Predictive analysis of electroconductive material parameters for system optimisation

DOI: 10.35530/IT.075.05.2022144

RALUCA MARIA AILENI CRISTINA STROE

ABSTRACT – REZUMAT

Predictive analysis of electroconductive material parameters for system optimisation

This paper presents mathematical modelling based on predictive and correlation analysis of independent and dependent variables of conductive materials to develop sensors or actuators. The resulting analysis and optimisation develop improved systems based on sensors or actuators, including selecting the appropriate conductive materials for development. Toward this purpose, 46 materials with electroconductive properties were selected and analysed. The independent variables considered were mass, air permeability and thickness, and the dependent variable was defined as the electrical surface resistance of the conductive fabric used.

Keywords: *textile, predictive, resistance, conductive, sensors, actuators*

Analiza predictivă a parametrilor materialelor electroconductive pentru optimizarea sistemului

Această lucrare prezintă modelarea matematică pe baza analizei predictive și corelației variabilelor independente și dependente ale materialelor conductive pentru dezvoltarea senzorilor sau actuatorilor. Analiza și optimizarea rezultată se utilizează pentru dezvoltarea unor sisteme îmbunătăţite bazate pe senzori sau actuatori, incluzând selectarea materialelor conductive adevate. În acest scop, au fost selectate și analizate 46 de materiale cu proprietăți electroconductive. Variabilele independente luate în considerare au fost masa, permeabilitatea la aer și grosimea, iar rezistența electrică a suprafeței țesăturii conductive utilizate a fost definite ca variabilă dependentă.

Cuvinte-cheie: *textil, predictiv, rezistenţă, conductiv, senzori, actuatori*

INTRODUCTION

Based on predictive analysis, decisions regarding the types of materials used for electrodes can be optimised according to the implemented monitoring system.

System optimization generally favours intelligent design based on metaheuristic algorithms [1–6]. Optimization can comprise evaluating multiobjective functions or single-objective functions [1–3] by:

- The transformation of a multiobjective optimization problem into a single-objective function optimization using the aggregation method and the method of displacements to arrive at the target values.
- Simultaneous approximation (using a population of candidate solutions) of several elements of the Pareto optimal set. An evolutionary algorithm approximates the Pareto set (and the corresponding Pareto front) in a single run. The approximation of the Pareto front must satisfy at least two characteristics: 1) be close to the real front and 2) be sufficiently diverse [4–6].

Here, we determine the parameters of conductive materials to maximize electrical conductivity and minimize electrical resistance for the development of surface electrodes for actuators and sensors. To solve these problems, we use the Pareto method. The Pareto optimal solution is x if there is no element x' such that f(x') dominates f(x). The set of all Pareto optimal elements of a multiobjective optimization problem is the optimal solution to the problem [7–10]. The set of objective function values (criteria to be optimized) associated with the elements of a Pareto optimal set is called a Pareto front (Pareto Frontier).

EXPERIMENTAL SETUP

For results analysis, mathematical models for the prediction of dependent variables based on independent variables and predictive analyses of composites of sensors and actuators were obtained in independent stages.

For predictive analysis, samples made by depositing conductive pastes comprising a polymer matrix with microparticles of Cu, Ni, Ag, magnetite (Fe_3O_4) or graphite were considered. The prediction of the dependent variable (electrical resistance) was made using multiple regression and by studying the correlations between the independent variables: mass M (g/m^2), thickness δ (mm), air permeability Pa ($l/m^2/sec$) and the dependent variable, surface resistance Rs.

Contributing to this study, 3D Electrotex has developed mathematical models for textile electrodes used for sensors/actuators.

For the development of our mathematical models, 46 samples (table 1) were made during phases 3–8. The textile supports were treated under hydrophilization using a classical method (alkaline boiling/bleaching).

The deposition step applied conductive paste comprising microparticles of nickel (Ni), copper (Cu), silver (Ag), polypyrrole (PPY), graphite or magnetite integrated into a polymeric matrix of polyvinyl alcohol (PVA) or polyethylene glycol (PEG). This step was carried out by rinsing.

