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STUDY ON THE MATHEMATICAL MODEL OF THE ELECTROSPINNING NANOFIBER DIAMETER

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Abstract

Since the diameter of the nanofiber affects the filtration efficiency and resistance of the nonwoven fabric, we use the BP neural network to study the Mathematical Model of the electrospinning nanofiber diameter about the distance (cm), the injection rate (mL/h), and the voltage (kV). First, based on the theory of statistical orthogonality, we make 30 sets of experiments and obtain 30 sets of nanofiber membranes. After, electron microscope images of the nanofiber membrane are got by the TM-1000 electron microscopy. Then, we use C++ to process the fiber images to get the diameter distribution of the nanofibers. The function relationship of the nanofiber diameter under three variables is obtained by MATLAB software to apply BP neural network knowledge. After obtaining the functional relationship, we random make three groups of experiments and compare the results with the experimental results and calculation results finding that the relative error is small, verify the function correct. The BP model predicted the minimum diameter (1,001nm) of electrospinning nanofiber membrane at the conditions of 19cm of spinning distance, 26kV of the applied voltage, and 0.8mL/h of volume flow rate.

1. Introduction

In recent years, with the rapid development of nanotechnology, electrospinning nonwovens have gained more usefulness. In people's daily lives, we can find traces of nonwoven products everywhere, such as medical equipment, medical materials, and chemistry. In the fields of catalysis, filter materials, protection products, and especially in consumer apparel, the requirements not only satisfy the need to keep warm, but also have a certain degree of comfort and decoration, and the rigid flexibility of the electrospinning fabric and the breathability of the fibers. The index directly affects its comfort, but the structure of the electro-spinning nonwoven fabric is very complicated and irregular, there is still some trouble in the research. According to the existing research results, we can know that for electrospinning nonwoven fabrics, the diameter of the fibers and the distribution of the diameter have a greater impact on the physical properties of the nonwoven, so we can study the distribution of the diameter to study the physical properties of electrospinning.

First, introduce how to measure the width of an irregular object. For this reason, let us review the geometric knowledge of the diameter. For a regular object, we can use the similarity principle measuring its diameter can be measured using the similarity principle in geometry, while the diameter measurement for an approximate regular object can be measured by the similar principle, but when the number of objects is excessive and the object is overlap, which use similar principles, it will be more complicated. In this article, we select the object rotation and overlay original image method to measure the diameter of the approximate regular object.

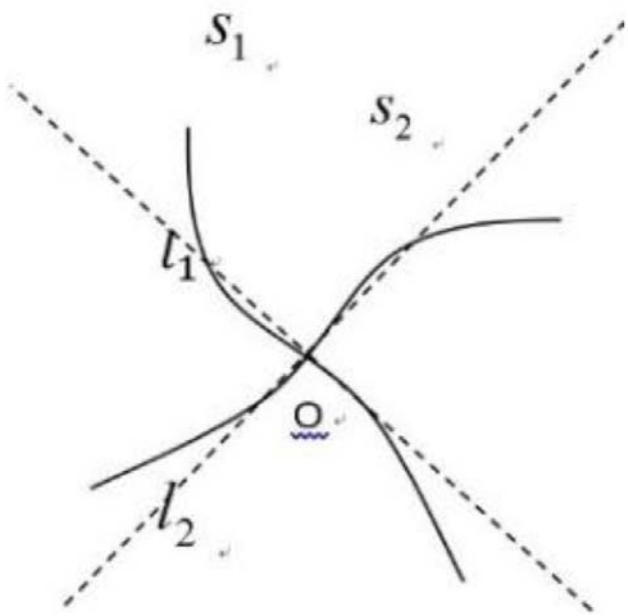


Figure 1.1. Curve rotation intersection.

