Istraživanja i projektovanja za privredu

ISSN 1451-4117

DOI:10.5937/jaes0-53043

www.engineeringscience.rs

publishing

Journal of Applied Engineering Science

Vol. 22, No. 4, 2024

Original Scientific Paper

Paper number: 22(2024)4, 1243, 804-809

OPTIMIZATION OF ELECTROSPINNING PARAMETERS USING AN ARTIFICIAL NEURAL NETWORK (ANN) MODEL FOR ENHANCED NANOFIBER PRODUCTION

Francisco Javier Laguna Luque[1], Sawan Shetty[2*], Animita Das[2], Chethan K N[3], Laxmikant G Keni[3], Sampath Suranjan Salins[4]

[1] Higher Technical School of Aeronautical and Space Engineers, Department of Aerospace Engineering, Madrid, Spain

[2] Manipal Academy of Higher Education, Manipal Institute of Technology, Department of Mechanical and Industrial Engineering, Manipal, Karnataka, India

[3] Manipal Academy of Higher Education, Manipal Institute of Technology, Department of Aeronautical & Automobile Engineering, Manipal, Karnataka, India

[4] Dubai International Academic City, Manipal Academy of Higher Education Dubai Campus, UAE

* sawan.shetty@manipal.edu

Electrospinning is a simple and cost-effective technique for creating nanofibers with diverse applications.Optimizing electrospinning parameters is crucial for producing nanofibers with desirable attributes, such as uniform diameter and bead-free morphology.Conventional trial-and-error strategies are frequently protracted and may not necessarily result in optimal outcomes. This investigation delineates the formulation of an artificial neural network (ANN) model specifically designed to systematically optimize electrospinning parameters. Crucial input variables, such as applied voltage, feed rate, and polymer concentration, were utilized to train the ANN model, which was constructed with multiple hidden layers to effectively encapsulate the intricate relationships between input parameters and the resultant nanofiber properties. In this research, an ANN was devised with a 4-3-1 architecture that was trained on a dataset extrapolated from experimental data documented in prior literature and employed the Levenberg-Marquardt algorithm to ascertain robust performance. Upon validation, the model proficiently predicted optimal parameters conducive to the production of smooth, bead-free nanofibers. The model achieved a root mean square error (RMSE) of 7.77%, which is lower than previous models for predicting electrospun Kefiran nanofiber diameter.The results indicate that the ANN-based methodology substantially augments the efficiency and precision of electrospinning parameter optimization, thereby providing a significant resource for researchers and engineers engaged in the domain of nanomaterials. Future investigations could delve into the application of this model to various polymer systems and further refine the ANN architecture to accommodate more intricate electrospinning configurations.

Keywords: artificial neural networks, electrospinning, nanofibers

1 INTRODUCTION

Nanofibers have attracted considerable scholarly interest among researchers owing to their unique characteristics and the multitude of advantages they offer across diverse disciplines. Also, Electrospun nanofibers offer advantages such as high surface area to volume ratio, customizable porosity, and functionalization capabilities, making them useful in healthcare applications like tissue engineering, regenerative medicine, wound treatments, and drug delivery solutions. Nanofiber structure is influenced by both external factors (voltage, tip-to-collector distance, feed rate) and internal factors (solution properties, such as conductivity, viscosity and concentration). Notwithstanding the advantageous traits of electrospun nanofibers, several challenges persist particularly the necessity of optimizing the aforementioned parameters to achieve a morphology devoid of beads. The comprehension of the concurrent influence of each parameter on the diameter of the nanofibers becomes increasingly complex during experimental investigations. Both experimental methods and computational approaches, such as artificial neural networks (ANN), can be employed to analyze the influence of various parameters on electrospinning.

ANNs, modeled after the human brain's neural architecture, are trained on experimental data to predict outputs based on input variables diameters [1]. In this study, ANN was applied to optimize electrospinning parameters for predicting nanofiber The ANN framework was constructed to examine the impact of four variables, including the concentrations of PEO and acetic acid, the applied voltage, and the temperature of the prepared solution, on the mean diameter of the fibers produced. The findings corroborated the robustness of the ANN model in elucidating the correlation between the average fiber diameter and the specified parameters [2]. The efficacy of the ANN model, alongside k-fold cross-validation, was evaluated for its predictive capability regarding the diameter of electrospun PEO nanofibers[3].Samadian et al. (2016) employed ANN methodologies to optimize the conductivity of carbon nanofibers by considering factors such as the concentration of simulated body fluid (SBF), immersion duration, and the diameter of the carbon nanofibers [4].