For these 46 samples, the dependent, surface resistance Rs (Ω) and independent, mass M (g/m^2), thickness δ (mm), and air permeability Pa (l/m^2/s), variables are presented in table 1. The surface resistance Rs (Ω) was measured as the ratio between the direct voltage applied between the two parallel electrodes on the surface of a sample and the current between these electrodes, neglecting the possible polarization of the electrodes.

RESULTS AND DISCUSSION

The problem to be solved is the elimination of high energy consumption by electrode prototypes that lack proper electrical conductivity. The realization of proper electroconductive materials involves a significant consumption of chemicals (e.g. polymers and metal powders) that are very water- and energy-intensive. Thus, to avoid using prototypes of materials that do not suffice for use as surface electrodes, we used predictive analysis. Our analysis started from the correlations between the obtained parameters to determine the prototype that delivers the desired electroconductive properties (e.g. 10^3–10^7 Ω) with reduced consumption of raw materials, energy and water. In general, using metal powders for electroconductive pastes increases the mass of the electroconductive paste compared to polymer-based paste (PEG, PVA, PPY). Thus, a material with reduced thickness, increased mass, low surface electrical resistance and implicitly high electrical conductivity indicates the predominant presence of metal powders. At the same time, a material with low mass but high thickness, with high surface resistance and implicitly without electrical conductivity indicates the excessive presence of polymers without conductive properties. Air permeability can also be increased by depositing polymer films on the fabric surface. However, in the case of films with integrated metal microparticles, continuity is no longer preserved, increasing the air permeability because the paste contains metal microparticles that do not form a continuous film.

Multiple regression modelling (equation 1) was used to develop the mathematical models describing the correlations between the independent variables:

$$Y = a_1 + b_1{*}X_1 + b_2{*}X_2 + b_3{*}X_3 + \ldots + b_kX_k \qquad (1)$$

where Y is the estimated value for the dependent variable, X1, X2, X3,..., Xk are the values of the k predictor variables, a1 is the point of origin and b1, b2, b3,..., bk are the coefficients for the k predictor variables.

Figures 1–4 show the 3D representations of the surface resistance Rs (Ω) as a function of thickness G and mass M, respectively. Air permeability and mass with residual values are included and excluded, respectively.