As shown in the Figure 1.1, the curve S_1, S_2 and the straight line l_1, l_2, where is the curve S_1, S_2 tangent at the point o, the curve S_2 is obtained by S_1 rotating the o point clockwise by 90 degrees, l_1 is S_1 a tangent line at the point o, l_2 is S_2 a tangent line at the point o, thus

$l_1 \perp l_2$. From the principle of differentiation, we can see that for any ε, exists $\delta > 0$, so that in the neighbourhood $O(o, \delta)$, then $f(l_1) - f(l_2) < \varepsilon$, $f(x)$ indicates the length of the curve of x in the neighbourhood $O(o, \delta)$. Therefore, when δ is sufficiently small, the length of the curve can be expressed by $f(l_2) \approx f(S_2)$. So for a relatively small bending object, the width of a certain place can be expressed approximately by the width of the intersection between the centerline rotation of the object and the object, as shown in the Figure 1.2:

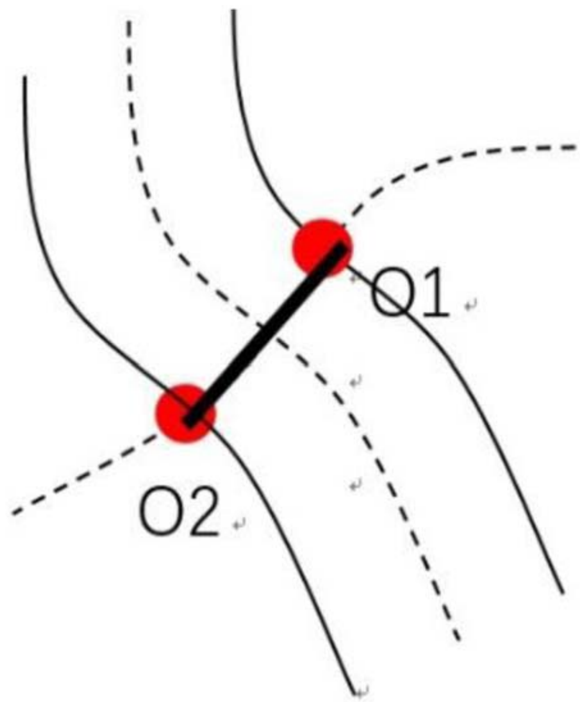


Figure 1.2. Approximate width measurement.

In this paper, what we want to study is the distribution of nanofiber diameters, so we will make a large number of diameter measurements. To increase the measurement efficiency, the method shown in Figure 1.2. Here is how to do diameter measure:

Step 1. Select a baseline from the left to the right through all fibers passing through the baseline, and count the left and right intersections of each fiber.

Step 2. Make the center of the line connecting the left and right points of each fiber as the center and the length of the line as the side length to make a square, in which the two sides of the square should be parallel to the baseline.

Step 3. Select the corresponding position of the refined image of the image to rotate counterclockwise by 90 degrees, and intersect the rotated square refined image with the corresponding position of the original image.

Step 4. After the intersection, there will be two intersection points. The distance between these two intersection points is the width of the fiber. The width value can be measured by the distance formula.

The algorithm is shown in Figure 1.3.

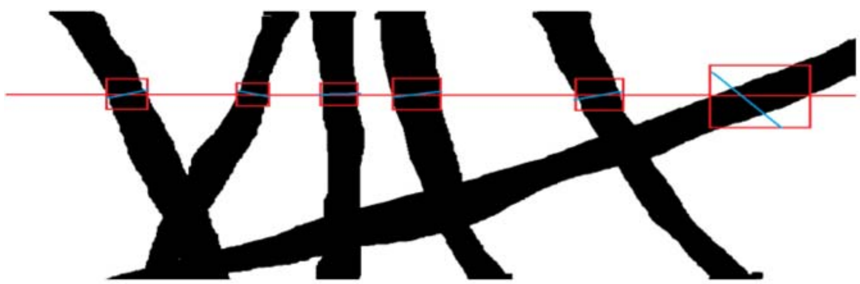
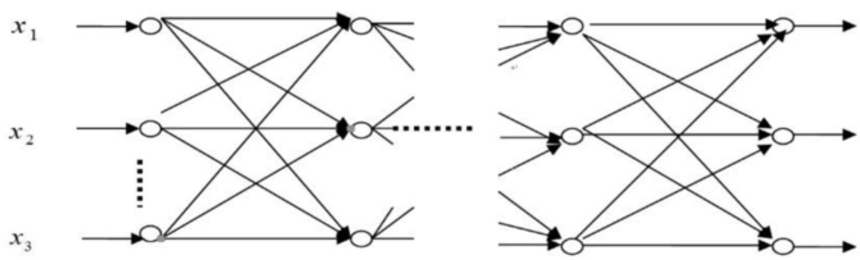


