Prediction of thermal and mechanical properties of acrylate-based composites using artificial neural network modeling

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Abstract

Poly(methyl methacrylate) (PMMA) has a broad spectrum of uses, especially in medical applications. The role of fine-grained alumina particles of PMMA composites was investigated in this study. The composites were based on PMMA modified with dimethyl itaconate (DMI) as a matrix and alumina particles (Al_2O_3) and alumina doped with iron (Al_2O_3-Fe) modified with 3-aminopropyl-trimethoxysilane (AM) and flax oil fatty acid methyl esters (biodiesel) as reinforcements. Three particle sizes were measured (~0.4, ~0.6 and ~1.2 μm). The highest thermal conductivity values were measured for the composite 5 wt.% Al_2O_3-Fe-AM. With the addition of 3 wt.% Al_2O_3-AM to the PMMA/DMI matrix, mechanical properties were improved (tensile strength, strain, and modulus of elasticity). An artificial neural network model based on the Broyden-Fletcher-Goldfarb-Shanno iterative algorithm was investigated for prediction of thermal conductivity and mechanical properties of the composites showing satisfactory results. This is relevant for applications for optimization of dental materials to produce dentures, which were exposed to variations in temperature during the application.

Keywords: Composite materials; thermal conductivity; Al_2O_3 particles.

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1. INTRODUCTION

Poly(methyl methacrylate) (PMMA) is a transparent thermoplastic polymer that has a wide range of applications, such as wide use of acrylic bone cements, based on PMMA in dentistry and orthopedic surgery [1-7].

A biomaterial intended for such purposes has to be biocompatible exhibiting certain properties, such as being non-toxic, non-injurious, and not causing immunological rejection. Biomaterials include various metals, ceramics, polymers and composites. Toxicity of a material is very important, especially in applications in which the material is in contact with the body. Biomaterials based on PMMA are often used because of their good biocompatibility, non-toxicity, good adhesion to human tissues, and easy handling.

Nevertheless, PMMA has several drawbacks such as poor thermal stability, low toughness, and toxicity of residual monomers. In the case of monomer leakage from the material, the surrounding tissue can be irritated. Also, such a leakage can create structural damages like cracks that could lead to mechanical fracture of the material [8]. The amount of residual monomers methyl methacrylate (MMA) can be significantly reduced by adding dimethyl itaconate to PMMA [9-10].

Physical and mechanical properties of polymer materials can be modified by incorporation of inorganic particulate fillers in the polymer matrix in order to control the shrinkage and mechanical properties of the material [11]. These fillers can be SiO_2, Al_2O_3, $Mg(OH)_2$ or $CaCO_3$ micro- or nanoparticles, which were shown to improve stiffness, strength, modulus and hardness of the resulting composite material [12-13]. Mechanical properties can be adjusted by using fillers with the controlled crystal structure [14-15]. Alumina or aluminum oxide (Al_2O_3) is often used in composites as reinforcement and

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as materials for high-temperature applications because of their extraordinary chemical properties (*e.g.* resistance to the action of chemical substances, insoluble in acids) Regarding composite materials, different structures and morphologies of aluminum oxide can be obtained by thermal treatment [16]. The aim of this work was to synthesize novel composite materials based on a matrix made of PMMA/itaconate copolymer and to investigate the possibility of predicting the thermal conductivity, tensile strength, strain and modulus of elasticity by using artificial neural network (ANN) modeling.

2. MATERIALS AND METHODS

Commercial PMMA (Biocril (Galenika AD, Serbia)), (chemical grade *p.a.*) and dimethyl-itaconate (DMI) (Sigma-Aldrich, USA) (*p.a.*) were used to produce samples. The procedure for obtaining PMMA starts with preparation of a two-component system: a liquid component consisting of methyl methacrylate (MMA) (*p.a.*) as a monomer and ethylene glycol dimethacrylate (EGDMA) (*p.a.*) as a modifier, and a powder component consisting of prepolymerized PMMA coated with benzoyl peroxide (*p.a.*) as the initiator. The powder component, has been characterized in literature as follows: molecular weight is $M_n = 1.27 \times 10^5$ g·mol^{-1}, $M_w = 3.82 \times 10^5$ g·mol^{-1}, and the polydispersity index PI = 3.01, with a 4.3 wt.% of monomer content and an average particle size of 55 µm [17].

