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Modeling and Prediction of Electrospun Fiber Morphology using Artificial Intelligence Techniques

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Abstract

This study presents the application of Artificial Intelligence (AI) techniques to predict the morphology of nanofibers produced by needless electrospinning method. Two straight and parallel copper wire electrodes electrospinning method was used to produce nanofibers. Using digital image processing software Image Journal, Mean Nanofiber Diameter (MFD) and Nanofiber Diameter Standard Deviation (NFSD) have been measured and recorded. Adaptive Neuro-Fuzzy Inference Systems (ANFIS), Support Vector Machines (SVMs) and Gene Expression Programming (GEP) methods were used for prediction of electrospun nanofiber morphology. Prediction results and experimental were compared. It was found that SVMs model has better predictive power in comparison with both ANFIS and Gene Expression Programming models. However, results provided by both GEP and ANFIS are also acceptable. The relative importance of process parameters as contributor to the nanofiber morphology was also investigated. It was found that nanofiber morphology was strongly or weakly dependent on processing parameters.

Keywords: Nanofiber; Adaptive Neuro-Fuzzy Inference Systems (ANFIS); Support Vector Machines (SVM)s; Artificial Intelligence (AI)

Introduction

Morphological properties of electrospun fibers such as fiber diameter and fiber diameter distribution are considered as the main parameter for quality control and small fiber diameter and higher fiber uniformity are desired in many applications. These properties depend on many different factors including processing parameters, polymer solution properties, and ambient parameters. However, one major issue with the process is the lack of a functional model that can link processing parameters and polymer solution properties to fiber morphology (fiber diameter and its distribution), which could allow these variables to be easily identified based on desired fiber properties. The electrospinning process is complex with the resulting fiber diameter being influenced by numerous material, design, and operating parameters. Therefore predicting the electrospun fiber morphology is very important from a technological point of view. Recent publications [1-5] provides a review of significant previous modeling attempts, as well as a detailed analysis of the effect of processing parameters and solution properties on the electrospinning process. Thompson's work identified important parameters but did not bridge the gap from a mathematical model to a functional model that could predict fiber diameter based on processing and solution conditions, a gap that remains to be filled. Response Surface Method (RSM), which is an empirical technique, has been used to establish the processing parameter-to-electrospun fiber diameter relationship in a few recent works. Ziabari et al. [6] used response surface methodology to predict the electrospun morphology based on processing variables. They established the quadratic models for mean fiber diameter and standard deviation of fiber diameter in terms of processing variables. They concluded that more uniform fibers were obtained at lower concentrations, lower voltage, and longer working distance. The flow rate was found to have an optimum value in order to form uniform fibers. The optimum flow rate value was affected by the other variables. The results have also shown that the relationship between electrospinning parameters and electrospun fiber morphology was nonlinear. Since the relationship between electrospinning parameters and electrospun fiber morphology is nonlinear, it is very difficult to use conventional techniques such as regression to predict morphology of electrospun fiber. However, in complex multi-variate problems such as electrospinning process, empirical model is not suitable. In fact, the relationship between electrospinning parameters and electrospun fiber morphology is nonlinear, therefore it is very difficult to use empirical techniques such as regression to predict morphology of electrospun fiber. One of the difficulties in regression model is that usually a linear model should be predefined. Intelligent control is a rapidly developing field with great practical importance and potential. An intelligent control system emerged from artificial intelligence and computer-controlled systems as an interdisciplinary field.

A neuro-fuzzy system can serve as a nonparametric regression tool, which models the regression relationship non-parametrically without reference to any pre-specified functional form [7-12]. Figure 1 shows the model linking processing parameters to electrospun fiber morphology. The main objective of this chapter is to use these new methodologies to predict the electrospun fiber diameter using the polymer solution properties and processing parameters. Such an approximation may then be used to determine the process and material parameters for a targeted fiber diameter. In this study, Adaptive Neuro-Fuzzy Inference Systems (ANFIS) and Support Vector Machines (SVMs) models were used to establish a relationship between PEO nanofiber diameter and electrospinning processing parameters. The predictive performances of the two models were estimated and compared to those of Gene Expression Programming (GEP). These approaches allowed finding information hidden in the data and their performance could be better than that of RSM.