Figure 1.3. Diameter measurement.

BP neural network has been successfully applied to the modelling and the control of electrospinning processes in recent years [15, 16]. BP neural network [1, 2, 6-12] is a unidirectional propagation multilayer forward network. As shown in the figure below, it includes the input layer, middle layer, and output layer. It is a neural network with three or more layers, it estimates the response based on the trained data in the inquired range. BP neural network can store a large number of mapping relationships between input and output modes, without previously revealing the mathematical equation describing the mapping relationship, the learning rule it applies is the steepest descent method, which is continuously adjusted by back propagation n, taking the BP network as an example. For any continuous function in a closed interval, it can be solved by a single hidden-layer BP neural network. The weights and thresholds of the network can minimize the squared error of the network. Therefore, any three-layer BP neural network can complete any m-dimensional N-dimensional mapping.



For the selection of the number of hidden neurons, we can use the existing formula, which is the number of hidden neurons, the number of input nodes, the number of output nodes, based on the number of hidden neurons as little as possible, speed is as fast as possible and the error is as small as possible. On the basis of multiple simulations, the number of hidden neurons is chosen 2 to 15, and 'transig' is selected as the transfer function. The 'transig' pair is a combination of transfer functions. To make the approximation error optimal, we select 'trainlm' as the training function in the same way.

2. Experimental

2.1. Materials

Polyacrylonitrile power (PVA), molecular weight 84000-89000, average degree of polymerization 1700-1800 Taiwan Changchun Petrochemical Co. Ltd.

2.2. Instruments

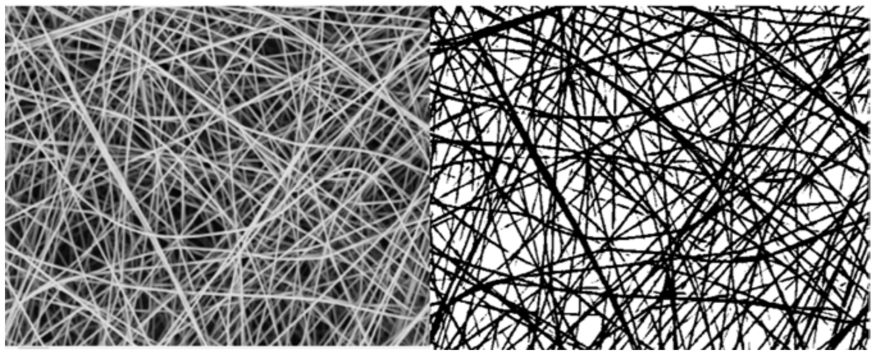
In this experiment, we used the equipment DXES-01 automatic electrospinning machine, produced by Shanghai Dongxiang Nanotechnology Co. Ltd.; TM-1000 desktop scanning electron microscope, Japan Hitachi Hi-tech Nagano Business Unit.

