NUMERICAL SIMULATION OF THE ELECTROSPINNING PROCESS USING THE TAGUCHI METHOD

TRIEU KHOA NGUYEN* , THO NGUYEN VAN *Faculty of Mechanical Engineering, Industrial University of Ho Chi Minh City *Corresponding author: nguyenkhoatrieu@iuh.edu.vn DOIs: https://doi.org/10.46242/jstiuh.v64i04.4890*

Abstract. This article presents a study on numerical simulation of the influence on operating parameters of an electrospinning device using the Taguchi method and analysis of variance (ANOVA). First, three parameters - voltage, the distance between the nozzle and collector, and collector size - that are important parameters affecting the electrospinning process are selected for the study. Through pre-feasibility simulations, three levels of values for each parameter are selected, and therefore, the L₉ orthogonal array is suitable for this investigation procedure. Using this orthogonal array, nine simulations of the electrospinning process were carried out. Then, the S/N ratio and ANOVA were used to determine the optimal levels of the factors and their influence on the normal current density. The results show that voltage has the most influence, accounting for 84.09%, on the output. An additional numerical simulation was carried out to validate the efficacy of the Taguchi method. The result obtained was -154.92 A/m², which was more optimal than the previous nine results. Hence, a conclusion could be drawn that the Taguchi method, with ANOVA, was a simple but powerful tool for studying the electrospinning process.

Keywords. Electrospinning, Numerical simulation, Taguchi method, Electrostatic force, Ultrathin fiber, Comsol.

1 INTRODUCTION

Electrospinning is the technique of producing super thin fibers from a solution, polymer melt, or polymer alloy in an electrostatic field [1]. The main properties of such fibers are their sub-micro- or nanometer thickness, high tensile strength, functionalization possibility, and the very large surface area-to-volume ratio [2]. Because of the unique features and properties of e-spun fibers from the electrospinning technique that distinguish it from other ultrathin fiber manufacturing techniques, e-spun fibers have been widely utilized in many industrial fields such as wound healing, engineering tissue, drug delivery, protective clothing, food packaging, electronic equipment, photovoltaic equipment, piezoelectric equipment, gas sensors, air purifiers, liquid filters, lithium batteries, fuel cells [3], ...

Because electrospinning is so widely applied, there have been many studies on electrospinning in general and electrospinning simulation in particular. In [1], the authors constructed electrospinning models applying three conservation quantities, namely that of the mass, the momentum, and the charge. These models figure the e-spun filament shape during its form during electrospinning. However, these models can contribute truly little to the optimization of operating conditions for the electrospinning device. In a similar way, Chun Lu et al. [4] built a molecular model and performed simulations of shear flow to study the effects of solvents on fiber diameter. And therefore, this study also did not bring much useful information for researchers who want to develop electrospinning devices. In [5], the influence of needle distance on the electric field force of the jet's stability section was investigated. This will be a piece of useful information for those who want to build a multi-nozzle electrospinning device. But not exhaustive, electrostatic force is just one of many input parameters in the process of optimizing equipment operating conditions. In more detail, to help understand the correlation between electric field distribution and nanofiber organization, COMSOL Multiphysics 4.4 was utilized to simulate the potentials of the electric field within the established electrospinning setup [6]. The parameters studied consist of the distance between the nozzle and the mesh surface of the collector and the applied voltage. Because these were two of the many important process parameters, this study provided useful information for process optimization. But the simulation process was not presented in detail, which made it difficult to reproduce the process and research results. Also studying electrostatic fields in electrospinning, Anna et al. [7] used a 3D model of a transmitter and collector. And also, this paper did not provide enough information for researchers to replicate the simulation. Also using 3D modeling, the authors in [8] built many different models to study the electrical field profiles. The authors gave important information for the selection of emitters and collectors for electrospinning devices. But again, no boundary conditions of the simulation were presented so it was not really helpful for further studies. In the next study, the authors investigated the impact of existing forces and the jet formation process in electrospinning providing a better understanding of this process, nanofiber formation, and its characteristics [9]. However, the results of this study could not be directly used for the operation of an electrospinning device. In another study, the authors in [10] used ANSYS to study the polymer fiber formation process and its effect on the electric field. The models in this study were not suitable for the research direction of process control. While in [11], theoretical simulations of electric and magnetic fields in an electrospinning device were performed to study the distribution of the electromagnetic field and ensure the experiment's rationality. And also again, this paper did not provide enough information for researchers to replicate the simulation. While Cheng Ge et al. [12] simulated the microbead shape of beaded fiber under different spinning voltages using the COMSOL Multiphysics software. After reviewing 479 articles on electrospinning, a recent review paper clearly shows the trend of research on this technique. In addition to solely experimental studies, simulations mainly focus on the molecular structure of the dissolved polymer, Taylor cone morphology, effect of solution concentration on jet behavior, fiber morphology, and effect of spinning voltage on the microbead shape of the beaded fiber [13].