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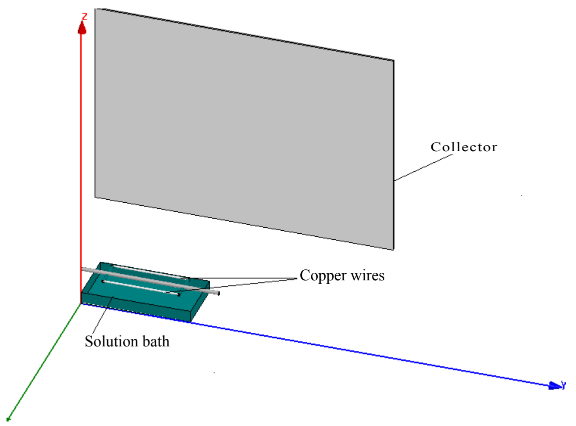

Figure 1: Two straight wires electrospinning setup.

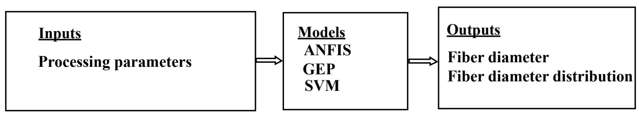

Figure 2: Model linking electrospinning processing parameters and electrospun fiber morphology.

Materials and Methods

Polyethylene oxide (PEO) is the polymers used in the completion of this work. Polyethylene oxide (PEO), with an average molecular weight (Mw) of 1,000,000, was obtained from Shanghai Liansheng Chemical (China) and used as received. Different PEO solution concentrations were prepared by dissolving the PEO in distilled water and each solution was stirred until homogenization. Different PEO solution concentrations (4, 6, 8, 9, 10) wt% were used. Polyethylene oxide (PEO) was used as it is an easily processible polymer and has a known and very well documented history of being processed. It is a polymer that is widely used in many biomedical applications and thus it was desirable to ascertain the ability of this polymer to be utilized in the electrospinning technique. The high voltage power supply FI 80-L was obtained from Fudan Middle School, Shanghai (China).

Electrospinning method

In this process, two straight and parallel copper wire electrodes mounted on a rotating metal spindle which is connected to a belt drive that is powered by a DC motor to allow for variable speed control. Figure 2 shows the setup of the method. As the spindle rotates along with the two copper wires, the wires are drawn through the polymer solution bath. The metal spindle is connected to a high voltage power supply (positive electrode) and the collector plate is connected to ground. As the wires move through the polymer solution bath, solution is entrained on the wires, resulting in a thin film of solution coating the wires. The forces such as gravity, surface tension, viscosity and inertia acting on polymer solution determine the amount of the solution entrained on the wire. Due to Plateau-Rayleigh instability, the coating breaks up into individual droplets of charged polymer solution on the wires. At the sufficiently high local electric field, the individual drops deform and jets are produced from the droplets, giving rise to a form of free surface electrospinning. As the wires rotate, electrospinning continues to occur until the supply of polymer solution is depleted plate.

Experimental design

Spinning distance (D=40, 50, 60) cm, applied voltage (V=50, 60, 70) kV, wire electrodes diameter (WD=0.37, 0.43, 0.55) mm, rotation speed (RS=6, 9, 12) rpm were considered in this study. Fractional factorial design, six factors at three levels (3^6-3=27) runs were used. All experiments have been carried out at a temperature of T=27.5 ± 1.5°C and under normal atmospheric pressure. Relative humidity varied between (20-55)% during experiment. Each experiment process was run for twenty-thirty minutes.

Characterization of nanofibers

Fiber formation and morphology of the electrospun PEO fibers were determined using a Scanning Electron Microscope (SEM). Samples were cut to obtain the SEM images Fiber diameters were measured with digital image processing software Image J [13] (National Institutes of Health, USA). This program measures the number of pixels and scales the length according to the calibration provided by the user. First the scale was set. Then, pixels between two edges of a fiber perpendicular to the fiber axis were counted. Each fiber diameter was measured at the location where the fiber was identified as a single fiber. There may be up to half a pixel error in both directions which should turn out up to 1-pixel error in measuring fiber diameter. The number of the pixels was converted to nanometers (nm) using the scale and the resulting diameters were recorded. Diameters of fibers of each SEM image were measured and average of fiber diameters (MFD) along with standard deviation of Fiber Diameters (FSD) values were then calculated.

