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Modeling tensile strength and suture retention of polycaprolactone electrospun nanofibrous scaffolds by artificial neural networks

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ABSTRACT

Electrospun polycaprolactone (PCL) scaffolds are broadly used in tissue engineering applications due to their superior biomechanical properties and compatibility with the cell matrix. The properties of PCL scaffolds depend on electrospinning parameters. The relationships between electrospinning process parameters and scaffold properties are complicated and nonlinear. In this study, we used the artificial neural networks (ANN) technique to estimate the tensile strength and suture retention of PCL scaffolds as a function of electrospinning parameters (polymer concentration, solution feed rate, applied voltage, and nozzle to collector distance). A standalone ANN software was developed, and the predicted properties were a good agreement with the experimental data. The present model has excellent learning precision for both training and testing data sets. The precise predictions revealed that the model could estimate the relationships between electrospinning parameters and properties of PCL scaffolds adequately.

1. Introduction

For the regeneration of lost tissue and damaged organs, tissue engineering is a multidisciplinary approach to provide tissue or organ. We are using scaffolds for regeneration of tissue and organs or filling the damaged sites. It will support the cell to transfer, connect, develop, propagate, distinguish, and finally form a functional tissue and organ [1]. A perfect scaffold for tissue engineering should be biocompatible and biodegradable, and it will contain similarity to the original matrix to provide tissues. Mechanical properties are a significant characteristic of the scaffolds functional for tissue engineering [2–4]. For replacement or regeneration of tissue, scaffolds should be satisfying unique mechanical properties depending on the kind of tissue or organ. For medical applications, a perfect scaffolding system must have enough tensile strength and the capability to withstand forces resulting from suturing when scaffolds are transplanted [5].

Electrospun nanofibrous mats are candidates for producing scaffolds due to their structural similarity to the original matrix of tissues [3]. Electrospinning is a popular method for producing scaffolds for tissue engineering. The mechanical properties of tensile strength and suture retention scaffolds are significant when scaffolds are transplanted. For example, a minimum tensile strength of 16 N/cm and suture retention strength of 20 N/mm necessary for scaffolds abdominal wall restore or hernia retention [6]. Various artificial and natural polymers were electrospun to make scaffolds for tissue engineering applications. Polycaprolactone (PCL) [3,4], FDA approved polymer is utilized to produce scaffolds for several applications such as bones, neural, nerve, cartilage, abdominal wall, and vascular tissue engineering [6–8].

The biomechanical properties (tensile strength and suture retention) are strongly dependent on the various factors related to process parameters (polymer concentration, solution feed rate, applied voltage, and nozzle to collector distance). An experimental study of these complex interactions is challenging and time-consuming [9]. The complicated relationship among the process parameters and the biomechanical properties can be correlated and explained by the artificial neural networks (ANN) method. ANN is a computational tool inspired by the biological nervous system. ANN model uses experimental data to correlate the complex relationships among the parameters without any

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specific equation.

Even though several studies are conveyed on the development of ANN models for predicting the mechanical properties of various materials, as per the author's best of knowledge, not considerable research has been reported on applying the ANN models to predict the biomechanical properties of PCL Scaffolds. Another significant limitation of the earlier studies is the lack of consideration to evaluate the relationship between independent variables and dependent variables quantitatively. Because of the prevailing gap, the present work focuses on developing an efficient artificial neural network software for modeling the tensile strength and suture retention of PCL scaffolds as a function of electrospinning parameters. The specific objectives of the present study were

- To predict properties at new instances and comparing with the existing equations of the same data sets
- To estimate the relationship between electrospinning parameters and properties qualitatively and quantitatively.
- To develop a standalone ANN software for ease of use without prior knowledge of neural networks or programming.