Submicron ferrous oxide (*p.a.*) doped alumina particles (Al_2O_3-Fe) were used as reinforcement. In specific, aluminium hydroxide chloride in crystallized state (Locron L; $Al_2(OH)_5Cl \times 2.5H_2O$, Clariant, Swiss) (*p.a.*) was used as alumina forerunner, while iron chloride ($FeCl_3 \times 6H_2O$) (Sigma Aldrich, USA), (*p.a.*) was used as a source of iron ions. The ferrous oxide doped alumina particles were prepared from these two components in demineralized water by a sol-gel technique, according to the previously described method [18]. In the end product the mass ratio of Al_2O_3 to Fe_2O_3 would be 90/10. The obtained gel was ground and calcined for two hours at 900 °C, The obtained particles were characterized by a particle size analyzer (Zetasizer Nano-ZS, Malvern, UK) yielding three fractions with average diameters: *d* (0.1) = 0.4 µm, *d* (0.5) = 0.6 µm, *d* (0.9) = 1.2 µm [19]. The crystal structure was determined previously by X-ray diffraction (XRD) analysis and it was as follows: η-Al_2O_3 (39.4 %), ƙ-Al_2O_3 (35.1 %) and α-Al_2O_3 (25.5 %) [14].

The particles were modified with 3-aminopropyl, trimethoxysilane (AM), (*p.a.*), (Sigma Aldrich, USA) and methyl esters of linseed oil fatty acids (biodiesel - BD, (*p.a.*) (Sigma Aldrich, USA) and denoted as Al_2O_3-AM, Al_2O_3-BD, Al_2O_3-Fe-AM, and Al_2O_3-Fe-BD. In order to enable the bonding of alumina particle to the matrix, first trimethoxysilane (AM) was attached to the surface of the particles by using the procedure described previously [20]. Commercial aluminum oxide (Al_2O_3) nanoparticles were used as fillers, doped with iron oxide, and then integrated in different content (1, 3 and 5 wt.%).

2. 1. Preparation of PMMA/DMI composites reinforced with alumina particles

DMI is added to the liquid monomer followed by addition of PMMA powder so to obtain the PMMA matrix with 5 wt.% DMI. To avoid agglomeration and to obtain a good dispersion, composite materials were prepared by adding alumina particles to the monomer followed by dispersion in an ultrasonic bath for 30 min. Next, the powder component (63 wt.%) was added into the liquid forming a paste poured into a mold made of aluminium alloy and stirred for 5 min. The mold was then closed and heated at 70 °C for 1 h. The polymerization was completed at 100 °C within 30 min. Using 1, 3 and 5 wt.% of different alumina particles (13 sample groups prepared with iron oxide and alumina nanoparticles with two surface modifications), were prepared as it was described in a previous work [17]. PMMA combined with DMI creates polymer matrix (PMMA/DMI), hereinafter referred to as DMI. The composition of all 13 tested samples is given in Table 1.

Table 1. Thermal conductivity of PMMA/DMI matrix and obtained composites [17]. Permissions under Attribution 4.0 International (CC BY 4.0)

Sample	λ / W m-1·K-1	Sample	λ / W m^{-1}·K^{-1}
PMMA/DMI	0.2	1 wt.% Al_2O_3-Fe-AM	0.7
1 wt. % Al_2O_3-AM	0.6	3 wt.% Al_2O_3-Fe-AM	0.7
3 wt. % Al_2O_3-AM	0.5	5 wt.% Al_2O_3-Fe-AM	0.8
5 wt. % Al_2O_3-AM	0.7	1 wt.% Al_2O_3-Fe-BD	0.7
1 wt. % Al_2O_3-BD	0.6	3 wt.% Al_2O_3-Fe-BD	0.7
3 wt. % Al_2O_3-BD	0.6	5 wt.% Al_2O_3-Fe-BD	0.7
5 wt. % Al_2O_3-BD	0.6		

2. 2. Experimental data for ANN modeling

In our earlier research, thermal conductivity and mechanical characterization (tensile strength, strain and modulus of elasticity) of all 13 samples were examined [17]. In order to determine the mechanical properties of the specimens, the testing machine (Instron Testing Machine, model 6025, China) was used. The samples were in the form of a block with dimensions 2×5 mm and 5 cm in length. The obtained results were used in the present work to investigate possibilities to predict thermal conductivity and mechanical properties of the composites by using artificial neural network modeling (ANN model).