Various ANN configurations have been devised to ascertain the optimal diameter of synthesized nanofibers. The input parameters were refined utilizing a genetic algorithm that incorporated four hidden layers, each comprising 20 neural nodes. The learning rate was established at 0.1, with the optimal fitting achieved at 1500 iterations [5]. The research conducted by Karimi et al. in 2015 involved the development of an artificial neural network characterized by four input parameters: the ratio of CS/PVA concentration, temperature, applied voltage, and the distance between the nozzle tip and the collector. This model was characterized by three hidden layers containing 8, 16, and 5 nodes in each respective layer [6]. An ANN predicated on a multilayer perceptron (MLP) architecture was formulated to forecast the average fiber diameter (AFD) of electrospun gelatin/bioactive glass (Gt/BG) scaffolds. The input parameters included one solution variable (BG content) along with two processing variables, namely, the distance from the tip to the collector and the feed rate. The aforementioned ANN architecture comprised two hidden layers, each comprising five neurons, and one output layer corresponding to the diameter[7].Numerous investigations assert that ANN methodologies have surpassed traditional techniques. Research shows that ANN is notably more adept and exact in estimating the diameter of electrospun PLGA nanofibers as opposed to the conventional Response Surface Methodology (RSM). An ANN model featuring four input layers, 14 hidden layers, and one output layer purportedly resulted in an absolute relative error of 2.24 percent, which is superior to the error produced by RSM [8]. A three-stage feed-forward ANN architecture was established and put into practice for predicting the diameter of electrospun PMMA nanofibers[9]. Collectively, the research underscores the effectiveness of ANNs as a promising instrument for predicting nanofiber diameter, particularly owing to their capacity to encapsulate intricate interactions among multiple input variables [10]. Kefiran is noted for being a natural, eco-friendly, water-dissolvable, and harmless heteropolysaccharide sourced from the vegetation found in kefir grains [11]. Investigative studies surrounding monosaccharides suggest that kefiran includes glucose (Glc) and galactose (Gal) in a molar ratio roughly calculated as 1.0:1.1 [12]. Recognized for its beneficial attributes, Kefiran aids in the battle against bacteria, fungi, and tumors, contributing positively to numerous healthcare applications, including the delivery of medications and the treatment of wounds, among others. In the current research investigation, we aim to develop an artificial neural network employing a Neural Networks Tool provided in MATLAB to predict the diameter of the electrospun Kefiran nanofibers.

2 MATERIALS AND METHODS

Kefiran nanofibers were synthesized employing the technique of electrospinning, and the dataset was subsequently constructed based on the data compiled from the previous literature [1]. The current analysis highlights the creation of an Artificial Neural Network (ANN) crafted to evaluate the diameter of electrospun nanofibers.

2.1 ANN model design

The artificial neural network (ANN) constructed facilitated the prediction of the nanofiber diameter based on the parameters, which include applied voltage, feed rate, distance from tip to collector, and polymer concentration. The architecture of the ANN, illustrated in Figure 1, was configured as 4-3-1, comprising four neural nodes within each of the hidden layers. The Neural Network Toolbox alongside the Parallel Computing Toolbox was employed in MATLAB version 2023 B to enhance the accuracy of the results. The hidden layers utilized the hyperbolic tangent sigmoid function while the output layer utilized the pure linear function as their default activation function.