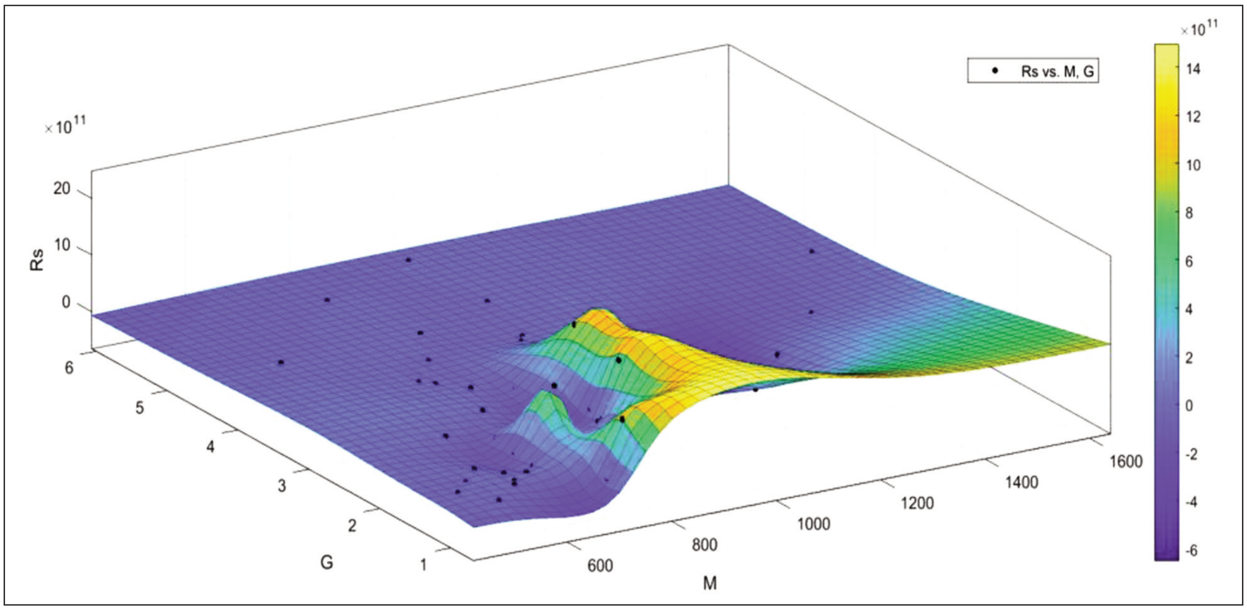

Fig. 1. 3D graphical representation of surface resistance values as a function of the thickness G and mass M, with residual values included

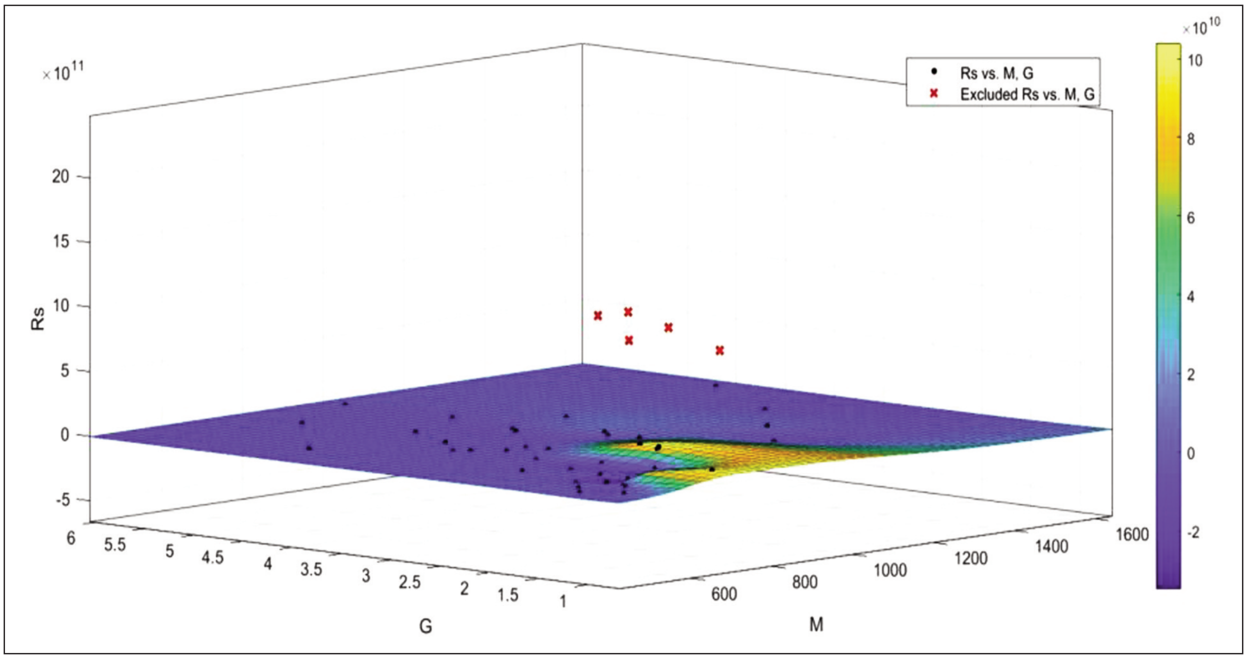

Fig. 2. 3D graphical representation of surface resistance values as a function of thickness and mass, with residual values excluded