2. 3. Artificial neural network modeling

The artificial neural network (ANN) model was developed in the form of a multi-layer perceptron model (MLP), which consisted of three layers (input, hidden, and output). It was used for prediction of thermal conductivity, tensile strength, strain, and modulus of elasticity based on the composite composition, addition of Fe and modifier. In the literature, the ANN model was proven as quite capable for approximating nonlinear functions [19-22]. Before the calculation, both input and output data were normalized (according to min - max normalization scheme) to improve the behavior of the ANN. During this iterative process, input data were repeatedly presented to the network [23-25]. The Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm was used as an iterative method for solving unconstrained nonlinear optimization during the ANN modeling.

The experimental database for ANN was randomly divided into training, cross-validation, and testing data (with 60, 20 and 20 % of experimental data, respectively). The training data set was used for the learning cycle of ANN and for the evaluation of the optimal number of neurons in the hidden layer and the weight coefficient of each neuron in the network. A series of different topologies were used, in which the number of hidden neurons varied from 5 to 20, and the training process of the network was run 100,000 times with random initial values of weights and biases. The optimization process was performed based on validation error minimization (the used error function was sum of square - SOS). It was assumed that successful training was achieved when learning and cross-validation curves approached zero.

Coefficients associated with the hidden layer (weights and biases) were grouped in matrices W_1 and B_1. Similarly, coefficients associated with the output layer were grouped in matrices W_2 and B_2. It is possible to represent the neural network by using matrix notation Eq. (1), (Y is the matrix of the output variables, f_1 and f_2 are transfer functions in the hidden and output layers, respectively, and X is the matrix of input variables) [25]:

$$Y = f_1(W_2 f_2(W_1 X + B_1)\ B_2 \qquad (1)$$

Weight coefficients (elements of matrices W_1 and W_2) were determined during the ANN learning cycle, which updated them using optimization procedures to minimize the error between the network and experimental outputs [23,26-27] according to the sum of squares (SOS) and BFGS algorithm, used to speed up and stabilize convergence [28]. The coefficients of determination were used as parameters to check the performance of the obtained ANN model. The ANN model calculation was performed using computer program StatSoft Statistica 12 (Tibsco software, USA) [29].

2. 4. Sensitivity analysis

In order to determine the relative influence (RI) of input variables (particle amount, addition of Fe and modifiers) on output variables (thermal conductivity, tensile strength, strain and modulus of elasticity), the Yoon's interpretation method was applied. The following equation was used, developed by Yoon, Swales, & Margavio [30]:

$$RI_{ij} = \frac{\sum_{k=0}^{n}\left(w_{ik}w_{kj}\right)}{\sum_{i=0}^{m}\left|\sum_{k=0}^{n}\left(w_{ik}w_{kj}\right)\right|}100 \qquad (2)$$

where, RI_{ij} is the relative importance of the i^{th} input variable on the j^{th} output, w_{ik} is the weight between the i^{th} input and the k^{th} hidden neuron, and w_{kj} is the weight between the k^{th} hidden neuron and the j^{th} output.

2. 5. Accuracy of the model

The numerical verification of the developed model was tested using the coefficient of determination (r^2), reduced chi-square (χ^2), mean bias error (MBE), root mean square error (RMSE), and mean percentage error (MPE). These commonly used parameters can be calculated as follows [31]:

$$\chi^2 = \frac{\sum_{i=1}^{N} (x_{\mathrm{exp},i} - x_{\mathrm{pre},i})^2}{N-n}, \tag{3}$$

$$\mathrm{RMSE} = \left[\frac{1}{N} \sum_{i=1}^{N} (x_{\mathrm{pre},i} - x_{\mathrm{exp},i})^2 \right]^{1/2}, \tag{4}$$

$$\mathrm{MBE} = \frac{1}{N} \sum_{i=1}^{N} (x_{\mathrm{pre},i} - x_{\mathrm{exp},i}), \tag{5}$$

$$\mathrm{MPE} = \frac{100}{N} \sum_{i=1}^{N} \frac{\left| x_{\mathrm{pre},i} - x_{\mathrm{exp},i} \right|}{x_{\mathrm{exp},i}} \tag{6}$$

where $x_{\mathrm{exp},i}$ stands for the experimental values and $x_{\mathrm{pre},i}$ are the predicted values calculated by the model, N and n are the number of observations and constants, respectively.