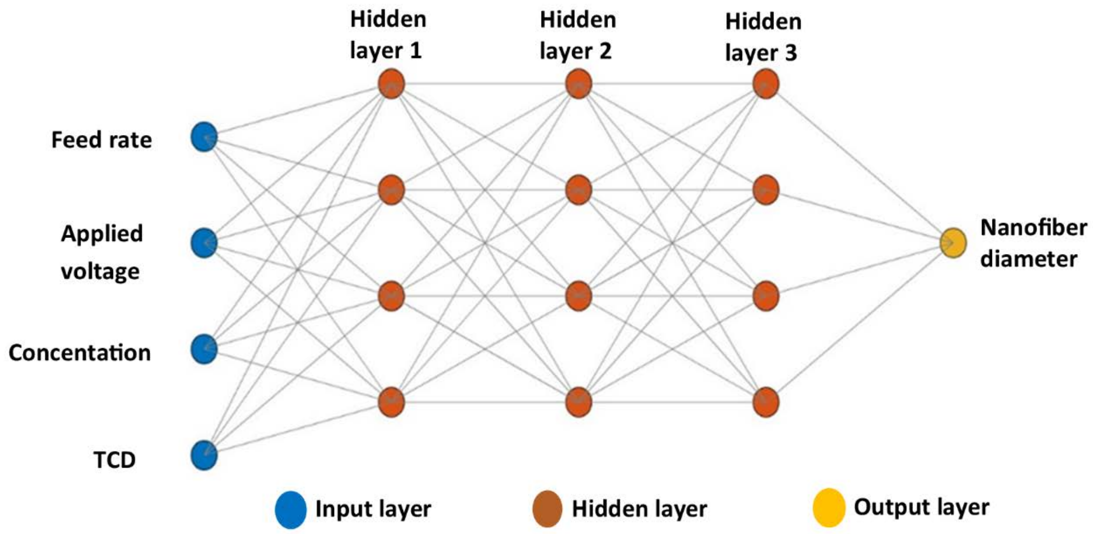

Fig. 1. The architecture of the ANN layout

In the beginning, the values were calibrated to lie within the limits of 0 and 1. Following the normalization process, the design of the ANN commenced. A primary consideration was that the relatively small size of the dataset rendered k-fold cross-validation an appropriate technique to implement. Even though k-fold cross-validation demonstrated pleasing performance, alternative techniques for splitting data were considered, resulting in superior outcomes. Thus, a suitable neural network function was applied with the information split into three unique categories: training (70%), validation (15%), and testing (15%). Furthermore, the optimization process for identifying the most effective training parameters was conducted utilizing the Parallel Computing Toolbox. The fixed parameters for this optimization comprised the ratios delineated previously and the structural configuration of the hidden layer, which consisted of a single hidden layer with a variable number of neurons.

The learning rate underwent modifications within a spectrum of 0.01 to 0.4, and the neuron count in the hidden layer was changed from 1 to 20. The optimization methodology is built upon a dual-loop architecture, whereby each iteration requires allocating two separate values to the learning rate and the neuron count, in that sequence. Training takes place for every distinct combination, and we assess the Root Mean Square Error (RMSE) for both the training group and validation group throughout each cycle. The optimal combination is determined based on the RMSE criterion; a lower RMSE indicates a more precise model. The final model and its optimized parameters are delineated in Table (1).

Table 1. Optimized ANN model parameters

Training Algorithm	Levenberg-Marquardt
Hidden Layers' Structure	[4,4,4]
Learning Rate	0.07
Number of Epochs	500

3 RESULTS AND DISCUSSION

3.1 ANN performance

Upon the acquisition of the optimized training parameters, the model underwent multiple training iterations utilizing the Parallel Computing toolbox. This particular toolbox was essential as the training was conducted until the cumulative Root Mean Square Errors (RMSEs) reached or fell below a predetermined threshold. To lessen the likelihood of an infinite loop occurring, the training setup was arranged to conclude after a certain number of cycles, fixed at 250 in this scenario when the desired RMSE was not fulfilled. Following a series of experimental trials, the model ultimately demonstrated commendable performance. The optimal outcomes of the model have been systematically presented in the subsequent Table 2.

Table 2. ANN model performance results.