2.3. Sample preparation

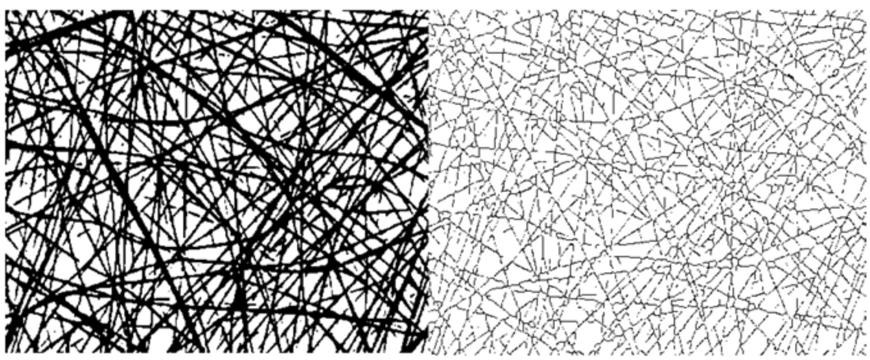
To study the properties of electrospinning nanofiber diameter, we used the experimental raw material polyvinyl alcohol (PVA) to make samples on a DXES-01 automatic electrospinning machine. The three important electrospinning factors are studied including the nozzle-collector distance (cm), applied voltage (kV), and the rejection rate (mL/h). In this experiment, we take time for 90 minutes, the polymer concentration is 12%; the distance (cm) to take 11, 13, 15, 17, 19; the voltage (kV) to take 15, 18, 20, 23, 26; the solution rejection rate (mL/h) is 0.5, 0.7, 1, 1.2, 1.5. In order to obtain more general experimental data and the number of trials is not excessive, we use an orthogonal experiment design method in mathematics and perform experiments on the basis of orthogonal tables, obtaining 30 sets of experimental samples.

2.4. Calculation of samples diameter distribution

Firstly, we use the TM-1000 desktop scanning electron microscope to take the electron microscope image and then use C++ to perform grayscale, image enhancement (Figure 2.1(a)), image binarization (Figure 2.1(b)), image denoising (Figure 2.1(c)), and image refinement (Figure 2.1(d)) in sequence on the original image, and then use refined images and binary values. The image is calculated for the diameter distribution, and the diameter of each fiber on the corresponding line of the pixel is measured every 10 pixels from the vertical 210-750 pixels. During the process of image processing, we find that some fibers are crossed together, which will lead to intersections. The numerical values are too large to affect the data, so we remove the diameters of these special anomalies and then calculate the average to obtain the diameter distribution of the experimental fibers. (Considering the above mentioned factors such as fiber crossover and the characteristics of the fiber diameter, the calculation does not exceed the average diameter of 70 pixels.) The whole process diagram is as follows Figure 2.1:



(a) image enhancement (b) image binarization



(c) image denoising (d) image refinement

Figure 2.1. The whole treatment process.

The nanofiber average diameter of 30 samples are obtained by the same method as above, and its corresponding diameter distribution is shown in Table 1.

Table 1

Number	Distance (cm)	Voltage (kV)	Speed(mL/h)	Diameter (cm)
1	11	15	0.5	6.830558627
2	13	15	0.7	9.013233424
3	15	15	1	7.54897634
4	17	15	1.2	7.686427585
5	19	15	1	8.576465396
6	19	15	1.5	7.60088917
7	11	18	0.5	8.763429997
8	11	18	0.7	11.2748824
9	13	18	1	8.312278035
10	15	18	1.2	9.959153423
11	17	18	1.5	9.308411285
12	19	18	0.5	9.70471888
13	11	20	1	9.413666504
14	13	20	1.2	9.715474569
15	15	20	0.7	10.96427777
16	15	20	1.5	8.794999672
17	17	20	0.5	10.04209325
18	19	20	0.7	6.844467498
19	11	23	1.2	9.358852779
20	13	23	1.5	9.666905455
21	15	23	0.5	7.764033572
22	17	23	0.7	7.064382946
23	17	23	1.5	11.50252052
24	19	23	1	5.350874311
25	11	26	1.5	10.22782614
26	13	26	0.5	14.73435264
27	13	26	1	9.098880443
28	15	26	0.7	11.13508447
29	17	26	1	6.849251517
30	19	26	1.2	13.50693568