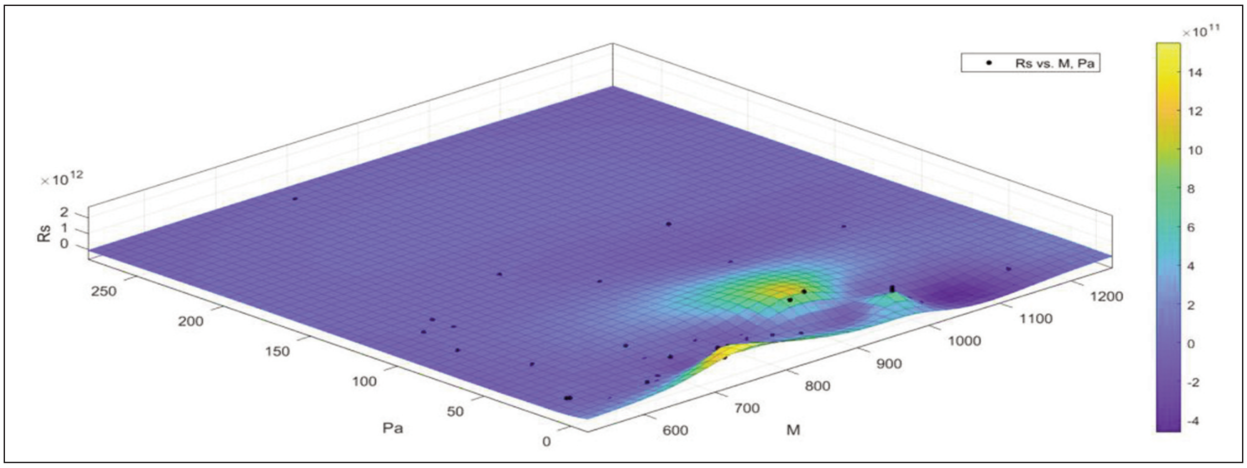

Fig. 3. 3D graphical representation of surface resistance values as a function of air permeability Pa and mass M, with residual values included

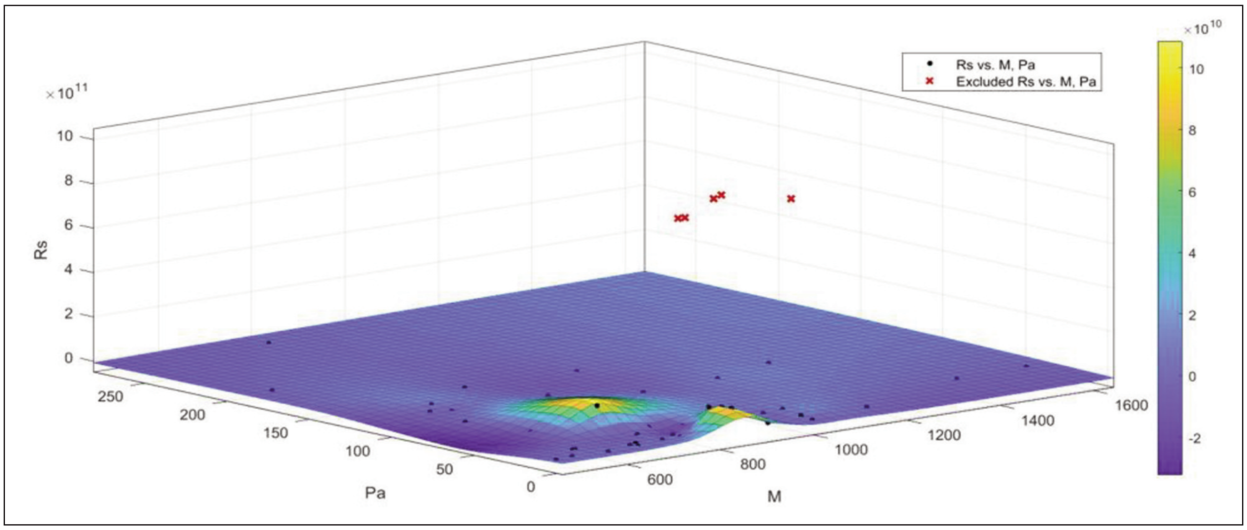

Fig. 4. 3D graphical representation of surface resistance values as a function of air permeability Pa and mass M, with residual values excluded