Training RMSE	2.08
Validation RMSE	4.46
Test RMSE	18.43
Test set r	0.997
RMSE for the Entire Dataset	7.77
Entire Dataset r	0.995

Moreover, it is widely acknowledged that graphical representations facilitate comprehension and interpretation; thus, several graphs were additionally constructed. Figure 2a indicates that a predominant number of predictions generated by the Artificial Neural Network (ANN) show minimal error, signifying that the network is proficient in maintaining a high accuracy level in relating inputs to outputs across the bulk of the dataset. More pronounced errors observed in a segment of the histogram may signify the presence of a systematic error in that specific region in the context of an ANN, potentially leading to either underdosing or overdosing with equal likelihood.

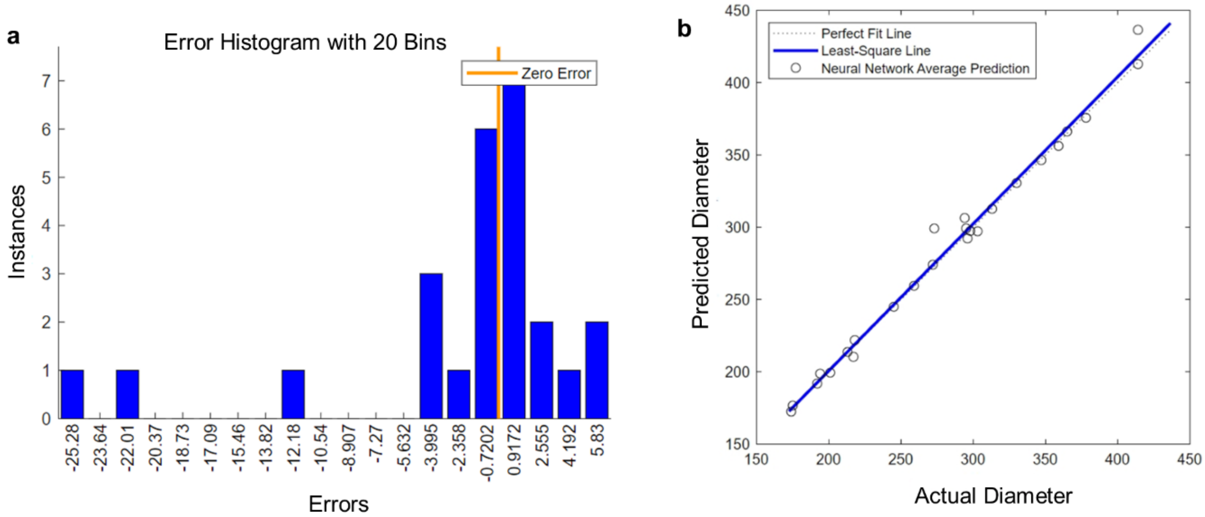

Fig. 2. The ANN model's: a) Error Distribution Histogram and b) Regression Analysis Plot

Figure 2b illustrates a regression plot. The evaluation of the regression diagram demonstrates that the actual and anticipated diameters have a strong positive relationship, with data points residing near the line that represents an exact fit. This suggests that the ANN performs effectively in predicting diameter. The alignment is nearly perfect, with the least-squares line closely adhering to the ideal fit line. Nonetheless, certain points reveal small discrepancies from the established line of best fit. These instances may indicate less optimal predictions by the ANN, possibly attributable to the presence of noisy data or restrictions in the model's capacity to generalize effectively. Table 3 illustrates a thorough assessment of the performance of our model in projecting the diameter of the electrospun Kefiran nanofibers, suggesting that our model has achieved superior results compared to the ANN model mentioned in earlier research.

Table 3. Training Data for ANN Modelling

Concentration (w/v (%))	Feed Rate (ml/h)	Voltage (kV)	TCD (cm)	Observed diameter (nm)	Predicted diameter (nm)	Predicted diameter from past literature (1) (nm)
6	1.7	10	14	175	176	185
6	1.7	10	20	192	192	188
6	2.3	10	14	217	210	221
6	2.3	10	20	213	214	192
6	2	15	17	194	199	297
6	1.7	20	14	174	172	177
6	1.7	20	20	201	199	358
6	2.3	20	14	218	222	248
6	2.3	20	20	245	245	221
8	2	10	17	259	259	246
8	1.7	15	17	313	313	261
8	2	15	14	296	292	314
8	2	15	17	295	299	298
8	2	15	17	273	299	275
8	2	15	20	294	306	297
8	2.3	15	17	303	297	135
8	2	20	17	272	274	248
10	1.7	10	14	330	331	264
10	1.7	10	20	365	366	304
10	2.3	10	14	378	376	358
10	2.3	10	20	414	413	372
10	2	15	17	414	436	382
10	1.7	20	14	298	297	314
10	1.7	20	20	359	356	377
10	2.3	20	14	347	346	376