3. Artificial Neural Networks Results

In the system involving three significant independent variables x1, x2, x3, the mathematical relationship between the response and these variables can be approximated by the BP neural network:

Y = 18.77/(exp(2.158/(exp(0.1803*conj(x2) – 0.277*conj(x1) – 11.24*conj(x3) + 9.738) + 1.0)
– 0.1542/(exp(0.5197*conj(x1) + 0.1255*conj(x2) – 11.85*conj(x3) – 5.784) + 1.0)
– 0.2577/(exp(0.8237*conj(x1) – 1.088*conj(x2) – 0.4984*conj(x3) + 11.01) + 1.0)
– 4.519/(exp(0.4169*conj(x1) – 0.8724*conj(x2) + 1.477*conj(x3) – 2.601) + 1.0)
– 5.12/(exp(0.1243*conj(x1) – 0.9889*conj(x2) + 2.518*conj(x3) + 20.76) + 1.0)
– 2.966/(exp(0.5777*conj(x1) + 0.2329*conj(x2) – 13.79*conj(x3) – 2.277) + 1.0)
+ 0.9069/(exp(1.513*conj(x1) + 0.3668*conj(x2) – 4.331*conj(x3) – 23.44) + 1.0)
– 6.73/(exp(1.15*conj(x2) – 0.5191*conj(x1) – 7.747*conj(x3) – 13.27) + 1.0)
– 0.2894/(exp(1.203*conj(x1) – 0.7558*conj(x2) – 3.808*conj(x3) – 2.008) + 1.0)
+ 19.89/(exp(0.6907*conj(x2) – 0.662*conj(x1) – 12.64*conj(x3) – 1.365) + 1.0)
+ 1.183/(exp(36.47 – 0.3644*conj(x2) – 10.59*conj(x3) – 1.053*conj(x1)) + 1.0)
– 1.591/(exp(28.27 – 0.8411*conj(x2) – 0.1293*conj(x3) – 0.8515*conj(x1)) + 1.0)
– 8.293) + 1.0) – 4.033,

where Y is the predicted response, x1 is the nozzle-collector distance (cm), x2 is the applied voltage (kV), and x3 is the rejection rate (mL/h). The equation is validated by the statistical tests called BP neural network analysis.

In the functional relationship, we also random do three other experiments, using the same method to obtain the average diameter, and compare the experimental results with the calculated results to analyze the relative error. The results of new offered and experimented conditions are showed in Table 2. The comparison results show that the relative error is small and the experimental results are ideal. In the other words, the BP neural network model is available.

Table 2. The Matlab and BP predicted electrospun nanofiber diameter

Number	Distance (cm)	Voltage (kV)	Rate (mL/h)	Matlab	BP	Error(%)
1	11	21	1.2	8.5301	7.634317	11.7%
2	15	26	0.6	12.1466	12.24703	0.82%
3	19	16	1.5	8.7115	9.245204	5.77%

