RESEARCH ARTICLE

Electrospinning of Polyacrylonitrile Nanofibers and Simulation of Electric Field via Finite Element method

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ABSTRACT

Objective(s): Since the electric field is the main driving force in electrospinning systems, the modeling and analysis of electric field distribution are critical to the nanofibers production. The aim of this study was modeling of the electric field and investigating the various parameters on polyacrylonitrile (PAN) nanofibers morphology and diameter.

Methods: FThe electric field profile at the nozzle and electrospinning zone was evaluated by Finite Element Method. The morphology and diameter of nanofibers were examined by Scanning electron microscopy (SEM).

Results: The results of the electric field analysis indicated that the electric field was concentrated at the tip of the nozzle. Moreover, in the spinning direction, the electric field was concentrated at the surface of the spinneret and decayed rapidly toward the surface of the collector. Increasing polymer solution concentration from 7 to 11wt.% led to increasing nanofibers diameter form 77.76 ± 19.44 to 202.42 ± 36.85.

Conclusions: TBase on our results, it could be concluded that concentration of the electric field at the tip of the nozzle is high and initiates jet and nanofibers formation. PAN nanofibers can be transformed to carbon nanofibers which have various applications in biomedicine.

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INTRODUCTION

Nanofibers with their enormous specific surface area, small pore size, high porosity, and the diameter of fibers offer great opportunities for their use in many areas. Different methods such as melt spinning, force spinning, self-assembly, electroblowing, template synthesis, and electrospinning can be used for nanofibers production. Electrospinning as a cost efficient, versatile, simple, and flexible method has attracted many attentions to fabricate fibers at micro and nanoscale (1-4). Electrospun nanofibers have various potential applications including tissue engineering, wound dressing, drug delivery, sensors, barrier textile, filtration, catalyst and enzyme carriers, energy storage, and other fields (5-11). Nanofibers with the different kind of compositions such as natural and synthesis polymers, metal, and ceramic can be produced via electrospinning (12). The different morphology, such as core-sheath,

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porous-surface, and side-by-side nanofibers can be made by using the electrospinning method (13-16). Generally, a typical electrospinning apparatus comprises of three main parts; a nozzle, a conductive rotating collector, and a high-voltage source to form high electric field between the collector and the nozzle (17). During the electrospinning process, the polymer solution is fed through the nozzle (a metal capillary) and under interaction with applied voltage the polymer jets/filaments form at the tip of the nozzle (18). It has been confirmed that the electric field as the main driving force in electrospinning has great effects on nanofibers formation, productivity, and morphology. However, due to the high-voltage involved, it is difficult to directly measure the electric field profile of an electrospinning setup. Then, modeling approaches can be useful to understand the electric field profile in electrospinning process. An assessment of the electric field profile in electrospinning framework was directed by Finite Element Method (FEM), a numerical technique which is utilized to discover solutions of incomplete differential condition equations (PDE). It gives an option approach to see high-electric field. Since, the practical dimensions and material properties can be used for the FEM calculation, it empowers to envision the electric field profile and to comprehend the impacts of material characteristics, dimension and physical geometry. In addition to applied voltage, the other involved parameters such as polymer solution concentration and nozzle to collector distance have a critical impact on nanofibers properties. If the polymer solution concentration is very low, electrospray occurs instead of electrospinning due to the low viscosity and high surface tensions, and micro (nano)-particles produce instead of fiber. As the polymer solution concentration is very high, helix-shaped microribbons will be obtained. Smooth nanofibers can be formed when the polymer solution is suitable (19-21). Nozzle to collector distance is the other parameter affecting nanofibers morphology and diameter. In short distance, the nanofibers cannot be solidified before reaching the collector and in long distance, beaded nanofibers will be produced (22, 23).

In the present study, the electric field profile and impacts of the various electrospinning processes on nanofibers diameter and morphology were investigated.

MATERIALS AND METHODS

Polyacrylonitrile (PAN) (MW: 80,000 g/mol) was purchased from Polyacryl Company (Iran). Dimethylformamide (DMF) was obtained from Merck Company. PAN/DMF solutions were prepared by dissolving PAN in DMF at 60°C for 12h with continuous and vigorous magnetic stirring to make a clear solution.

Electric Field Analysis

The status and potential profile of the applied electric field in electrospinning setup was manifested by COMSOL3.5, a FEM based program that was used for meshing and solving purposes. The physical characteristics of the electrospinning constituents including; the polymers solutions, the nozzle, and the collector were determined based on their size, relative permittivity, dimension, and position in the system. The collector and the boundaries at the infinite distance were defined as zero potential and the others set as continuity. The electric field profile was calculated using the Laplace equation, because there was no charge within the system. The boundary conditions were determined according to system parameters.