Data collection

The experimental results data produced with two rotating straight and parallel wire electrodes electrospinning methods were used to train the models. The results are summarized in Table 1. A total of 26 data pairs were used. The data has been divided into two sets, namely, training (estimating) and checking (validation) data sets. Table 2 shows the processing parameters selected. Five processing parameters: solution concentration (C), working distance (D), applied voltage (V), wire diameter (WD) and rotation speed (RS) been chosen based on their high influential degree on the electrospun fiber morphology. Processing parameters were used as inputs (independent variables). Mean nanofiber diameter (MFD) and a standard deviation of electrospun fiber diameters (FSD) were the targets (outputs). For implementation, Commercial DTREG software [14] was used to execute SVMs and GEP while Matlab software [9] was used to execute ANFIS model.

Prediction of nanofiber morphology with ANFIS: Details on ANFIS can be found in reference [9]. For implementation, the Fuzzy Toolbox in MATLAB software, which provides functions of constructing, editing and training of ANFIS, was employed. Since the input data set has a high dimension, we used clustering function as a pre-processor to ANFIS (Figure 3) for determining the initial rules. An important advantage of using a clustering method to find rules is that the resultant rules are more tailored to the input data than they are in a FIS generated without clustering. This reduces the problem of combinatorial explosion of rules when the input data has a high dimension. The ANFIS used here contains the 32 rules (32=25) with 2 membership functions being assigned to each input variable. In the experiment, there was totally dataset of 26 pairs. These data were divided into two sets: training (75%), and test (25%) in order to meet the requirements of generalization. After the 10 epochs, the final results are expressed by the Root Mean Squared Error (RMSE). At the end of training, RMSE was 1.66178 and was quite small but the final comment

#	WD	V	D	C	RS	RH	Min	Max	MFD	FSD
C1	0.43	40	50	6	6	42	247	667.57	358.91	99.11
C2	0.43	40	50	6	9	42	236	396.69	299.4	44.39
C3	0.43	40	50	6	12	42	234	432.71	321.87	63.41
C4	0.43	50	60	8	6	25	329	552.49	449.12	66.46
C5	0.43	50	60	8	9	25	480	817.81	618.59	106.15
C6	0.43	50	60	8	12	25	313	677.4	513.61	88.35
C7	0.43	60	70	10	6	45	236	420.73	308.35	47.42
C8	0.43	60	70	10	9	40	281	676.15	383.96	97.96
C9	0.43	60	70	10	12	46	288	731.1	530.79	160.36
C10	0.55	40	60	8	6	46	349	662.98	509.39	94.5
C11	0.55	40	60	10	9	42	165	890.86	365.54	213.12
C12	0.55	40	60	10	12	42	215	874.77	533.14	218.1
C13	0.55	50	70	6	6	35	304	594.99	401.91	82.57
C14	0.55	50	70	6	9	35	281	480.23	393.97	55.6
C15	0.55	50	70	6	12	32	221	678.41	350.1	119.48
C16	0.55	40	60	10	6	40	444	614.14	508.88	65.68
C17	0.55	60	50	8	9	20	537	809.28	636.58	110.63
C18	0.55	60	50	8	12	20	199	747.16	430.41	140.79
C19	0.37	40	70	8	6	20	576	825.11	704.46	79.12
C20	0.37	40	70	8	9	20	376	668.29	550.55	114.49
C21	0.37	40	70	8	12	20	258	478.82	316.48	56.84
C22	0.37	50	50	10	6	55	233	461.51	336.3	64.04
C23	0.37	50	50	10	9	45	152	334.15	267.9	49.15
C24	0.37	50	50	10	12	42	215	665.23	377.53	167.85
C25	0.37	60	60	6	6	30	266	444.34	348.4	57.1
C26	0.37	60	60	6	9	28	221	479.7	321.01	80.12
C27	0.37	60	60	6	12	28	NaN	NaN	Nan	NaN

Table 1: Electrospinning conditions and statistics of responses for two straight wires electrospinning (Method C).

Processing parameters	Description of parameters	Units
C	Concentration	C (wt %)
D	Distance	cm
V	Applied voltage	kV
WD	Wire diameter	mm
RS	Rotation speed	rpm

Table 2: Processing parameters selected.

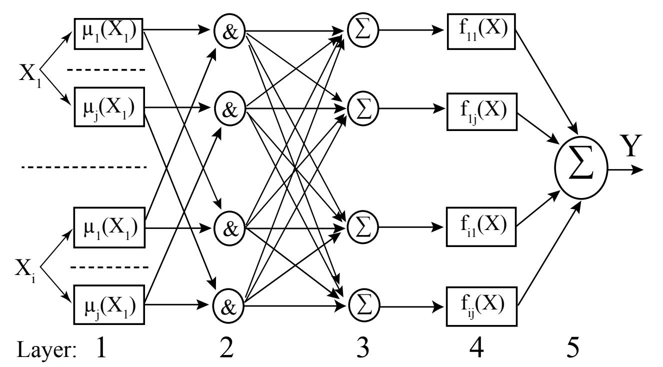

Figure 3: ANFIS architecture.

on overall prediction performance should be made by analyzing the testing results.