The analysis and mathematical modeling were performed using StatSoft Statistica 12 (Tibsco software, USA) [29]..

3. RESULTS AND DISCUSSION

Thermal stability is crucial for materials, with applications in dentistry and medicine. It is acknowledged that aluminum oxide particles exhibit superior thermal conductivity in comparison to PMMA matrix. This difference is attributed to the variance in their crystal structures, [32-34]. Consequently, integrating these particles into the matrix can alter its thermal conductivity, as demonstrated by the results presented in Table 1, [17].

Compared to PMMA/DMI, an evident increase in thermal conductivity was obtained by the addition of fillers (Table 1). The addition of 1 wt.% particles increased heat conductivity in all samples, while the lowest value was found for the composite with 1 wt.% Al_2O_3-BD. As alumina exhibits higher thermal conductivity (12-38.5 W m^{-1}·K^{-1}) as compared to PMMA (0.167-0.25 W m^{-1}·K^{-1}) [34], further addition of particles induced higher thermal conductivity values. Due to the difference in chemical structure, dense crystal structure with a content of alpha phase in alumina, contributes to better thermal conductivity. It should be noticed that the highest conductivity values were determined for composites with Al_2O_3-Fe particles. The presence of BD on alumina surfaces decreases the thermal conductivity when compared to modification with AM and impedes further increase in the thermal conductivity [17].

Mechanical tests of all 13 were performed previously to examine the influence of different amounts of alumina particles on the tensile properties [17]. The values of tensile strength at break (R_m), strain ($\mathcal{E}$) and modulus of elasticity (E) are shown in Table 2. All specimens with the incorporation of 3 wt.% particles reveal an important increase in some of tested mechanical properties (R_m, $\mathcal{E}$ and E). This increase may be attributed to the efficient scattering of Al_2O_3-Fe particles [35]. A larger number of dipol/dipol intermolecular synergy was created by hydroxyl groups on surface and polar groups of PMMA/DMI matrix. The newly created material with addition of 3 wt.% Al_2O_3-Fe AM, compared to PMMA/DMI, had the modulus of elasticity increased by 37 %. As it was shown in our previous work, new materials strengthened with particles modified with AM had improved compatibility in the PMMA/DMI matrix compared to those modified with BD [17].

It is important to mention that these are our first investigations of polymer composite material and that differences in the obtained results are expected. The obtained results represent the basis for further research and contribution in this research area.

Table 2. Mechanical properties of the PMMA/DMI matrix and the obtained composites: tensile stress, strain and modulus of elasticity depending on the amount and type of particles [17]. Permissions under Attribution 4.0 International (CC BY 4.0)

Sample	R_m / MPa	ε / %	E / MPa
PMMA/DMI	39.8	7.9	802.4
1 wt.% Al_2O_3-AM	48.9	7.6	761.7
3 wt.% Al_2O_3-AM	49.4	11.4	839.1
5 wt.% Al_2O_3-AM	36.2	5.2	550.5
1 wt.% Al_2O_3-BD	38.0	9.7	567.9
3 wt.% Al_2O_3-BD	46.9	12.8	592.2
5 wt.% Al_2O_3-BD	25.9	8.6	471.9
1 wt.% Al_2O_3-Fe-AM	36.7	6.1	897.3
3 wt.% Al_2O_3-Fe-AM	47.1	5.6	1096.7
5 wt.% Al_2O_3-Fe-AM	35.2	4.4	827.3
1 wt.% Al_2O_3-Fe-BD	37.1	9.9	745.8
3 wt.% Al_2O_3-Fe-BD	42.1	9.5	774.8
5 wt.% Al_2O_3-Fe-BD	29.6	8.2	630.8

3. 1. Artificial neural network model

The artificial neural network (ANN) model was developed in the form of multi-layer perceptron model (MLP), with 5 inputs (input variables were particle amount and addition of ferrous oxide as continuous variables, and addition of modifier as a categorical variable, with logical values 0, AM and BD), 9 neurons in the hidden layer and 4 output variables (thermal conductivity, tensile strength, strain and modulus of elasticity). The acquired optimal neural network model showed a good generalization capability for the experimental data and could be used to accurately predict the output values based on the input variables. To obtain the highest values of r^2 (during the training cycle r^2 for output variables were: 0.998; 0.999; 0.999; and 0.999, respectively), shown in Table 3.