2. Materials and methods

The experimental data reported for PCL scaffolds were used in the present work consists of polymer concentration (PC), solution feed rate (SF), applied voltage (AV), and nozzle to collector distance (NCD) with respective biomechanical properties as taken from the literature [1]. From 27 data points, 21 data sets were being used for the model development, and the remaining 6 data sets are used for testing the model performance. The statistics and the entire data are presented in Tables 1 and 2, respectively. All the variables are normalized between 0.1 to 0.9. The normalization process is expressed as the following equation shown below [10]:

$$Xn = \left(\frac{(X - Xmin)*0.8}{(Xmax - Xmin)}\right) + 0.1 \tag{1}$$

Where Xn is the normalized value of *X; Xmax and Xmin* are the minimum and maximum values of X, respectively, in the entire data sets. Once the best network was found, all the transformed data were put back into their original value by the following equation [10]:

$$X = \left(\frac{(Xn - 0.1)*(Xmax - Xmin)}{8}\right) + Xmin \tag{2}$$

2.1. Modeling procedure

In the present study, the ANN model was trained with a backpropagation algorithm using the sigmoid function as an activation function [11–14]. A full explanation of the backpropagation algorithm and training method has been well reported [15]. The ANN model training program and the graphical user interface design were written in C and Java.

The model consists of four neurons (polymer concentration, solution feed rate, applied voltage, nozzle to collector distance) in the input layer and two neurons (biomechanical properties) in the output layer, as shown in Fig. 1. The model training involves adjusting the coefficients associated with each connection among the neurons until the input data set has calculated properties equal to the experimental data. To define the ANN model's ideal architecture and to find the model's assurance, the data sets are divided into training and testing data sets.

ANN model consists of the learning rate, momentum term, neurons in the hidden layers, the number of hidden layers, and the number of iterations. The optimum ANN model with 4−6-6−2 architecture consists of 0.65 momentum term and 0.6 learning rate with 21,000 iterations produced a minimum RMSE [16]. Tensile strength and suture retention strength average prediction error of training data and testing data is 0.21, 0.17, 0.16, and 1.44. The comparison of ANN model predictions and existing equation predictions with experimental values are presented in Table 2.

Table 1
Statistics of the database variables used in the present study.

Variable	Minimum	Maximum	Mean	Std.dev
PC (%)	10	20	15	3.396
SF (ml/h)	2	5	3.5	1.019
NCD (mm)	120	160	140	13.587
Voltage (kV)	15	25	20	3.396
Tensile strength (MPa)	0.4	3	1.485	0.653
Suture retention (N/mm)	1.5	47.9	20.49	15.458

3. Results and discussion

3.1. Validation and performance of the ANN model with experimental data

After ANN model development, performance is carried out with Pearson's r and Adj. R-squared value between experimental, published, and ANN model predicted properties of the train and test datasets. Fig. 2 (a, b) shows the correlation between the ANN predicted, experimental, and calculated biomechanical properties. From the equation and experimental tensile strength and suture retention, Pearson's r, and adj. R-squared are 0.964, 0.927, 0.984, and 0.967, respectively. Whereas the ANN model predicted tensile strength and suture retention, it was nearly equal to one with the R-Squared (0.999 and 0.999), respectively. From these, we can say the ANN predicted biomechanical properties are in good agreement with experimental properties. The percentage error of calculated [1] tensile strength and suture retention from the equation is -6.81 % and 7.27 %. Whereas the ANN model predictions, tensile strength, suture retention training data, and testing data are 0.21 %, 0.17 %, 0.16 %, and 1.44 %, respectively. The predicted and experimental tensile strength and suture retention were represented in Table 2 for the training and testing datasets.

3.2. Transformation of coefficients of the ANN model

The input, hidden, and output layers in the ANN model have connected through weights, and these weights have information about the relationship between process parameters and biomechanical properties. The model's prediction efficiency depends upon the nature and magnitude of the weights of the ANN model [17,18]. The minimum errors in ANN model predictions were obtained with 21,000 iterations. The values of initial and transformed weights were shown in Fig. 3. The ANN architecture, 4−6-6−2 yields, a total of 86 weights ((4 + 1) X 6+((6 + 1) X6+((6 + 1) X2 = 86). Initial weights were randomly generated between -0.5 to +0.5. The best model values of the weights varied from -7.9 to +5.9. These weights are capable of mapping the relationship between the process parameters and properties.