Table 1

PHYSICO-MECHANICAL AND ELECTRICAL CHARACTERIZATION OF CONDUCTIVE EXPERIMENTAL SAMPLES

No.	PPY	Ni	Al	Ag	Zn	Fe3O4	Graphite	Cu	PEG	PVA	M*	δ**	Pa***	Rs****
1		x							x	x	1159	2.13	9.29	10^4
2								x	x	x	1587	4.48	33.9	107
3								x	x	x	1431	3.34	31.7	$1.1 \cdot 10^7$
4							x		x	x	709	0.915	45.46	10^{11}
5						x				x	515	1.011	5.755	10^7
6								x		x	752	1.011	4.31	10^{12}
7		x								x	556	4.385	16.8	10^3
8								x		x	650	1.527	8.876	10^7
9								x		x	658	1.847	6.123	10^3
10				x						x	476	1.304	4.27	10^8
11				x						x	586	1.317	3.88	10^3
12					x					x	741	1.894	5.656	10^{12}
13								x		x	863	2.28	7.55	10^{11}
14								x		x	858	2.07	12.2	10^{11}
15								x		x	897	2.13	27.83	10^{12}
16								x		x	720	2.75	9.03	10^9
17								x		x	816	3.25	19.15	10^8
18								x		x	824	3.05	25.94	10^9
19								x		x	995	5.82	25.64	10^9
20								x		x	760	2.25	9.52	10^3
21								x		x	776	1.77	33.16	10^3
22								x		x	670	2.19	11.1	10^3
23								x		x	761	3.22	14.35	10^3
24								x		x	721	3.42	24.54	10^3
25								x		x	702	3.52	31.92	10^3
26								x		x	780	5.38	264.8	10^3
27								x		x	1276	2.68	101.99	10^{10}
28								x		x	925	2.96	31.22	10^{12}
29								x		x	1020	2.93	9.83	10^{10}
30								x		x	841	2.01	15.07	10^{11}
31								x		x	1033	3.34	24.72	10^{10}
32		x								x	828	4.42	109.1	10^3
33								x		x	992.8	2.932	8.148	10^{12}
34		x								x	950.4	3.9	10.148	10^3
35				x						x	1020.4	3.248	3.248	10^3
36								x		x	1125.2	4.106	90.3	10^{10}
37		x								x	966.4	4	90.383	10^3
38				x						x	1002.8	4.762	141	10^3
39		x								x	590.8	1.5	113.4	10^3
40		x						x		x	623.2	1.424	109.4	10^7
41								x		x	623.6	1.42	121.8	10^{10}
42	x									x	513.6	1.472	187.4	10^8
43						x				x	602.8	2.408	55.73	10^8
44		x	x							x	769.6	3.878	143	10^3
45			x							x	577.2	1.25	88.14	10^5
46					x					x	559.2	1.684	16.2	10^5

Note: * M (g/m^2) – mass per unit length; ** δ (mm) – thickness of the textile material; *** Pa (l/m^2/sec) – air permeability at 100 Pa pressure; **** Rs (Ω) electrical resistance.

The correlation coefficient (equation 2) between the vector Rs and the mass vector M shows a positive value ($R_{Rs,M}$ = 0.0619), resulting in a direct correlation between the mass and the electrical resistance of the surface. The correlation coefficients between the Rs vector and thickness G and air permeability Pa respectively show negative values ($R_{Rs,G}$ = –0.1714, $R_{Rs,Pa}$ = –0.2093), and it follows that there is an inverse correlation signifying that when air permeability increases, the thickness of the conductive layer and the electrical surface resistance decrease and the electrical conductivity of the textile surface increases.