Prediction of nanofiber morphology with Support vector machines: The foundations of Support Vector Machines (SVM) have been developed by Vapnik [10], and are gaining popularity due to many attractive features, and promising empirical performance. The formulation embodies the Structural Risk Minimization (SRM) principle, as opposed to the Empirical Risk Minimization (ERM) approach commonly employed within statistical learning methods. SRM minimizes an upper bound on the generalization error, as opposed to ERM which minimizes the error on the training data. It is this difference that equips SVMs with a greater potential to generalize, which is our goal in statistical learning. Details on SVMs are found in [10].

As the problem is nonlinear, we first apply the RBF kernel function to map the data into a different space where a hyperplane can be used to do the separation. The RBF function nonlinearly maps samples into a higher-dimensional space, so, unlike the linear kernel, RBF can handle the case when the relation between class labels and attributes are nonlinear. Furthermore, the linear kernel and sigmoid kernel behave like RBF for certain parameters [10-12]. To find the optimal parameter we used grid and pattern search methods. As the complexity increases by the number of support vectors, SVM is constructed through trading off decreasing the number of training errors and increasing the risk of over-fitting the data. Since SVM captures geometric characteristics of feature pace without deriving weights of network from the training data, it is capable of extracting the optimal solution with the small training set size. We conducted grid search and pattern search methods using ten-fold cross-validations on the training data and reported the validation results. One subset is chosen for testing and remaining 9 subsets are used for training and the process is repeated until all the subsets are chosen for the testing. For implementation, the DTREG software was used to execute the SVM. We used both grid and pattern search methods on ε=0.001, 165.684766 and 0.41591837, p=21.0604513 for MFD,ε=0.001, 43.4424563 and 102.857194, p=21.6661033 for FSD, both using 10-folds cross-validation. The results including the number of support vectors (Figure 4) and analysis run time are reported in Table 2.

Prediction with Gene expression programming: More details on GEP are found in Ferreira's work [14]. It is a development of genetic algorithms and genetic programming. It uses a population of individuals, selects them according to their fitness and luck of roulette wheel, and introduces genetic variation in the individuals using various genetic operators resulting in the development of an expression, which describes the data that is input. GEP evaluation was performed using 10-fold cross-validation. The Generations required to the training of model, the complexity of model before simplification, the complexity of model after simplification, the generations required for simplification and the number of evaluations of the fitness function were optimized on trial and error based. The optimal values of these parameters for both MFD and FSD are given in Table 3. The mathematical expressions, as the models to represent the interactions between the different variables in consideration, were generated for both MFD and FSD and are given by equations (1) and (2), respectively:

$$\mathrm{MFD(nm)}=\left(\left(\left(\left(\frac{93.176954}{\mathrm{WD}}\right)+\left(1.7077874\times(\mathrm{D+V})\right)+\frac{(-421.64372)}{\mathrm{D}}\right)-10.387579\right)+\left(\left((-5.0039359)\times\mathrm{C}\right)+\left(\frac{\left(\left(\frac{\mathrm{V}}{\mathrm{WD}}\right)+\mathrm{WD}\right)}{\mathrm{WD}\sqrt{\mathrm{RS}}}\right)\right)\right) \tag{1}$$

$$\mathrm{FSD(nm)}=\left(3.0249211\times\left(\mathrm{C}-(\mathrm{WD}\times\mathrm{V})\right)\right)+\left(\mathrm{C}-\left(\mathrm{WD}\times\left(\mathrm{D}+(5461.1092)\right)\right)\right)+\left((2.462077\times\mathrm{V})+\left(\frac{28964.329}{\mathrm{RS}}\right)\right)-\mathrm{D}+2561.2366+\left(-7387.4802\sqrt{\mathrm{WD}}\right)+\left(\frac{(\mathrm{D}+68246.209+\mathrm{V}+(-97154.841))}{\mathrm{RS}}\right) \tag{2}$$

From equations (1) and (2), one can see that the relationship between processing parameters and nanofiber diameter is nonlinear.