3.3. Single variable sensitivity analysis

Sensitivity analysis provides insight into the impact of a single process parameter on biomechanical properties keeping other parameters constant. Carrying out of these types of experiments requires much time and needs to spend more resources. The present ANN model can extract massive information from limited and valuable experimental data. The developed ANN model can produce infinite results; we will report a few representative results. Fig. 4(a, b) the estimated effect of polymer concentration on biomechanical properties varied from 10 % to 20 % (w/v). The biomechanical properties will increase because of increases in polymer concentration, increasing the polymeric solution's viscosity, which results in thick fibers [19]. The predictions with the increase in

Table 2
The experimental PCL properties of the RSM and ANN model predicted PCL Properties.

					Tensile Strength, MPa					Suture retention, N/mm				
S.No	PC	SF	AV	NCD	Exp	ANN	%Error	RSM	%Error	Exp	ANN	%Error	RSM	%Error
1	10	2	20	140	0.7	0.70	0.01	0.84	19.67	4.2	4.20	0.00	3.49	16.71
2	20	2	20	140	1.3	1.20	0.01	1.54	18.30	20	19.90	0.03	20.60	−3.06
3	10	5	20	140	0.9	0.80	0.01	0.71	20.50	5	5.02	0.02	2.11	57.70
4	20	5	20	140	3.03	3.00	0.01	2.95	2.77	48	47.90	0.04	46.40	3.27
5	15	3.5	15	120	2	2.00	0.04	1.98	1.00	39	39.00	0.11	37.40	4.06
6	15	3.5	25	120	1	0.50	0.02	1.15	15.26	20	6.02	0.03	25.10	25.81
7	15	3.5	15	160	1.61	1.60	0.02	1.49	7.36	32	30.40	0.01	29.90	6.27
8	15	3.5	25	160	1.36	1.30	0.02	1.41	−3.95	18	18.10	0.10	17.70	1.42
9	10	3.5	20	120	0.5	0.40	0.03	0.83	66.60	6	6.06	0.21	7.99	33.10
10	20	3.5	20	120	2.27	2.20	0.02	2.30	−1.29	39	38.90	0.04	38.70	0.75
11	10	3.5	20	160	0.5	0.50	0.02	0.72	43.80	2	1.74	0.07	0.57	71.42
12	20	3.5	20	160	1.9	1.90	0.00	2.19	15.00	33	32.90	0.06	31.20	5.19
13	15	2	15	140	1.42	1.40	0.01	1.41	0.39	25	24.80	0.06	26.10	−4.47
14	15	5	15	140	2.26	2.20	0.03	2.06	9.00	38	3.04	0.06	38.30	−0.88
15	15	2	25	140	1	1.00	0.00	0.96	3.77	14	13.80	0.12	13.80	0.93
16	15	5	25	140	1.55	1.50	0.03	1.60	−3.49	23	22.80	0.07	26.00	13.41
17	10	3.5	15	140	0.66	1.90	0.00	0.84	26.50	12	3.96	0.16	15.80	26.96
18	20	3.5	15	140	2.6	2.50	0.01	2.64	1.35	42	41.90	0.19	46.50	10.91
19	10	3.5	25	140	0.83	0.80	0.12	0.72	13.64	4	4.09	1.03	3.62	9.49
20	20	3.5	25	140	2.1	2.00	0.11	1.85	11.92	36	36.30	0.96	34.30	4.62
21	15	2	20	120	1	0.90	0.00	0.85	14.90	20	1.52	0.06	18.20	8.79
22*	**15**	**5**	**20**	**120**	**2.06**	**2.00**	**0.11**	**2.28**	**10.79**	**34**	**33.90**	**0.89**	**30.40**	**10.41**
23*	**15**	**2**	**20**	**160**	**1.8**	**1.80**	**0.00**	**1.53**	**15.19**	**10**	**10.00**	**1.59**	**10.80**	**−8.20**
24*	**15**	**5**	**20**	**160**	**1.28**	**1.20**	**0.10**	**1.38**	**−7.67**	**18**	**1.50**	**1.30**	**23.00**	**24.52**
25*	**15**	**3.5**	**20**	**140**	**1.65**	**1.60**	**0.40**	**1.51**	**8.52**	**35**	**34.80**	**2.08**	**33.00**	**5.59**
26*	**15**	**3.5**	**20**	**140**	**1.73**	**1.60**	**0.37**	**1.51**	**12.75**	**36**	**34.80**	**2.78**	**33.00**	**8.21**
27*	**15**	**3.5**	**20**	**140**	**1.5**	**1.60**	**0.04**	**1.51**	**−0.62**	**134**	**34.80**	**0.04**	**33.00**	**2.81**

22* – 27* data sets were treated and designated as test data sets.