Table 3 Artificial neural network model summary (performance and errors), for training, testing, and validation cycles

Network name	ANN performance			Error			Training algorithm	Error function	Hidden activation	Output activation
	Train.	Test.	Valid.	Train.	Test.	Valid.				
MLP 5-9-4	0.999	0.998	0.998	0.001	0.003	0.002	BFGS[a] 226	SOS	Logistic sigmoidal	Identity

Train. –TTraining cycle; Test. – Testing cycle, Valid. – validation cycle during ANN developing.
Performance term represents the coefficients of determination, while error terms indicate a lack of data for the ANN model
BFGS - Broyden-Fletcher-Goldfarb-Shanno algorithm

The obtained ANN model for prediction of output variables was complex (94 weights-biases) because of the high nonlinearity of the observed system [36,37].

The accuracy of the ANN model could be visually assessed by presenting dispersion of points from the diagonal line in the graphics shown in Figure 1. For the ANN model, the predicted values were very close to the measured values in most cases, in terms of r^2 values. SOS values obtained with the ANN model were of the same order of magnitude as experimental errors for the outputs i.e. thermal conductivity, tensile strength, strain, and modulus of elasticity.

The elements of matrix W_1 and vector B_1 (presented in the bias column) are presented in Table 4, while in Table 5 are shown the elements of matrix W_2 and vector B_2 (bias) for the hidden layer, used for calculation in Eq. 2.

The goodness of fit between experimental measurements and model-calculated outputs, represented as ANN performance (sum of r^2 between measured and calculated output variables), during training, testing and validation steps, are shown in Table 6.

A high r^2 is indicative that the variation was accounted for and that the data fitted the proposed model satisfactorily [38].

The residual analysis of the developed model was presented in Table 7. The ANN model had an insignificant lack of fit tests, which means the model satisfactorily predicted the thermal and mechanical properties of the acrylate-based composites.

The ANN model predicted experimental variables reasonably well for a broad range of the process variables.

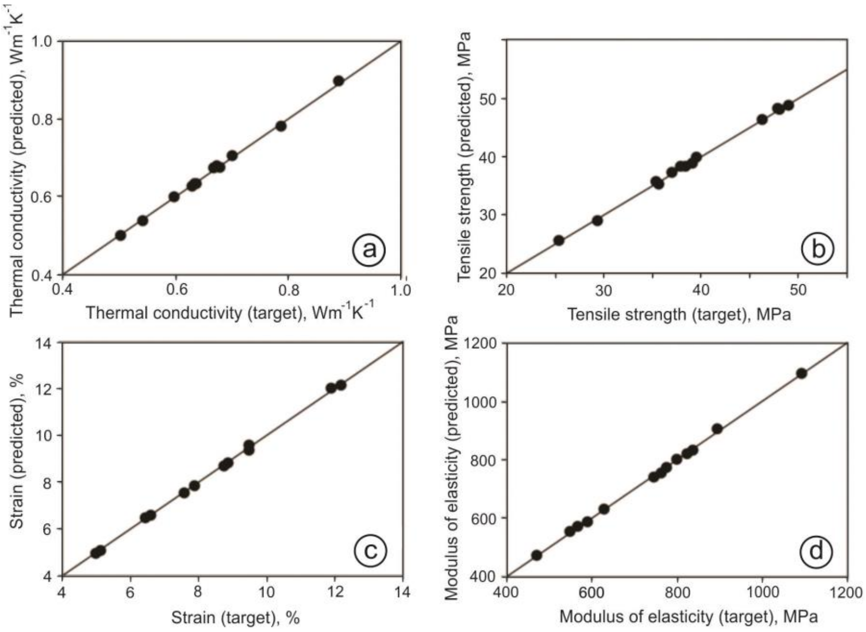

Figure 1. Comparison between experimental and calculated values of thermal conductivity (a), tensile strength (b), strain (c) and modulus of elasticity (d)

Table 4 Elements of matrix W_1 and vector B_1 (presented in the bias column)

Input variables	Neurons								
	1	2	3	4	5	6	7	8	9
Particle amount	-3.069	-6.347	-0.327	-7.049	-3.393	-0.294	-3.355	-1.601	-3.239
Addition of Fe	1.775	1.296	-0.113	-3.405	-1.850	2.122	5.535	4.369	-0.343
Addition of modifier (0)	-0.565	-1.429	0.891	-0.218	1.619	-0.513	-0.287	0.789	-0.430
Addition of modifier (AM)	0.333	0.496	-0.951	0.614	-0.717	1.129	-1.135	-1.874	-0.429
Addition of modifier (BD)	0.192	0.217	2.267	4.222	1.543	-0.287	-1.879	5.152	1.515
Bias	-0.004	-0.790	2.235	4.696	2.571	0.311	-3.291	3.886	0.809