Validation and comparison of prediction performances of the three models: After the training, all the three models have been subjected to the unseen testing data. The goal was comparing ANFIS, SVMs and GEP models. Three methods of comparison were used to judge the performances of the three models: the Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Mean Absolute Percentage Error (MAPE). RMSE and MAE are the measures of the deviation between the actual and predicted values. The smaller the values of RMSE and MAE, the closer are the predicted values to the actual values. These three functions are widely used in evaluating the effect of fitting. All these methods of comparison are defined as the following:

$$\mathrm{RMSE}=\sqrt{\frac{1}{n}\sum_{i=1}^{n}(o_i-o_p)^2} \tag{3}$$

$$\mathrm{MAE}=\frac{1}{n}\sum_{i=1}^{n}|o_i-o_p| \tag{4}$$

$$\mathrm{MAPE}=\frac{1}{n}\sum_{i=1}^{n}\frac{|o_i-o_p|}{|o_i|}\times 100\% \tag{5}$$

where n is the number of pairs; O_i is i-th desired output O_p is i-th predicted value and, is the mean of a dependent. As it can be seen from Tables 4 and 5, SVMs have provided a good performance compared to both ANFIS and GEP.

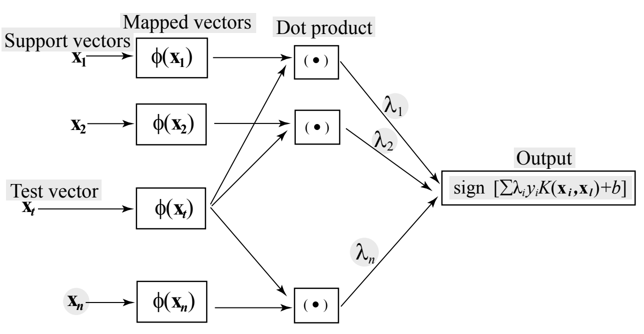

Figure 4: Structure of the support vector machines.

Nanofiber diameter property	NCVF	NSV	RMSE	MAE	MAPE	ART
MFD	10	17	41.26	36.92	9.21	04:00.0
FSD	10	15	27.28	21.54	24.33	00:06.2

Table 3: Processing parameters selected.

Results and Discussion

Importance of processing parameters on electrospun fiber morphology

Figures 5-8 show the order of computed importance of the individual processing parameter for the electrospun fiber morphology obtained by each method. The models determine the most important processing parameter. From figures one can see that the electrospun fiber morphology is influenced, to a greater or lesser degree, by processing parameters. Wire Diameter (WD) is ranked first in importance as a contributor to both MFD and FSD by both SVM and GEP models. Polymer solution concentration (C) may contribute to both MFD and FSD to a lesser degree. In fact, in the range of polymer solution concentrations where a polymer solution is spinnable, the polymer solution concentration may have a little influence in ℃ the variation of electrospun fiber diameter.

Fiber properties	GR1	GR2	CM1	CM2	NE
MFD	1140	107	56	27	230900
FSD	1910	1	75	30	110150

Table 4: GEP optimal parameters for both MFD and SDFD.

Statistical parameter	ANFIS model	SVMs model	GEP model
RMSE	55.8	48.27	49.98
MAE	50.1	36.81	40.12
MAPE	35.22	42.56	45.07

Table 5: Comparison analysis of the prediction performances of the three models for FSD.

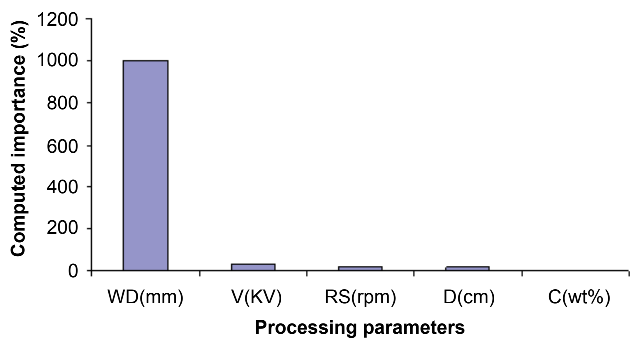

Figure 5: Computed importance (%) of processing parameters on MFD by SVMs.