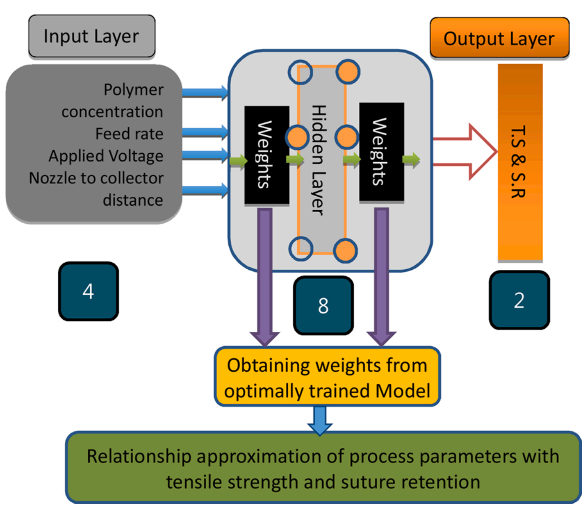

Fig. 1. Schematic representation of the ANN model.

the applied voltage decrease the tensile strength and suture retention, as shown in Fig. 4(c,d). The electrified strength is inversely proportional to the nozzle to collector distance and at the distance's low values. When the applied voltage is high, it will cause beads that will affect the biomechanical properties [20,21].

Further, the ANN model was used to estimate the combined impact of two electrospinning parameters on properties, as shown in Fig. 5. The increase in applied voltage results in the decrease of biomechanical properties because of the electrostatic repulsive forces on the charged jet increases the fiber diameter favors the narrowing of properties. In addition to this phenomenon, when the applied voltage around the optimum value increases the probability of bead formation. The increase in NCD increases the tensile strength and decrease in suture retention due to the electrified strength is applying in reverse to the NCD, so thick beads will form at lows distance. Fig. 5(c,d) illustrates the 3D surface plots of biomechanical properties by using PC and SF. The responses show that changes in both biomechanical properties are highly responsive at Polymer concentration and SF.

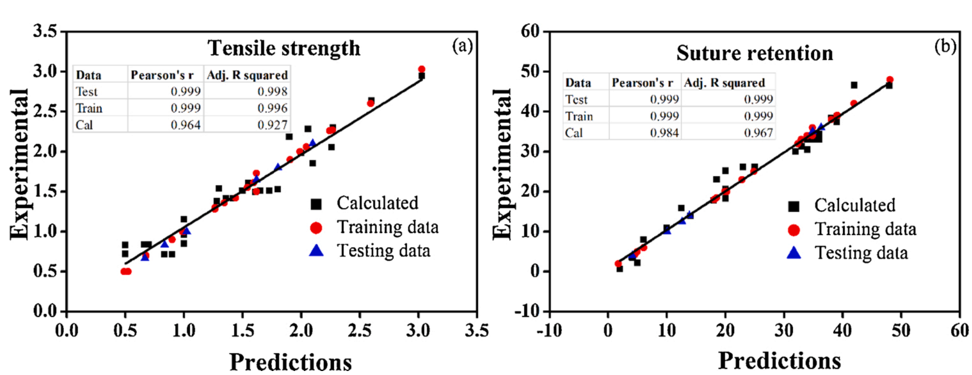

Fig. 2. Comparison between experimental biomechanical properties with predcitions by RSM and ANN models (a) Tensile strength, and (b) Suture retention.