Therefore, there is a gap in the application of numerical simulation to the design and development of electrospinning equipment, optimizing the operating conditions of the device. Some articles mentioning the machine's operating parameters were a little sketchy. They did not provide enough information for researchers to replicate the simulation. Hence, this study was carried out to clearly reveal the boundary conditions for electrospinning process simulation. This is an indispensable step in developing an electrospinning device. At the same time, this study contributes to expanding the application of numerical simulation for electrospinning, especially for beginners.

2 MATERIALS AND METHODS

2.1 Electrospinning Process

Electrospinning is a technique that produces micro- and nanofibers through a jet of an electrically charged polymer solution or molten polymer [2]. The simplest form of electrospinning device has two electrodes, a syringe to hold and supply the polymer solution, and a high DC voltage supply, usually in the kV range. Due to the high voltage, the polymer drop from the metallic nozzle of the syringe is formed into a Taylor cone. The top of this Taylor cone is spun into a charged jet. And the charge makes the fiber bend in such a way that its diameter is reduced each time the polymer fiber is looped. The e-spun fiber is formed as a web on the surface of the grounding collector [3].

Figure 1 presents a schematic of a typical electrospinning device. The factors affecting the electrospinning process are also demonstrated in Figure 1. Environmental factors include humidity and temperature. The factors related to the solution are concentration, molecular weight, molecular structure, conductivity, viscosity, and solvent volatility. While the distance, voltage, flow rate, and type of collector factors are device settings. Criteria for evaluating an electrospinning process include physical, chemical, or biological parameters to make adequate summations of in vitro studies. From a physical point of view, there are the average fiber diameter, pore size distribution, porosity, and mechanical testing. For characterization of espun in chemical properties, one may utilize one of the following: contact angle analysis, differential scanning calorimetry, thermogravimetric analysis, gelpermeation chromatography, X-ray photoelectron spectroscopy, X-ray diffraction, Fourier transform infrared spectroscopy.

Figure 1: Schematic of a typical electrospinning device [3].

2.2 Numerical Simulation via Comsol Multiphysics

COMSOL Multiphysics is a commercial simulation software solution for various physics and engineering applications. This software facilitates finite element analysis using differential equations (PDEs). The Electric Currents module was utilized for electric field distribution between a nozzle and a grounded collector. The distance between the metallic nozzle and the collector was set at 10 cm. And the space between them was filled with air. While the applied voltage was 20 kV. The affair of electromagnetic analysis at the macroscopic level is to solve Maxwell's equations according to certain boundary conditions. Maxwell's equations are a suite of equations, which were indicated in integral or differential form. These equations are to state the correlations between the fundamental electromagnetic quantities. Simulations were performed based on three equations:

$$
\nabla \cdot J = Q_{J,V} \tag{1}
$$

$$
J = \sigma E + J_e \tag{2}
$$

$$
E = -\nabla V \tag{3}
$$

where ∇ : Laplace operator means divergence; J: current density (A/m²); Q_{J,V}: boundary current source (A/m²); σ: electrical conductivity (S/m); V: the voltage applied (V); E: electric field intensity (V/m). The relation defining the current density is generalized by using an externally generated current $J_e(A/m^2)$.