Table 5 Elements of matrix W_2 and vector B_2 (presented in the bias column)

Outputvariables	Neurons									Bias
	1	2	3	4	5	6	7	8	9	
Thermal conductivity	1.812	-2.589	0.640	-1.416	2.018	-1.226	1.760	-1.022	-1.290	1.414
Tensile strength	-1.051	-4.847	-1.441	0.545	1.380	1.425	3.989	-1.102	0.904	0.740
Strain	1.200	-2.736	-0.094	2.033	-2.613	-0.871	-0.097	-1.713	1.109	2.325
Modulus of elasticity	0.866	-3.052	-1.944	-0.110	0.241	-0.729	1.728	0.921	0.531	1.300

Table 6. The "goodness of fit" tests for the developed ANN model

Output variable	χ^2	RMSE	MBE	MPE	r^2
Thermal conductivity	0.000	0.004	0.001	0.577	0.998
Tensile strength	0.043	0.172	0.038	0.362	0.999
Strain	0.004	0.054	-0.027	0.607	1.000
Modulus of elasticity	16.999	3.430	0.444	0.355	1.000

Table 7. The residual analysis of the ANN model

Output variable	Skew	Kurt	Mean	SD	Var
Thermal conductivity	-1.141	0.736	0.001	0.004	0.000
Tensile strength	0.492	-0.443	0.038	0.174	0.030
Strain	0.704	-0.695	-0.027	0.049	0.002
Modulus of elasticity	-0.513	-0.239	0.444	3.541	12.535

Skew - skewness, Kurt - kurtoisis, Mean - mean value of residuals, SD - standard deviation of residuals,
Var - variation of residual values

3. 2. Global sensitivity analysis- the Yoon's interpretation method

In this section the influence of input variables (particle amount, addition of Fe and modifier) on relative importance (*RI*) for thermal conductivity, tensile force, strain, and modulus of elasticity was studied. According to Figure 2, particle amount (wt.%) was the most influential parameter with approximately relative importance of 34 % for thermal conductivity calculation, while the influence of modifier BD was negative (-29 %). The particle amount (wt.%) was the most influential parameter with approximately relative importance of 28 % for tensile strength calculation, while the influence of modifier BD was negative (-31 %). Similarly, the particle amount (wt%) was the most influential parameter for strain calculation with approximately relative importance of 25 %, while the influence of addition of Fe was negative (-44 %). Finally, the particle amount (wt.%) and addition of Fe were the most influential parameters for modulus of elasticity calculation with approximately relative importance of 25 and 35 %, respectively, while the influence of modifier AM was negative (16 %).