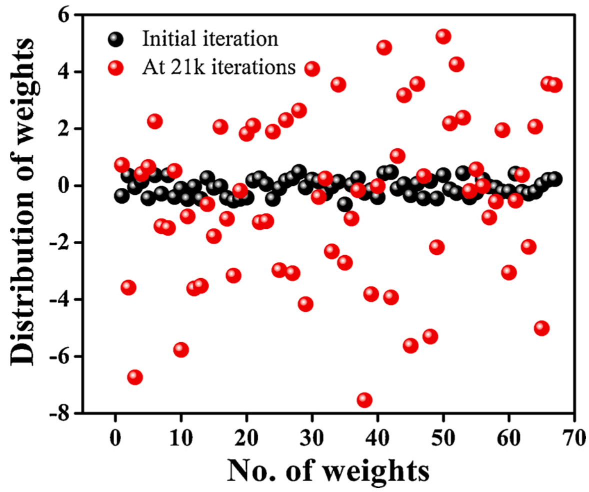

Fig. 3. Distribution of initial and optimally trained model weights of the ANN model.

3.4. Creation of an imaginary electrospinning system

We created an imaginary electrospinning experimental system with the datasets' minimum values, which are not available in experimental data. These values are fed to the ANN software developed, as shown in Fig. 6, and estimated the biomechanical properties. Fig. 6 shows the ANN model's graphical user interface with virtual electrospinning experimental conditions and respective predicted properties. The ANN model uses the weights reported in Fig. 1. The predicted values of the tensile strength and suture retention are 0.512 MPa, and 6.22 N/mm respectively. More importantly, the predictions are also within the range of the experimental biomechanical properties. This proves the model's ability to correlate the relationship between process parameters and properties. There is an infinite number of experiments possible within the range of the electrospun parameters. Our ANN model can predict the biomechanical properties of PCL Scaffolds for these infinite experimental conditions with reasonable accuracy.

Table 3 shows the quantitative estimation of biomechanical properties by the virtual addition of input parameters. The change in polymer concentration from 10 to 15 % increased tensile strength (0.512–1.431) and suture retention (6.22–29.75), and these results are in good agreement with the single and two-variable plots. At an average of a 1% increase in polymer, concentration increases tensile strength and suture retention by 0.184 MPa and 4.71 N/mm, respectively. Changing in solution feed (mL/h) from 2 to 3.5 mL/h by keeping other parameters constant, we predicted the two properties. There is not enough time available for evaporation of starch; hence, the larger fibers increase tensile strength and suture retention. At an average of a 0.5 % increase in solution feed rate increases tensile strength and suture retention by 0.186 MPa and 3.13 N/mm, respectively. Increasing applied voltage from 15 to 20 kV resulted in a decrease in tensile strength and suture retention due to beads' formation.

Suppose we are increasing in NCD, and the remaining parameters are kept constant. It will usually affect the fiber thickness and morphology by modifying the electric field strength so that tensile strength and suture retention will increase. The experimental values of tensile strength and suture retention are 1.650 MPa and 35 N/mm (See in Table 2). The prediction values of tensile strength and suture retention are 1.618 MPa, and 34.83 N/mm. The percentile of error was tiny, so our predicted values are also suitable for making scaffolds.

3.5. Index of the relative importance

The qualitative effect of individual process parameters on properties can be estimated by using the index of relative importance (I_{RI}) method. A detailed explanation of this method has been reported [10,22]. In this study, we selected two samples, which are higher and lower tensile

