviations from each other, varables with larger ranges of variation may dominate those with smaller ranges. To normalize the variables in the current sample, the values of the variables with greater variation are subtracted. After normalization, the variables are transformed to equal scales.

Step 2: Calculation of the covariance matrix

The covariance matrix consists of the covariances between all possible pairs of variables. The (i,j) element represents the covariance between the i-th and j-th variable. The covariance matrix is of size p x p, where p represents the number of variables. Since the covariance of a variable with itself is its variance, the elements on the main diagonal of the covariance matrix represent the variances of each variable. Covariance is commutative, and the elements of the covariance matrix are symmetric with respect to the main diagonal, which means that the upper and lower parts are equal.

This matrix shows how the variables in the input dataset vary from their mean values relative to each other or indicates the presence of correlations between them. Correlation, in turn, denotes the relationship between two variables. The correlation value varies from -1 to +1.

The presence of a positive value in an element of the covariance matrix indicates that increasing the value of one variable in the considered pair of variables leads to an increase in the value of the other variable.

The presence of a negative value in an element of this matrix indicates that increasing the value of one variable leads to a decrease in the value of the other variable.

The presence of an element in the matrix with a value of 0 indicates that the variables are orthogonal or have no correlation between them.

On the other hand, the absolute value of each element of the covariance matrix indicates the strength of the relationship between the variables.

Table 1. Distribution of the investigated non-reinforced test specimens.

Group	Code	NS[1]	Subgroup Material/Supplier	Code	N	Storage conditions	Code	NS[1]
Solid laboratory specimens	3.1	180	HP – PMMA[3] Superpont C+B (Spofa Dental, Czech Republic)	3.1.1	60	Dry DW[2]	3.1.1.A 3.1.1.B	30 30
			CAD-CAM pre-polymerized PMMA DD temp MED (Dental Direkt GmbH, Germany)	3.1.2	60	Dry DW	3.1.2.A 3.1.2.B	30 30
			CAD-CAM printing resin Temporary CB Resin (FormLabs, USA)	3.1.3	60	Dry DW	3.1.3.A 3.1.3.B	30 30
Solid clinical specimens	3.2	180	Self-polymerizing PEMA DENTALON plus (Kulzer, Germany)	3.2.1	60	Dry DW	3.2.1.A 3.2.1.B	30 30
			Light-curing composite Revotek LC (GC, Japan)	3.2.2	60	Dry DW	3.2.2.A 3.2.2.B	30 30
			Dual-curing composite TempSpan (Pentron, USA)	3.2.3	60	Dry DW	3.2.3.A 3.2.3.B	30 30

[1]Number of specimens;
[2]Distilled water;
[3]Heat polymerizing PMMA Superpont C+B (Spofa Dental, Czech Republic).

Table 2. Distribution of tested reinforced specimens.

Reinforcement	Code	NS[1]	Subgroup Material/Supplier	Code	N	Storage conditions	Code	NS[1]
Fiber glass thread Fiber Splint One Layer (Polydentia, Switzerland)	4.1	180	HP – PMMA[3]	4.1.1	60	Dry	4.1.1.A	30
						DW[2]	4.1.1.B	30
			CAD-CAM PMMA[4]	4.1.2	60	Dry	4.1.2.A	30
						DW	4.1.2.B	30
			CAD-CAM resin[5]	4.1.3	60	Dry	4.1.3.A	30
						DW	4.1.3.B	30
Polyethylene thread Ribbond Regular 4.0 mm (Ribbond Inc., USA)	4.2	180	HP - PMMA	4.2.1	60	Dry	4.2.1.A	30
						DW	4.2.1.B	30
			CAD-CAM PMMA	4.2.2	60	Dry	4.2.2.A	30
						DW	4.2.2.B	30
			CAD-CAM resin	4.2.3	60	Dry	4.2.3.A	30
						DW	4.2.3.B	30
Metal triple-braided wire for splinting 015" Leone (Leone S.p.a., Italy)	4.3	180	HP - PMMA	4.3.1	60	Dry	4.3.1.A	30
						DW	4.3.1.B	30
			CAD-CAM PMMA	4.3.2	60	Dry	4.3.2.A	30
						DW	4.3.2.B	30
			CAD-CAM resin	4.3.3	60	Dry	4.3.3.A	30
						DW	4.3.3.B	30
Aesthetically coated ligature wire 012" Leone (Leone S.p.a., Italy)	4.4	180	HP - PMMA	4.4.1	60	Dry	4.4.1.A	30
						DW	4.4.1.B	30
			CAD-CAM PMMA	4.4.2	60	Dry	4.4.2.A	30
						DW	4.4.2.B	30
			CAD-CAM resin	4.4.3	60	Dry	4.4.3.A	30
						DW	4.4.3.B	30
Glass fiber threads coated with light-curing resin Interlig 8,5 x 0,2 mm (Angelus, Brazil)	4.5	180	HP - PMMA	4.5.1	60	Dry	4.5.1.A	30
						DW	4.5.1.B	30
			CAD-CAM PMMA	4.5.2	60	Dry	4.5.2.A	30
						DW	4.5.2.B	30
			CAD-CAM resin	4.5.3	60	Dry	4.5.3.A	30
						DW	4.5.3.B	30