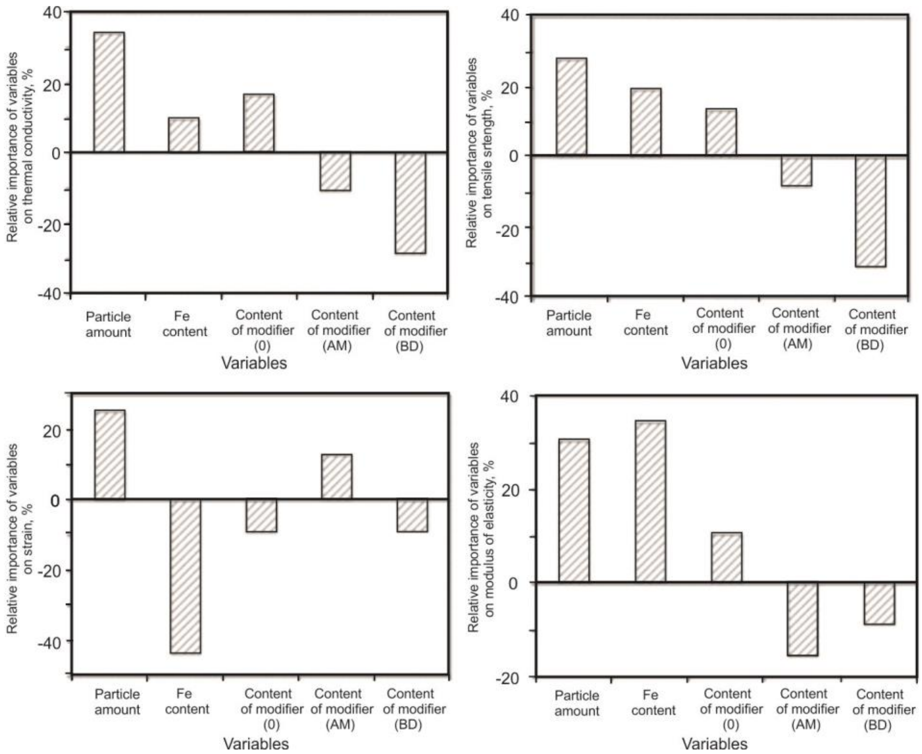

Figure 2. The relative importance of the molecular descriptors on RI, determined by using the Yoon interpretation method

Review of the available literature has shown that application of the ANN model in this field is lacking, and it can be considered that a database for this model is newly formed in the present work. Based on the results of the developed model, it was shown that the model is well suited and that filling the database with new experimental data will enable its wider validation and utilization. It was shown that the particle amount has the greatest influence on all tested properties, and that the addition of Fe has a high influence on the modulus of elasticity. Very high values of the coefficient of determination (r^2), obtained by the model, show the matching of the calculated values with the experimental results.

4. CONCLUSION

Based on the results of this study, thermal conductivity, tensile strength, strain, and modulus of elasticity of PMMA/DMI composites were improved by adding alumina-based reinforcement to the polymer matrix. Aluminum oxide-based particles were used as reinforcement modified with organosilane-3-aminopropyl-trimethoxylane (AM) and in the second stage with fatty acid methyl esters (biodiesel). Surface modification provided better bonding of particles with the polymer matrix by covalent and hydrogen bonds and dipole-dipole interactions. Mechanical and thermal properties of the newly obtained composites were improved by adding these particles.

The artificial neural network model was shown to be adequate for prediction of thermal and mechanical properties (i.*e.* thermal conductivity, tensile force, strain, and modulus of elasticity) as output variables as functions of input variables (*i.e.* particle amount, addition of Fe and modifier) (the r^2 values during training cycle for these variables were: 0.998; 0.999; 0.999 and 0.999, respectively). It has been established that there are evident overlaps between the predictions of the applied mathematical models and the obtained experimental data, so we can conclude that the artificial neural network model has a good perspective in predicting thermal and mechanical properties in this field of composite materials.

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Predviđanje termičkih i mehaničkih svojstava kompozita na bazi akrilata korišćenjem modela veštačke neuronske mreže

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Izvod

Poli (metil metakrilata) (PMMA) ima široku upotrebu, posebno u stomatologiji i medicini. Kompoziti su napravljeni od PMMA modifikovanog dimetil itakonatom (DMI) kao matrice. Kao pojačanje korišćene su čestice glinice (Al_2O_3) i glinice dopirane oksidom gvožđa (Al_2O_3-Fe) modifikovanim sa 3-aminopropil-trimetoksilanom (AM) i metil estrima masnih kiselina lanenog ulja (biodizel – BD). Prema merenjima toplotne provodljivosti, najveće vrednosti toplotne provodljivosti imao je kompozit sa česticama glinice 5 wt.% Al_2O_3-Fe-AM. Dodatkom modifikovanih čestica glinice u PMMA/DMI matricu, poboljšane su mehaničke osobine (zatezna čvrstoća, deformacija i modul elastičnosti). Razvijen je model veštačke neuronske mreže zasnovan na iterativnom algoritmu predloženom u literaturi (Broiden-Fletcher-Goldfarb-Shanno), za predviđanje toplotne provodljivosti i mehaničkih svojstava kompozita na bazi akrilata u kombinaciji sa česticama na bazi glinice, u zavisnosti od masenog udela čestica, i dodatka oksida gvožđa i modifikatora. Pokazano je da ovi matematički modeli mogu predvideti mehanička i termička svojstva kompozitnih materijala. Ovo je posebno relevantno za predviđanje toplotne provodljivosti materijala koji se koriste u stomatologiji za izradu proteza i koji su izloženi temperaturnim promenama tokom primene.

Ključne reči: kompozitni materijali; toplotna provodljivost; Al_2O_3 čestice