3.2 3D plots for parameter interpretation

Three-dimensional surface representations aid in fully comprehending the detailed interactions that occur between electrospinning settings and the size of the resulting nanofibers. Consequently, several plots were generated to elucidate the relationship between two parameters while maintaining the other two at a constant and intermediate value.

Initially, the TCD and the feed rate were maintained at constant values of 17 cm and 2 mL/h, respectively, as depicted in Figure 3a. The surface plot presented therein exhibits considerable variability and complexity. It can be deduced from this evaluation that a higher voltage application is probably correlated with a widening of the nanofiber diameter. Nevertheless, this correlation ceases to be true when the concentration is either significantly low or significantly high. The diameter is minimized at medium voltage levels. In contrast, boosting concentration doesn't always lead to an equivalent enlargement of the nanofibers' diameter. The maximum diameter attainable is generated at an intermediate polymer concentration coupled with a high applied voltage.

Figure 3b illustrates the scenario where the polymer concentration and the feed rate are held constant at 8 w/v(%) and 2 mL/h, respectively. The figure distinctly indicates a nonlinear relationship between the parameters and the diameter. Additionally, it can be inferred that an increase in the applied voltage invariably leads to an increase in diameter. However, the TCD does not exhibit a similar trend as the voltage, as the diameter tends to diminish when the TCD is maintained at an intermediate value. In addition, the constants illustrated in this Figure 3c comprised the applied voltage, which was standardized at 15 kV, and the TCD, which was designated at 17 cm. The diameter exhibits a relatively direct proportionality to the feed rate. In contrast, the relationship pertaining to concentration is markedly more intricate. For diminished feed rates, the diameter tends to augment concomitantly with an increase in concentration. However, under conditions of elevated applied voltage, the diameter will initially expand, attain a maximum threshold, and subsequently experience a reduction.

For Figure 3d, both the feed rate and the applied voltage were maintained at constant values of 2 mL/h for the feed rate and 15 kV for the applied voltage. It is evident that for any specified value of the TCD, the diameter enlarges as the concentration increases. Conversely, the TCD does not consistently escalate for fixed values of concentration. Initially, the diameter experiences a slight increase with the rise of the TCD; however, it subsequently declines. Following this, for a specific TCD value, the diameter increases substantially, after which it remains unchanged. The maximal diameter achievable is produced from a solution characterized by high concentration in conjunction with the collector far from the tip.

To generate Figure 3e, the concentration and TCD were maintained at constant levels of 8 w/v (%) and 17 cm, respectively. It is discerned that the diameter expands with an escalation in applied voltage for any designated value of the feed rate. Nevertheless, regarding the feed rate, the correlation diverges. At elevated applied voltages, variations in feed rate exert negligible influence on the nanofiber diameter. As the applied voltage decreases, a minimum diameter is observed for an intermediate feed rate. Lastly, Figure 3f was constructed utilizing previously unutilized constants, specifically the applied voltage and the polymer concentration. Each parameter was fixed at values of 15 kV and 8 w/v (%), respectively. The figure permits the inference that regardless of the feed rate value, an increase in the TCD will precipitate an increase in the diameter. The interrelationship can be characterized as quadratic, given the graph's consistent pattern. For lower TCDs, the increment is pronounced; however, this increase tends to moderate for larger TCDs. Conversely, as the feed rate escalates, the diameter correspondingly increases.