[1]Number of specimens;
[2]Distilled water;
[3]Heat polymerizing PMMA Superpont C+B (Spofa Dental, Czech Republic);
[4]CAD-CAM factory pre-polymerized PMMA DD temp MED (Dental Direkt GmbH, Germany);
[5]CAD-CAM printing resin Temporary CB Resin (FormLabs, USA).

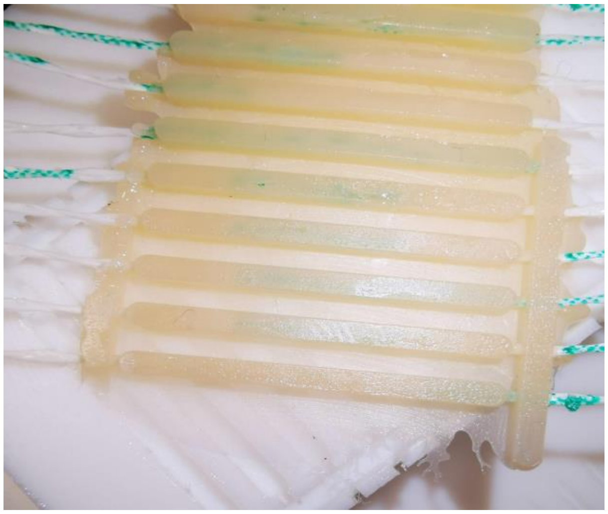

Fig. 1. Test series of specimens with a dual-curing clinical material for PNRPC reinforced with glass fibers for industrial use.

Step 3: Calculation of eigenvectors and eigenvalues of the covariance matrix

The eigenvalues are the coefficients in the eigenvectors. They indicate the amount of variance carried in each principal component. By arranging the eigenvectors in order of their eigenvalues, from highest to lowest, the principal components are obtained in order of significance.

Step 4: Calculation of principal components

Principal components are constructed in such a way that the first principal component captures the largest possible variation (variance) in the dataset. The second principal component captures the next largest variance, and so on until the last component. The number of principal components is equal to the original number of variables. Organizing the information into principal components allows for dimensionality reduction of the data array with minimal loss of information and the removal of components that carry little information. After determining the principal components, the percentage of variance (information) accounted for by each component is calculated by dividing the eigenvalue of each component by the sum of all eigenvalues.

Step 5: Determination of feature vectors

At this step, the decision is made regarding which principal components (with larger values and eigenvalues) should be retained and which ones should be discarded (those with smaller values and eigenvalues). The principal components that are retained form a matrix of vectors called the feature vector. The feature vector is a matrix whose columns represent the eigenvectors of the components that have been chosen to be preserved. This process reduces the dimensionality of the data.

Step 6: Data transformation along the principal components

In the final step, the data is transformed from the original axes (variables) to those represented by the principal components by multiplying the transpose of the original dataset by the transpose of the feature vector.

RESULTS

The PCA method was applied for statistical analysis of the experimental data obtained from testing 1260 specimens of the three physico-mechanical characteristics: bending strength (FS) in MPa; maximum force before fracture (Fmax) in N, and modulus of elasticity (E) in MPa, using the aforementioned materials, their reinforcements, and storage conditions. As a result, the values of two principal components, PC1 and PC2, were determined, which account for 87.56% and 12.43% of the variance in the experimental data, respectively.

The results obtained from applying PCA are presented in tables below. Table 3 displays the results of the covariance analysis. There is a high degree of correlation (r = 0.999) between FS and Fmax.

Table 3. Correlation matrix containing correlation coefficients.