$$R_{Rs,M} = \begin{vmatrix} 1.0000 & 0.0619 \\ 0.0619 & 1.0000 \end{vmatrix} \Leftrightarrow$$

$$\Leftrightarrow R1,2_{Rs,M} = R2,1_{Rs,M} = 0.0619 \qquad (2)$$

$$R_{Rs,G} = \begin{vmatrix} 1.0000 & -0.1714 \\ -0.1714 & 1.0000 \end{vmatrix} \Leftrightarrow$$

$$\Leftrightarrow R1,2_{Rs,G} = R2,1_{Rs,G} = -0.1714 \qquad (3)$$

$$R_{Rs,Pa} = \begin{vmatrix} 1.0000 & -0.2093 \\ -0.2093 & 1.0000 \end{vmatrix} \Leftrightarrow$$

$$\Leftrightarrow R1,2_{Rs,Pa} = R2,1_{Rs,Pa} = -0.2093 \qquad (4)$$

For the prediction of the surface electrical resistance values (Rs [Ω]), the following mathematical models were developed using the established independent variables (M, δ, Pa) in MATLAB:

- the mathematical model M1 (equation 5) for the prediction of surface electrical resistance values (Rs[Ω]) for copper-based materials depending on the air permeability Pa (l/m^2/sec) and the mass of the functionalized material M (g/m^2):

$$\begin{gathered} z = 5.263*10^{11} + 2.912*10^{11}x + 2.532*10^{12}y + \\ + 4.969*10^{11}*x^2 - 1.732*10^{11}*x*y + 6.883*10^{10}*y^2 - \\ - 1.039*10^{12}x^3 + 4.651*x^2*y - 1.35*10^{12}x*y^2 - \\ - 8.421*10^{12}*y^3 - 5.837*10^{11}*x^4 + 1.793*x^3*y + \\ + 4.998*10^{12}x^2*y^2 - 4.84*10^{12}*x*y^3 - \\ - 3.689*10^{12}*y^4 + 1.917*10^{11}*x^5 - 1.63*10^{12}x^4*y + \\ + 4.303*10^{12}x^3*y^2 - 4.848*10^{12}*x^2*y^3 - \\ - 4.84*10^{12}*x*y^4 + 4.264*10^{12}*y^5 \qquad (5) \end{gathered}$$

  where z is surface electrical resistance Rs, x – thickness G and y – mass M.

- the mathematical model M2 (equation 6) for the prediction of surface electrical resistance values Rs (Ω) for copper-based materials depending on the air permeability Pa (l/m^2/sec) and the thickness of the functionalized material G (mm]):

$$\begin{gathered} z = 4.726*10^{13} + 3.296*10^{12}*x - 1.232*10^{14}*y - \\ - 2.457*10^{13}*x^2 - 4.113*10^{12}*x*y + 1.128*10^{14}*y^2 - \\ - 9.435*10^7*x^3 + 2.484*10^{10}x^2*y + 1.79*10^{12}x*y^2 - \\ - 4.677*10^{13}*y^3 + 9.799*10^6*x^4 - 7.338*10^8*x^3*y + \\ + 8.721*10^9*x^2*y^2 - 4.173*10^{11}*x*y^3 + \\ + 9.04*10^{12}*y^4 - 4.331*10^4*x^5 + 1.295*10^6*x^4*y + \\ + 8.924*10^7*x^3*y^2 - 2.178*10^9*x^2*y^3 + \\ + 3.549*10^{10}*x*y^4 - 6.346*10^{11}*y^5 \qquad (6) \end{gathered}$$

  where z is Rs, x – air permeability Pa and y – G.

- the mathematical model M3 (equation 7) for the prediction of surface electrical resistance values Rs (Ω) depending on the air permeability Pa (l/m^2/sec) and the mass of the functionalized material M (g/m^2):

$$z = 2.119*10^6 - 4.353*10^5x + 1.142*10^6y \qquad (7)$$

  where z is Rs, x – Pa and y – M.

- the mathematical model M4 (equation 8) for predicting the electrical resistance values Rs depending on the mass M and the thickness G of the conductive material:

$$\begin{gathered} z = 1.435*10^5 *x + 2.238*10^4y - 1.435*10^5*x^2 - \\ - 42.15*y^2 + 0.02128*y^3 \qquad (8) \end{gathered}$$

  where z is Rs, x – G and y – M.