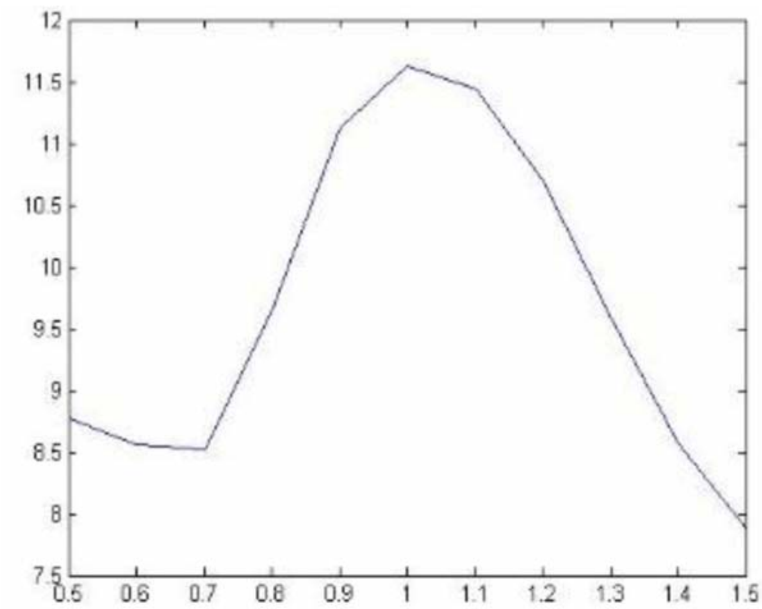
4. Results Analysis

According to the function relation $f(x1, x2, x3)$, the effects of all the single and dual factors on the diameter of the nanofiber membrane were studied. The effect plots, which describe the effects of single factor and dual factors on the diameter of the nanofiber membrane, are shown in Figure 4.1 and Figure 4.2, respectively.

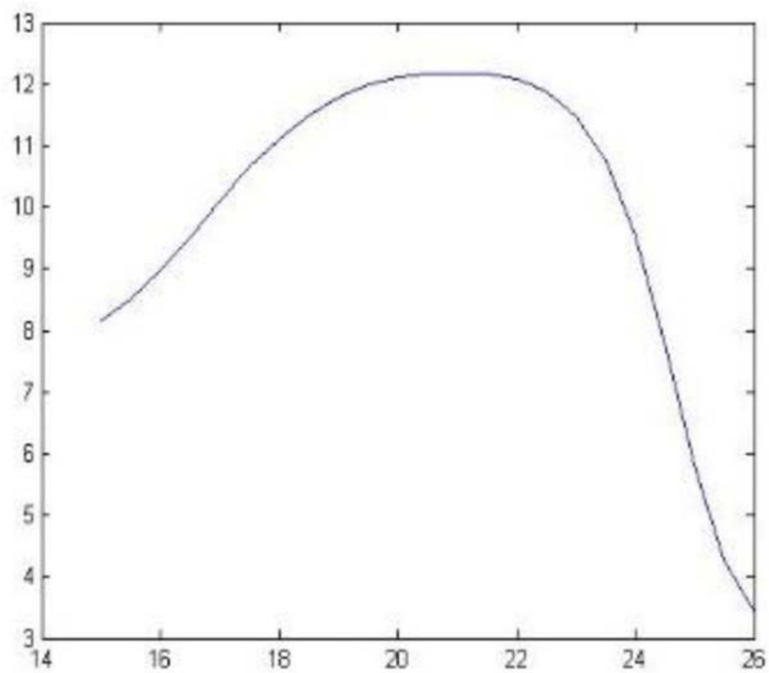
Fix x1 = 16, x2 = 18, change of diameter to x3 (Figure 4.1(a));

Fix x1 = 16, x3 = 0.9, change of diameter to x2 (Figure 4.1(b));

Fix x2 = 18, x3 = 0.9, change of diameter to x1 (Figure 4.1(c));


12
11.5
11
10.5
10
9.5
9
8.5
8
7.5
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5

(a)