Variables	FS (MPa)	Fmax (N)	E (MPa)
FS (MPa)	1	0.999	0.713
Fmax (N)	0.999	1	0.714
E (MPa)	0.713	0.714	1

In Table 3, FS (MPa) represents the bending strength, Fmax (N) represents the maximum force before fracturing, and E (MPa) represents the modulus of elasticity.

In Table 4, the summarized contribution of the dependent variables to the statistical model is presented. The highest percentage, 87.56%, is associated with the bending strength FS (MPa), followed by a contribution of 12.43% from the maximum force before fracturing Fmax (N). The eigenvalues of the matrix are shown in Table 4.

From the results presented in Tables 3, 4, and 5, it can be observed that there is a very strong correlation between the two variables FS and Fmax, indicating a close relationship between them. This means that an increase in one variable will inevitably lead to an increase in the other. The observed relationship is directly proportional, corresponding to a correlation coefficient of approximately +1. This provides a basis to consider that one of the two variables, FS or Fmax, can be chosen for further analysis while excluding the other variable from subsequent consideration. In this case, the variable Fmax is selected. A weaker correlation is observed between the variables E and FS.

Table 4. Eigenvalues of the correlation matrix.

Component	Eigenvalue	Variance	Cumulative Probability
FS (MPa)	2.626	87.56%	87.56%
Fmax (N)	0.372	12.43%	99.98%
E (MPa)	$5.39.10^{-4}$	0.02%	100%

Table 5. Extracted eigenvectors.

Vectors	Coefficients of PC1	Coefficients of PC2
FS (MPa)	0.600	-0.374
Fmax (N)	0.600	-0.372
E (MPa)	0.527	0.849

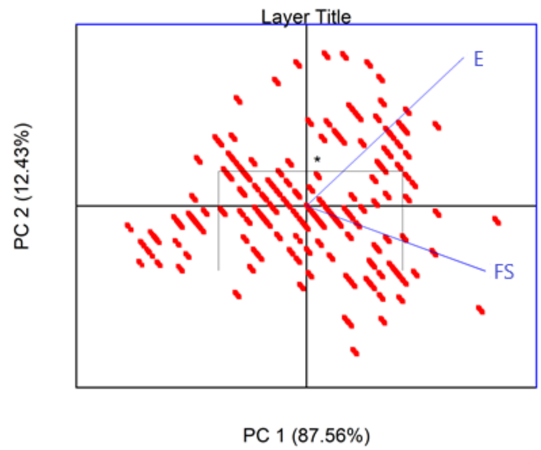

Fig. 2. Plot of the two principal components in two dimensions and visual identification of clusters of closely related data points.

Table 6. Obtained optimal results for the investigated polymer materials, reinforcements, and storage conditions after applying the PCA method.

Exp.	Sample Code	Reinforcement	Polymer	Storage conditions	F max/N	FS/MPa	E/MPa
Cluster with the highest modulus of elasticity E (MPa)							
484 492	4.1.3.A	Glass fibers - Fiber Splint One Layer (Polydentia, Switzerland)	CAD-CAM resin for printing Temporary CB Resin, (FormLabs, USA)	at room temperature	24.2 24.8	91.5 92.1	10894.8 10895.4
Cluster of data points with the highest modulus of elasticity E (MPa) and good flexural strength FS (MPa)							
154 157 164 174 181	3.1.3.B	Laboratory plain without reinforcement	CAD-CAM resin for printing Temporary CB Resin, (FormLabs, USA)	in distilled water at room temperature	26.4 26.5 26.6 26.9 26.8	99.9 100 100.1 100.4 100.3	11205.4 11205.5 11205.6 11205.9 11205.8
Cluster of data points with the highest flexural strength FS (MPa) and good modulus of elasticity E (MPa)							
785 789 795 804 807 810	4.3.2.B	Braided orthodontic wire for splinting - 015" Leone (Leone S.p.a., Italy)	CAD-CAM prefabricated PMMA DD temp MED (Dental Direkt GmbH, Germany)	in distilled water at room temperature	32.2 32.3 32.4 32.8 32.7 32.6	121.7 121.8 121.9 122.3 122.2 122.1	10893.6 10893.7 10893.8 10894.2 10894.1 10894
Cluster of data points with the highest flexural strength FS (MPa)							
786 793 797 799 801 805	4.3.2.B	Braided orthodontic wire for splinting - 015" Leone (Leone S.p.a., Italy)	CAD-CAM prefabricated PMMA DD temp MED (Dental Direkt GmbH, Germany)	in distilled water at room temperature	28.8 28.9 29 29.4 29.3 29.2	108.8 108.9 109 109.4 109.3 109.2	9337.8 9337.9 9338 9338.4 9338.3 9338.2

Figure 2 represents the distribution of data in two dimensions - the two principal components. Based on this visualization, clusters of closely related data points have been identified. In Table 6 are systematized the clusters of data points corresponding to the optimal results obtained for the two variables: modulus of elasticity E (MPa) and flexural strength FS (MPa), which determine more durable dental polymer materials.