- the mathematical model M5 (equation 9) for the prediction of electrical resistance values Rs depending on the thickness of the conductive material G and air permeability Pa:

$$\begin{gathered} z = 12.49x - 2.292*10^6xy + 5.78*10^5y^2 - \\ - 5313y^3 - 12.49y - y^3 - yx^4 \qquad (9) \end{gathered}$$

  where z is Rs, x – G and y – Pa.

Table 2 shows the elements defining the predictive power of mathematical models, such as the coefficient of determination, which quantifies the square of the multiple correlation coefficient (R^2), and the adjusted coefficient of determination (adjusted R^2).

Table 2

DEFINING ELEMENTS FOR THE PREDICTIVE POWER OF MATHEMATICAL MODELS

Model	R^2	Ajusted R^2
M1	0.9353	0.7504
M2	0.9191	0.6879
M3	0.844	0.8367
M4	0.7729	0.7567
M5	0.7464	0.7233

CONCLUSIONS

In conclusion, the values of the adjusted coefficient of determination (adjusted R2), show that the predictive power of models M1, M3, M4 and M5 is reasonable. We observed that the coefficient of determination (R^2) values are close to 1 for mathematical models M1, M2, and M3, with the best prediction provided by models M1 and M2.

ACKNOWLEDGEMENTS

The research presented in this paper was prepared in the INCDTP laboratories. Funds support this work from MCID, National Project "Electroconductive composite textile materials based on 3D polymer matrices for sensor systems for monitoring and attenuation of electromagnetic waves (3D ELECTROTEX)", Grant Agreement PN 19 17 01 01.

REFERENCES

[1] Micota, F., *Algoritmi metaeuristici*, note de curs, Facultatea de Informatica, Universitatea de Vest din Timisoara

[2] Ivanciu, L.N., *Sistem inteligente de suport decizional*, note de curs, Facultatea de Electronică, Telecomunicații și Tehnologia, Informației, Universitatea Tehnica din Cluj-Napoca

[3] Kumar, V., Ram, M. eds., *Predictive Analytics: Modeling and Optimization*, CRC Press, 2021

[4] Boschetti, M.A., Maniezzo, V., Roffilli, M., Bolufé Röhler, A., M*atheuristics: Optimization, simulation and control,* In: International Workshop on Hybrid Metaheuristics, Springer, Berlin, Heidelberg, 2009, 171–177

[5] Maniezzo, V., Stützle, T., Voß, S., *Matheuristics*, New York, NY, USA: Springer International Publishing, 2021

[6] Toklu, N.E., *Matheuristics for robust optimization: application to real-world problems,* Doctoral dissertation, Università della Svizzera Italiana, 2014

[7] Cheng, L., Zhang, T., Guo, M., Li, J., Wang, S., Tang, H., *Electromagnetic shielding effectiveness and mathematical model of stainless steel composite fabric*, In: The Journal of The Textile Institute, 106, 6, 2015, 577–586

[8] Bahadır, S.K., *Identification and modeling of sensing capability of force sensing resistor integrated to e-textile structure*, In: IEEE Sensors Journal, 2018, 18, 23, 9770–9780

[9] Chattopadhyay, R., *A Review on Mathematical Modeling for Textile Processes*, In: Journal of The Institution of Engineers (India): Series E, 96(2), 89–98

[10] Sedighi, A., Montazer, M., Mazinani, S., *Fabrication of electrically conductive superparamagnetic fabric with microwave attenuation, antibacterial properties and UV protection using PEDOT/magnetite nanoparticles*, In: Materials & Design, 2018, 160, 2015, 34–47

Authors:

RALUCA MARIA AILENI, CRISTINA STROE

The National Research & Development Institute for Textiles and Leather,
Lucretiu Patrascanu 16, 030508 Bucharest, Romania

Corresponding author:

RALUCA MARIA AILENI
e-mail: raluca.aileni@incdtp.ro