13
12
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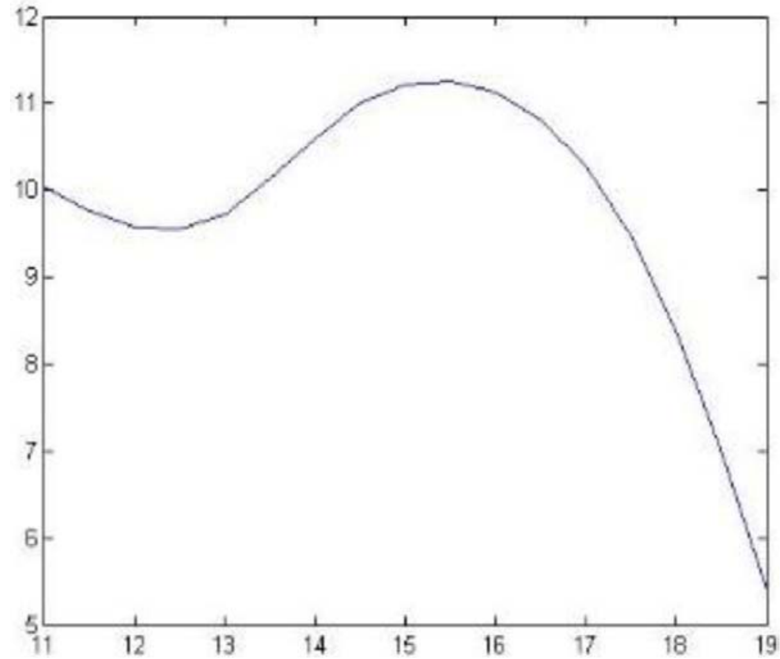
26

(b)



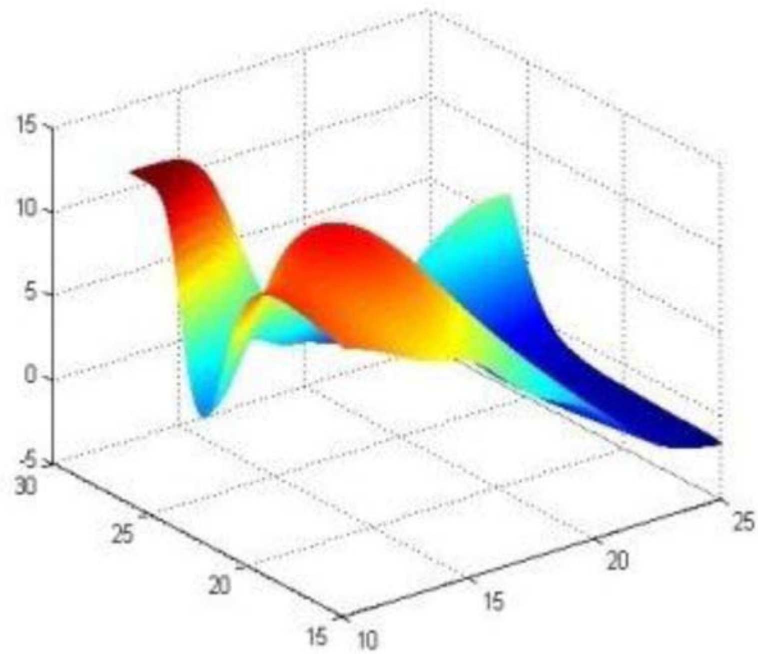
(c)

Figure 4.1. The change of the resistance of two variables to third variables.

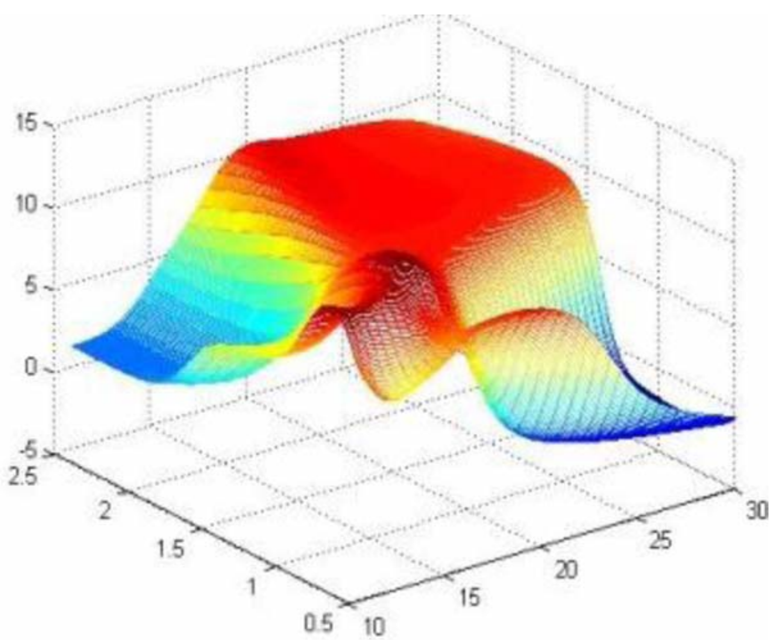
Fix x3 = 0.8, nanofiber diameter change with x1, x2 (Figure 4.2(a));