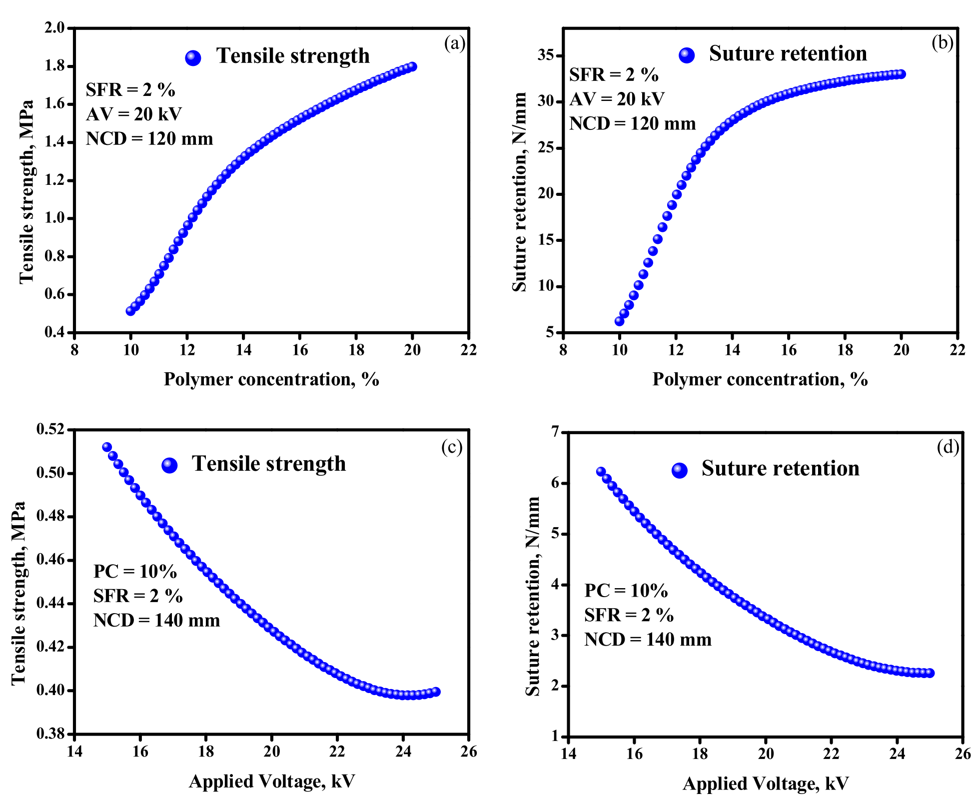

Fig. 4. Predicted Tensile strength and suture retention as a function of (a) and (b) polymer concentration, (c) and (d) applied voltage, keeping other parameters are constant.

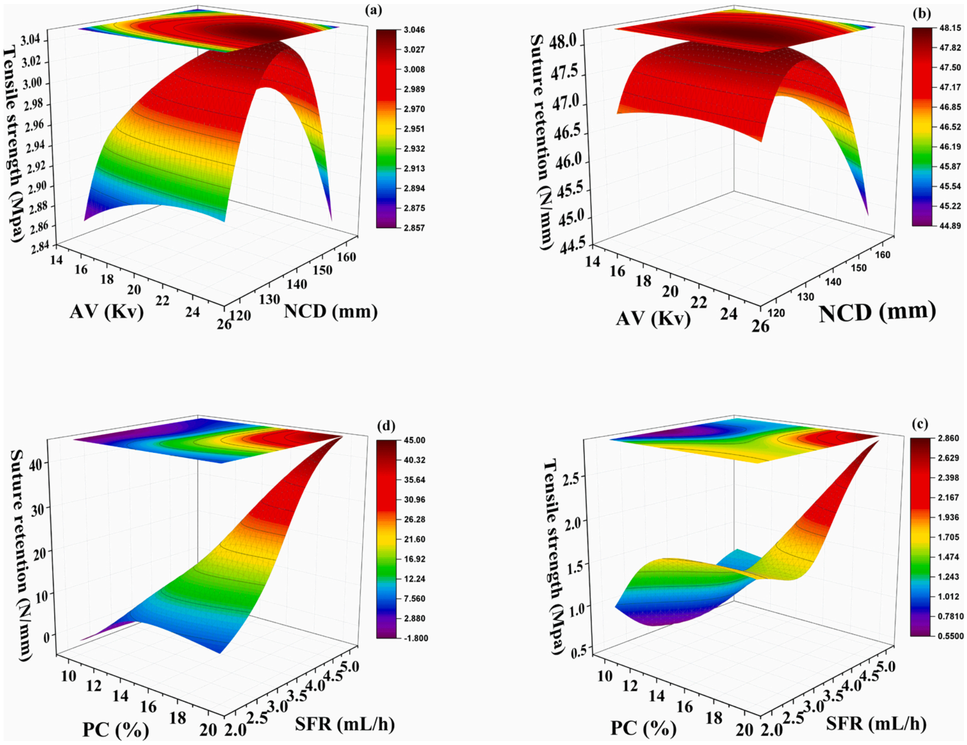

Fig. 5. 3D surface plots showing the effect of process parameters on biomechanical properties.