The normal current density is applicable to exterior boundaries that present either a source or a sink of current. The following equation provides a condition for specifying the normal current density as an inward or outward current flow:

$$
J_n = -n \cdot J \tag{4}
$$

2.3 Taguchi method

Nowadays, the Taguchi method has been more and more widely applied in experimental planning [14]. This method contributes to improving productivity in the research and development process, creating highquality products at low cost. Dr. Taguchi has developed a method based on the Orthogonal Array experiment to reduce the number of experiments with the appropriate arrangement of the most favorable conditions of the controllable parameters [15]. The orthogonal arrays create a trade-off between the experiments. And the Signal-to-Noise (S/N) ratio is a logarithmic function of the desired output, satisfying

the optimization purpose, making the analysis, and predicting results. In the Taguchi method the term "Signal" refers to the mean (desired value) of the output target and the term "Noise" refers to the unwanted value [16]. Therefore, the S/N ratio is used to calculate the deviation from the desired value. The following are the formulas to calculate the S/N ratio [17]:

- Larger is better:

$$
S/N = -10lg \left[\frac{1}{n} \sum \left(\frac{1}{y_i^2} \right) \right] \tag{5}
$$

- Smaller is better:

$$
S/N = -10lg[1/n \Sigma(y_i^2)]
$$
 (6)

The design of experiments using the Taguchi method is more effective than that of other statistical methods. Via choosing the right fit of different independent variables, the quantity of experiments is significantly decreased. In addition, there is no loss of any information due to a reduction in the number of experiments. The goal of the Taguchi method was to minimize variation around the goal and improve quality. Using this technique allows scientists, engineers, and researchers to spend less time on experimental planning and analyzing results. With improvements in computer technology, it is becoming easier to use the Taguchi method in applications. The most common is a technical analysis using computer software, such as Minitab.

3 RESULTS AND DISCUSSIONS

3.1 Selection of Factors and Orthogonal Arrays

The electrospinning process simulation was performed with the boundary conditions shown in Figure 2. From these boundary conditions, the factors for numerical investigation of the electrospinning process are selected as shown in Table 1. From the pre-feasibility experiments and simulations, the ranges of values of the electric potential, distance, and size of collector parameters in Table 1 were selected.

Figure 2: Boundary conditions for numerical simulation.

Table 1: Factors for numerical investigation.

| No. | iymbols | Factors | Level 1 | evel 2 | Level 3 | Unit |
|-----|---------|--------------------|---------|--------|---------|------|
| | A | Electric potential | | | | kΑ |
| | | Distance | 80 | 100 | 120 | mm |
| | | Collector | 80 | 100 | 120 | mm |

The construction of the orthogonal array is based on the number of elements and the number of levels of each element. In the current study, with 3 elements, 3 levels each, the orthogonal array has the L_9 structure as shown in Table 2.

NUMERICAL SIMULATION OF THE ELECTROSPINNING PROCESS …

In Table 2, MSD stands for mean squared deviation. The simulation results in Table 2 show that case #7 has the highest absolute value output. A higher absolute value of the normal current density (A/m^2) means a greater electric field force [11].

3.2 S/N Ratio

The purpose of the current work is to investigate the influence of factors on the electrospinning process, so the "bigger-better" principle is chosen and represented by equation (5). The results of the analysis of the S/N ratio are shown in Figure 3, showing that the absolute value of normal current density increases with increasing voltage, the smaller the distance between the nozzle and the collector, and the smaller the collector size. The S/N results also show that "electric potential'' was the factor that has the most influence on the output, followed by "distance", and the factor that had the least impact was the size of the collector.

Figure 3: The analysis of the S/N ratio shows the simulation parameters' influence on the normal current density.

3.3 ANOVA Results

To further study the effect of relative parameters, the ANOVA method was carried out as demonstrated in Table 3. Consistent with the analysis of the S/N ratio, voltage has the greatest effect on the increase in normal current density. In addition, the ANOVA method only introduces the voltage factor, since a value of *F* greater than $F_{(0.05,2,3)}$ is statistically significant. At the same time, the result from P% shows the contribution of factors. Accordingly, factor A, voltage, contributes up to 84.09% to the variation of the

normal current density. Factor B, the distance between the nozzle and the collector, contributes 13.49%. While factor C, the size of the collector, has a negligible effect on the normal current density, only 1.62%.