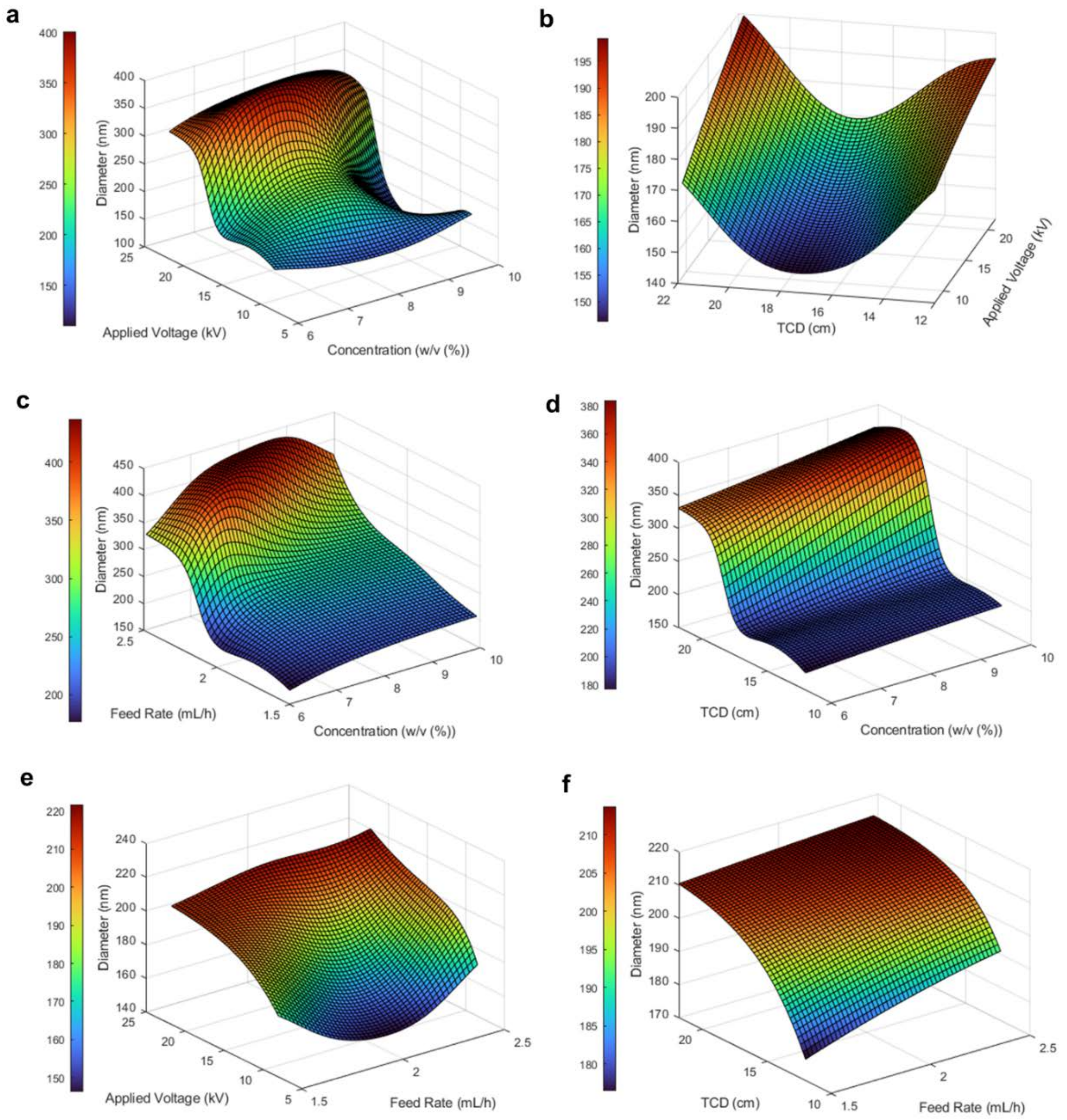

Fig. 3. Three-dimensional representations of the diameters of nanofibers, as forecasted by Artificial Neural Networks (ANN), were established at the specified parameters (a-f)

4 CONCLUSIONS

To encapsulate the findings, the model demonstrated commendable efficacy with an architecture comprising three hidden layers, each containing four neurons, and a learning rate established at 0.04. These specific parameters emerged as the most effective when evaluated against the entire spectrum of alternatives. Subsequently, the model underwent extensive training until it reached optimal performance utilizing the parameters derived through the optimization process. This culminates in a highly optimized artificial neural network (ANN) model. The Pearson correlation coefficient, which evaluates the correlation between the recorded and predicted diameters of nanofibers, was computed to be 0.995, as opposed to a coefficient of 0.671 cited in another research study. Moreover, the R-squared measurement for the testing dataset was determined, producing a value of 0.994. In summation, the model articulated and developed in this manuscript demonstrates enhanced performance when compared to the model from which the data was initially sourced.