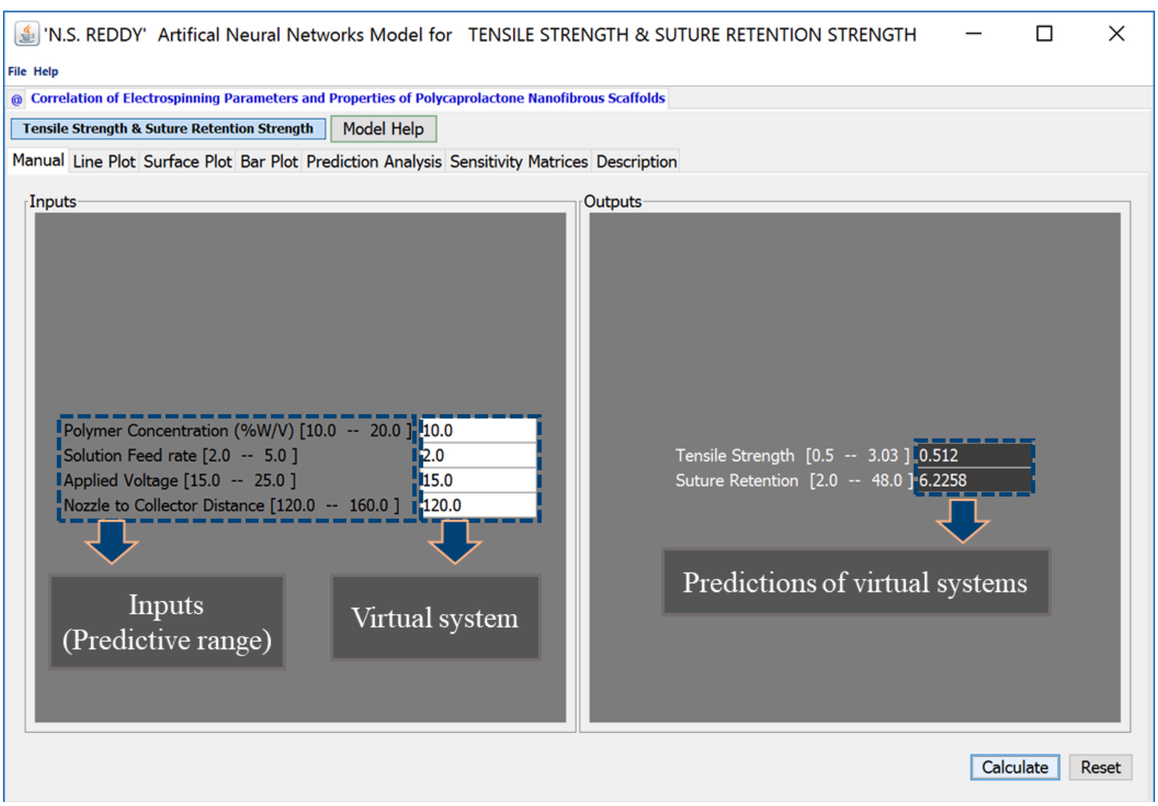

Fig. 6. The graphical user interface of the model with an imaginary electrospinning experimental conditions and respective predictions.

strength and suture retention. Fig. 7 shows the I_{RI} for the biomechanical properties of the tensile strength (3.030 and 0.70 MPa) and suture retention strength (48 and 4.20 N/mm), respectively.

The higher values of tensile strength and suture retention (Fig. 7 (a&c)) are due to the positive effect of polymer concentration, solution feed rate, and nozzle to collector distance. The decrease in polymer concentration (20 to 10) and solution feed rate (5 to 2) resulted in lower values (Fig. 7(b&d)) of both the tensile strength and suture retention.

Table 3
Quantitative estimations of the relationships between electrospun process parameters and biomechanical properties. (Grey shades indicates the components of Virtual Electrospun System.)