DISCUSSION

In the present study, the PCA method was applied to investigate the physico-mechanical characteristics (maximum force before fracture, flexural strength, and modulus of elasticity) of polymer dental composites, used for preformed non-removable prostheses with or without reinforcing fibers.

Principal component analysis is a statistical method applied to process large datasets that contain a high number of measurements/observational features. Its application aims to reduce the dimensionality of the data while increasing interpretability and minimizing information loss. This is achieved by creating new uncorrelated variables, known as principal components, which sequentially maximize the variance. Finding such new variables involves solving an eigenvalue/eigenvector problem, where the new variables are defined based on the available dataset. In most cases, the analysis focuses on identifying the first two principal components, representing the data in two dimensions and visually identifying clusters of closely related data points.

When applying PCA, a strong correlation was found between two of the investigated mechanical properties - flexural strength and maximum force before fracture. The results obtained from the analysis of the experimental data for the remaining two properties - flexural strength and elastic modulus, allowed the identification of the three types of test specimens made of polymer materials with and without reinforcement, which exhibited the highest values for these properties. They are:

1) Plain test specimens made of CAD-CAM resin for 3D printing, specifically Temporary CB Resin from (FormLabs, USA).

2) Test specimens made of CAD-CAM resin for 3D printing, specifically Temporary CB Resin from (FormLabs, USA), reinforced with a single layer of glass fiber splint (Fiber Splint One Layer) from Polydentia (Switzerland).

3) Test specimens made of CAD-CAM factory PMMA (polymethyl methacrylate) material, specifically DD temp MED from Dental Direkt GmbH (Germany), reinforced with a triple-braided chrome-cobalt wire for splinting, specifically 0.015" wire from Leone (Italy).

CONCLUSIONS

The presented sequence of materials and reinforcements, determined based on PCA as the materials and combinations with the highest strength qualities, directs clinical thinking towards the need for validation of these data in a clinical experiment. This, along with the presented in vitro study, is the subject of scientific research in a dissertation titled "Reinforcement of materials for preliminary constructions - laboratory and clinical investigation".

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REFERENCES

1. J. Ivanova, V. Valeva, T. Petrova, W. Becker, *Mechanics of Advanced Materials and Structures*, **22**(10), 813 (2015).
2. J. Ivanova, V. Valeva, T. Petrova, W. Becker, Piezo health monitoring of adhesive joints, in: Proceedings of the 9th Conference on Sustainable Development of Energy, Water and Environment Systems SDEWES, September 20 - 27, 2014, Venice-Istanbul, article 0194.
3. S. F. Rosenstiel Land, M. F. Fujimoto, J. Contemporary Fixed Prosthodontics, Fifth edn. St. Louis, Missouri, Elsevier, 2016.
4. P. Pfeiffer, L. Grube, *The Journal of Prosthetic Dentistry*, **89**(2), 170 (2003).
5. Z. N. Al-Dwairi, K. Y. Tahboub, N. Z. Baba, C. J. Goodacre, *J. Prosthodont.*, **29**(
6. *The International Journal of Prosthodontics*, **17**(3), 318 (2004).
7. T. A. Hamza, S. F. Rosenstiel, M. M. Elhosary, R. M. Ibraheem, *J. Prosthet. Dent.*, **91**(3), 258 (2004).
8. M. Pantea, R. C. Ciocoiu, M. Greabu, A. Ripszky Totan, M. Imre, A. M. C. Țâncu,... A. E. Petre, *Materials*, **15**(9) 3075 (2022).
9. L. I. Smith, A Tutorial on Principal Components Analysis, 2002. https://ourarchive.otago.ac.nz/bitstream/handle/10523/7534/OUCS-2002-12.pdf
10. https://builtin.com/data-science/step-step-explanation-principal-component-analysis