5 ACKNOWLEDGEMENT

The authors would like to thank the Department of Mechanical and Industrial Engineering, Manipal Institute of Technology Manipal, Manipal Academy of Higher Education, Manipal for carrying out this research work.

6 REFERENCES

[1] Esnaashari SS, Naghibzadeh M, Adabi M, Faridi-Majidi R (2017) Evaluation of the effective electrospinning parameters controlling Kefiran nanofibers diameter using modelling artificial neural networks. Nanomedicine Research Journal 2:239–249. https://doi.org/10.22034/NMRJ.2017.04.005

[2] Mirzaei E, Amani A, Sarkar S, et al (2012) Artificial neural networks modeling of electrospinning of polyethylene oxide from aqueous acid acetic solution. Journal of Applied Polymer Science 125:1910–1921. https://doi.org/10.1002/app.36319

[3] Sarkar K, Ghalia M Ben, Wu Z, Bose SC (2009) A neural network model for the numerical prediction of the diameter of electro-spun polyethylene oxide nanofibers. Journal of Materials Processing Technology 209:3156–3165. https://doi.org/10.1016/j.jmatprotec.2008.07.032

[4] Samadian H, Zakariaee SS, Adabi M, et al (2016) Effective parameters on conductivity of mineralized carbon nanofibers: an investigation using artificial neural networks. RSC Advances 6:111908–111918. https://doi.org/10.1039/c6ra21596c

[5] Ma M, Zhou H, Gao S, et al (2023) Analysis and Prediction of Electrospun Nanofiber Diameter Based on Artificial Neural Network. Polymers 15:2813. https://doi.org/10.3390/polym15132813

[6] Karimi MA, Pourhakkak P, Adabi M, et al (2015) Using an artificial neural network for the evaluation of the parameters controlling PVA/chitosan electrospun nanofibers diameter. E-Polymers 15:127–138. https://doi.org/10.1515/epoly-2014-0198

[7] Yilmaz C, Ustun D, Akdagli A (2017) Usage of artificial neural network for estimating of the electrospun nanofiber diameter. IDAP 2017 - International Artificial Intelligence and Data Processing Symposium 1–5. https://doi.org/10.1109/IDAP.2017.8090329

[8] Abdelhady SS, Atta MM, Megahed AA, et al (2022) Modeling electrospun PLGA nanofibers' diameter using response surface methodology and artificial neural networks. Journal of Industrial Textiles 52:1–23. https://doi.org/10.1177/15280837221142641

[9] Khanlou HM, Sadollah A, Ang BC, et al (2014) Prediction and optimization of electrospinning parameters for polymethyl methacrylate nanofiber fabrication using response surface methodology and artificial neural networks. Neural Computing and Applications 25:767–777. https://doi.org/10.1007/s00521-014-1554-8

[10] Nasouri K, Shoushtari AM, Khamforoush M (2013) Comparison between artificial neural network and response surface methodology in the prediction of the production rate of polyacrylonitrile electrospun nanofibers. Fibers and Polymers 14:1849–1856. https://doi.org/10.1007/s12221-013-1849-x

[11] Moradi Z, Kalanpour N (2019) Kefiran, a branched polysaccharide: Preparation, properties and applications: A review. Carbohydrate Polymers 223:. https://doi.org/10.1016/j.carbpol.2019.115100

[12] Ghasemlou M, Khodaiyan F, Jahanbin K, et al (2012) Structural investigation and response surface optimisation for improvement of kefiran production yield from a low-cost culture medium. Food Chemistry 133:383–389. https://doi.org/10.1016/j.foodchem.2012.01.046

Paper submitted: 28.08.2024.
Paper accepted: 16.12.2024.