Fix x2 = 21, the change in nanofiber diameter with respect to x1, x3 (Figure 4.2(b));

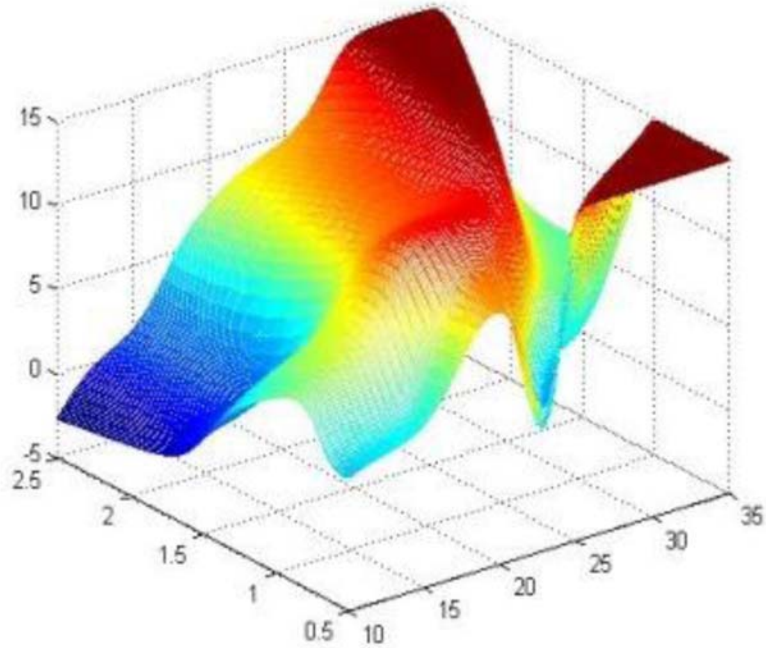
Fix x1 = 16, nanofiber diameter change with x2, x3 (Figure 4.2(c)).



(a)



(b)



(c)

Figure 4.2. Fix one independent variable, the change of the resistance of the remaining two independent variables.

5. Optimizing the Nanofiber Diameter

In this work, our goal is to minimize the average of nanofibers diameter optimization finds a good set of conditions that will meet the minimum diameter. The BP model predicted the minimum diameter (1,001nm) of electrospinning nanofiber membrane at the conditions of 19cm of spinning distance, 26kV of the applied voltage and 0.8mL/h of volume flow rate.

6. Conclusion

This article presented a study the Mathematical Model of the electrospinning nanofiber diameter on the effects of processing variables, including the injection rate (mL/h), applied voltage (kV), and nozzle-collector distance (cm). Though using BP neural network, we find the relationship between nanofiber average diameter and variables. The diameter of the nanofiber measured by the Matlab software is close to the nanofiber diameter simulated by the BP neural network, indicating that the performance of BP neural network model for predicting is good. On the basis of the function, the finest value for each process variables is also determined for PVA the rate ($x3 = 0.8$mL/h), applied voltage ($x2 = 26$kV), and nozzle-collector distance ($x1 = 19$cm). The result analysis also showed that injection rate and the voltage have a greater influence on the diameter of the nanofiber mat.

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