3.4 Verification using Minitab

Using the S/N ratio analysis as well as ANOVA results, it can be affirmed that a larger value of the normal current density can be obtained from the process parameter condition A3-B1-C1 as shown in Figure 3. This result was verified by Minitab software, product version 18.1. The validation results (Figure 4) were consistent with the manual calculation results using Excel. This demonstrated the correctness of the process of applying the equations. The practice has shown that engineers in production workshops only utilize software solutions, such as Maple, Minitab, or Matlab, to reduce the time for experimental planning as well as analysis of outcomes.

3.5 Confirmation using Numerical Simulation

One more numerical simulation was performed, using these conditions as a confirmation, Figure 5. The results show that the normal current density obtained from this additional numerical simulation was -154.92 A/m². This value is lower than the normal current density of all the cases considered in the orthogonal array listed in Table 2. From this confirmation numerical simulation, it can be inferred that the Taguchi method can produce a better combination of process factors that can increase the absolute value of the normal current density. Thus, the simulation results also showed that the voltage had the greatest influence on the plastic fiber formation. Basically, the higher the voltage, the better. However, the higher the voltage, the

higher the possibility of electrical leakage and the greater the possibility of the coils in the power supply getting hot and burning.

Figure 5: The results of the additional simulation using the recommended combination setting.

4 CONCLUSIONS

In the current work, the Taguchi method was utilized to numerically study the influence of process parameters on the normal current density of a self-development electrospinning device. The simple technique employed in this investigation basically consists of the OA of the Taguchi method used in conjunction with the analysis of variance (ANOVA). In the basic electrospinning process using a single nozzle, three process parameters were considered. From the study of the S/N ratio as well as ANOVA based on the Taguchi method with an OA L_9 (3³), voltage is identified as the most important parameter for increasing the absolute value of the normal current density. The result shows that the optimal normal current density has been reached at the minimum input. This result was validated by commercial software, Minitab, and an additional numerical validation simulation. The results of this study provide the foundations for further research and application of the electrospinning technique in both academic and industrial settings in our country.

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MÔ PHỎNG QUÁ TRÌNH QUAY ĐIỆN HÓA DÙNG PHƯƠNG PHÁP TAGUCHI

NGUYỄN KHOA TRIỀU* , NGUYỄN VĂN THỌ *Khoa Công nghệ Cơ khí, Đại học Công nghiệp Thành phố Hồ Chí Minh * Tác giả liên hệ: nguyenkhoatrieu@iuh.edu.vn*

Tóm tắt. Bài báo này trình bày nghiên cứu mô phỏng số ảnh hưởng của các thông số vận hành của thiết bị quay điện bằng phương pháp Taguchi và phân tích phương sai (ANOVA). Đầu tiên, ba thông số bao gồm điện áp, khoảng cách giữa vòi phun và bộ thu và kích thước bộ thu là những thông số quan trọng ảnh hưởng đến quá trình quay điện được lựa chọn cho nghiên cứu. Thông qua các mô phỏng tiền khả thi, ba mức giá trị cho mỗi tham số được quyết định. Và do đó, mảng trực giao L⁹ phù hợp cho nghiên cứu này. Dựa trên mảng trực giao này, 9 mô phỏng của quá trình quay điện đã được thực hiện. Sau đó, tỷ số S/N và ANOVA được sử dụng để tìm mức tối ưu của các tham số và tác động của chúng đối với mật độ dòng điện chính phương. Kết quả cho thấy điện áp có ảnh hưởng nhiều nhất, 84,09%, đến đầu ra. Một mô phỏng số bổ sung đã được thực hiện để xác nhận tính hiệu quả của phương pháp Taguchi. Kết quả mật độ dòng điện chính phương thu được là -154,92 A/m², tối ưu hơn so với 9 kết quả trước đó. Do đó, có thể rút ra kết luận rằng phương pháp Taguchi, ANOVA là một công cụ đơn giản, dễ thực hiện, nhưng hiệu quả để nghiên cứu quá trình quay điện.

Từ khóa. Quay điện hóa, Mô phỏng, Phương pháp Taguchi, Lực tĩnh điện, Sợi siêu mảnh, Comsol.

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