PC	SF	AV	NCD	TS	Change	SR	Change
10 min	2.0 min	15.0 min	120 min	0.512	0	6.22	0
15	2.0	15.0	120	1.431	0.912	29.75	23.53
15	3.5	15.0	120	1.989	0.558	39.09	9.34
15	3.5	20	120	1.430	-0.559	30.69	-8.4
15	3.5	20	140	1.618	0.188	34.83	4.14

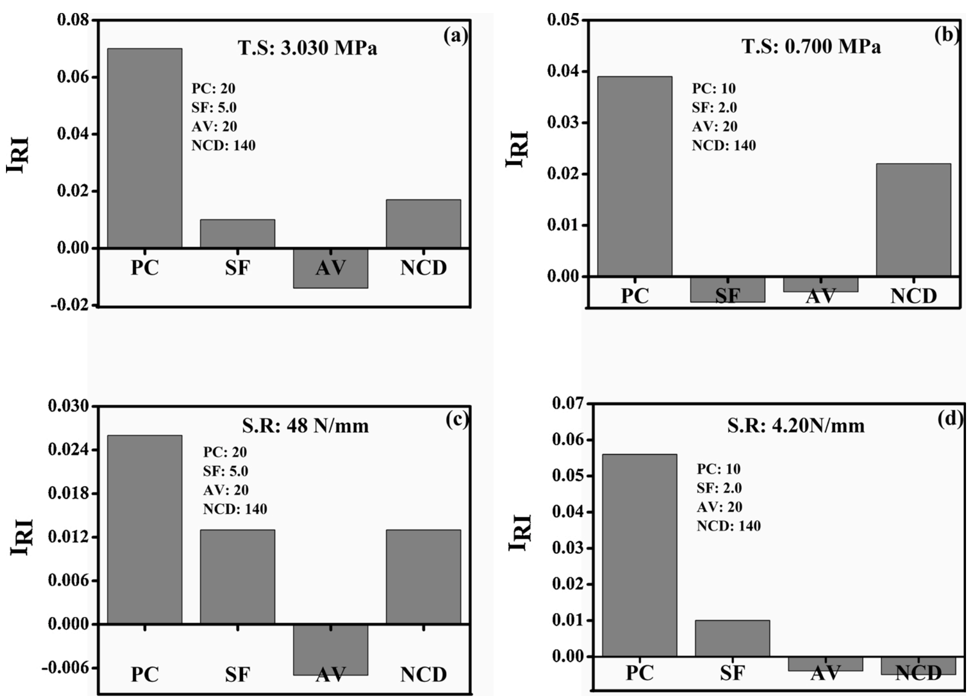

Fig. 7. The index of relative importance (I_{RI}) of polymer concentration, solution feed rate, applied voltage, and nozzle to collector distance on (a) 3.03 MPa tensile strength, (b) 0.70 MPa, (c) 48 N/mm suture retention, and (d) 4.20 N/mm suture retention.

Even though the applied voltage is having an adverse effect in all the four cases, the degree is different due to changes in the other two parameters. The lower values of polymer concentration and solution feed rate parameters result in larger fiber diameter and decrease the suture retention and tensile strength.

4. Conclusion

1) This work outlines the use of an artificial neural network to model the tensile strength and suture retention of PCL scaffolds from their electrospinning parameters. The predicted results are in good agreement with the experimental results than the published model.
2) The ANN model estimated a minimum nanofibrous tensile strength and suture retention 0.70 MPa and 4.20 N/mm. These results can be achieved with 10 % polymer concentration, 2.0 ml/h feed rate, high voltage 20 kV, and nozzle to collector distance is 140 mm. The proposed model is an efficient technique for optimizing process parameters for the desired scaffold's biomechanical properties.
3) Electrospun nanofibrous biomechanical properties prediction is difficult owing to its complex interactions between various parameters. We created imaginary electrospinning to estimate the impact of electrospun parameters on properties quantitatively. It is a new and simple technique to identify the significance of input parameters on the nanofibrous scaffold's properties.

CRediT authorship contribution statement

B.S. Reddy: Methodology, Writing - original draft. **Kim Hong In:** Investigation. **Bharat B. Panigrahi:** . **Uma Maheswera Reddy Paturi:** Writing - review & editing. **K.K. Cho:** Supervision, Writing - review & editing. **N.S. Reddy:** Methodology, Supervision, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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