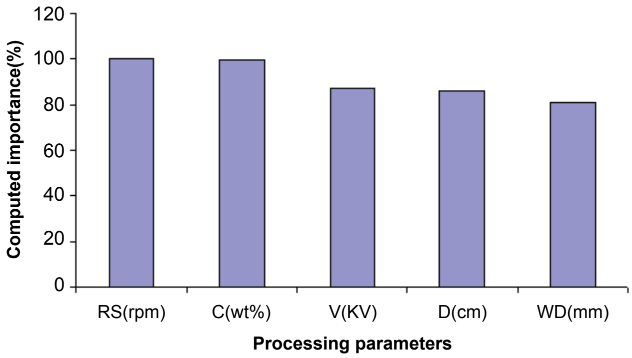

Figure 6: Computed importance (%) of processing parameters on FSD by SVMs.

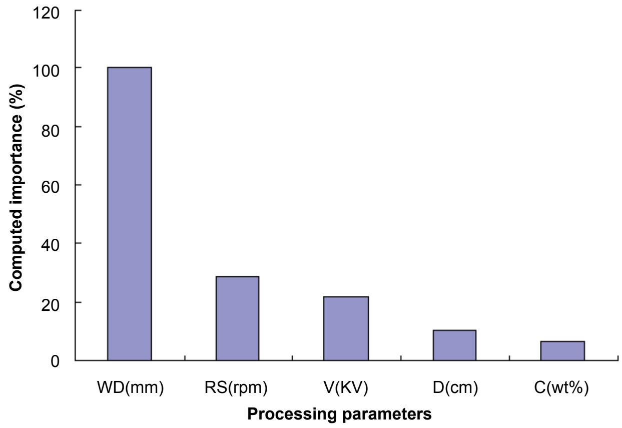

Figure 7: Computed importance (%) of processing parameters on MFD by GEP.

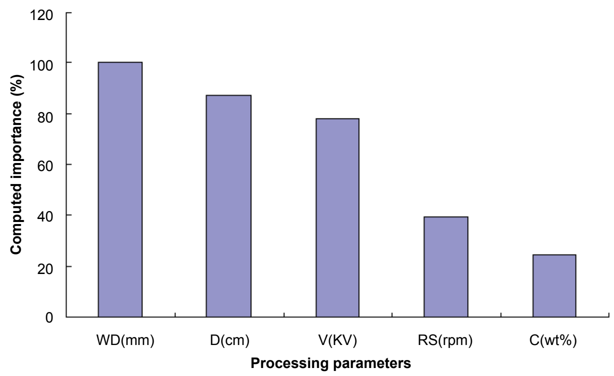

Figure 8: Computed importance (%) of processing parameters on FSD by GEP.

In this study, we have evaluated the electrospun fiber diameter with adaptive neuro-fuzzy inference systems (ANFIS) (Figure 3), Support Vector Machines (SVMs) and Gene Expression Programming (GEP). It was found that SVMs model has better predictive power in comparison with both ANFIS and Gene expression programming models. However, results provided by both GEP and ANFIS are also acceptable. These methods provide the advantage of modeling a nonlinear and complicated system without the need of finding suitable functional forms for the system, and their neural network learning ability also equips them with high efficiency in nonlinear system modeling. The relative importance of process parameters as contributor to the fiber morphology was also investigated. It was found that nanofiber morphology was strongly or weakly dependent on processing parameters. The results of this study need to be repeated and compared to others from similar analysis. As we know that the relationship between processing parameters and nanofiber diameter is nonlinear, these new artificial intelligent methods should be potentially better data analytic methods that need to be explored more in-depth to assess the practical impact of processing parameter on the electrospun nanofiber morphology and compared to more techniques that are already in use in nanofiber engineering.

Conclusion

In this study, we have evaluated the electrospun fiber diameter with Adaptive Neuro-Fuzzy Inference Systems (ANFIS), Support Vector Machines (SVMs) and Gene Expression Programming (GEP). It was found that SVMs model has the better predictive power in comparison with both ANFIS and Gene Expression Programming models. However, results provided by both GEP and ANFIS are also acceptable. These methods provide the advantage of modelling a nonlinear and complicated system without the need of finding suitable functional forms for the system, and their neural network learning ability also equips them with high efficiency in nonlinear system modelling. Relative importance of process parameters as contributor to the fiber morphology was also investigated. It was found that nanofiber morphology was strongly or weakly dependent on processing parameters. The results of this study need to be repeated and compared against others from similar analysis. As we know that the relationship between processing parameters and nanofiber diameter is nonlinear, these new artificial intelligent methods should be potentially better data analytic methods that need to be explored more in depth to assess the practical impact of processing parameter on the electrospun nanofiber morphology and compared to more techniques that are already in use in nanofiber engineering.

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