Electrospinning

PAN solution was electrospun using needle-based electrospinning apparatuses (Fanavaran Nano Meghyas Ltd., Co., Tehran, Iran). The PAN solution was fed to the tip of the nozzle, a blunted 18-gague stainless needle, using the electronically controlled injection module. An electrical field was applied between nozzle and collector at a high voltage of 20 kV to direct and accelerate the jet flow of PAN solution toward the collector.

Characterization of Nanofibers

The nanofibers morphology was revealed by SEM (Philips XL-30, at 20 kV), after sputtering with gold. The mean diameter of nanofibers was calculated by Image J (1.47v, National Institute of Health, USA) software.

RESULTS AND DISCUSSION

Electric Field Analysis

The electric field as the main driving force for nanofibers formation has a great impact on nanofibers formation and morphology. In this

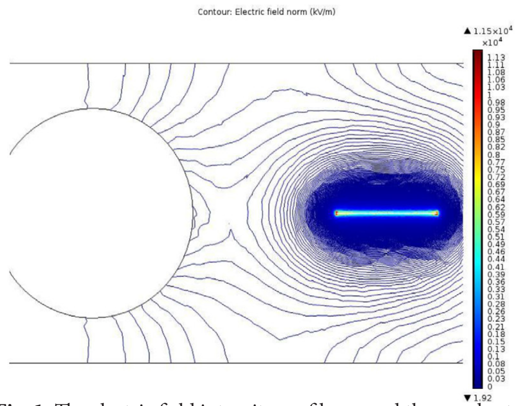

Fig. 1. The electric field intensity profile around the nozzle at 20 kV applied voltage.

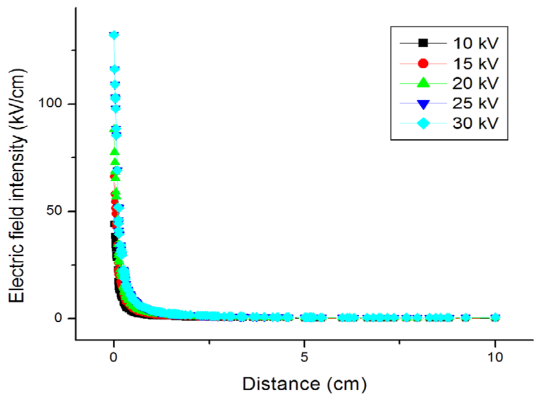

Fig. 2. The intensity of electric field along the spinning direction at different applied voltage.

regard, understanding the distribution of electric field is critical for appropriate nanofibers processing in electrospinning systems. Finite element analysis was used to calculate the electric field intensity at the nozzles surface and in the electrospinning zone (from the tip of the nozzle to the collector) to understand the electrospinning results (Figs. 1 and 2).

As shown in Fig. 1, the electric field intensity vector distributes symmetrically, the electric field lines are concentrated around the electrospinning nozzle, and the direction of electric field intensity is toward the collector. Around and a little far from the nozzle the value of electric field intensity is the same which is critical for the production of a stable jet. The electric field profile in electrospinning direction at various applied voltage are shown in Fig.2.

Fig.2 demonstrates the electric field intensity in the electrospinning direction (the nozzle to the collector) in the electrospinning system at different applied voltage. The highest electric field intensity was at the surface of the nozzle and decayed rapidly in the direction of spinning toward the collector surface.

Electrospinning Process

Electrospinning was performed considering the applied voltage, the polymer concentration, and distance between the nozzle and collector to tailor formation and morphology of the fibers. Table 1 summarizes experiments conducted in this study to investigate the effects of different electrospinning parameters on PAN nanofibers diameter and morphology.

Table 1 summarized the effects of different electrospinning parameters on nanofibers morphology and diameter in needle electrospinning system.

The concentration of polymer solution as the most important parameter has a great effect on nanofibers diameter, morphology, and electrospinning process. Increasing PAN concentration led to the formation of uniform and bead free nanofibers (Fig 3).

Increasing the polymer concentration from 7 to 9 and 11wt.% increased the fiber diameter from 77.76 ± 19.44 to 115.77±29.10 and 202.42 ± 36.85, respectively (Fig.4 (a)). The previous studies showed that there is a direct relation

Table 1. Effects of electrospinning parameters on the diameter and morphology of PAN nanofibers

Concentration wt.%	Distance (cm)	Voltage (kV)	Diameter (nm)	SD (nm)	Morphology
7	10	15	60.96	25.11	Beaded nanofibers
7	10	20	77.76	19.44	Beaded nanofibers
7	10	25	79.91	29.94	Beaded nanofibers
7	13	20	80.91	18.22	Beaded nanofibers
7	16	20	83.54	18.82	Beaded nanofibers
9	10	20	115.77	29.10	Nanofiber
11	10	20	202.42	36.85	Nanofiber

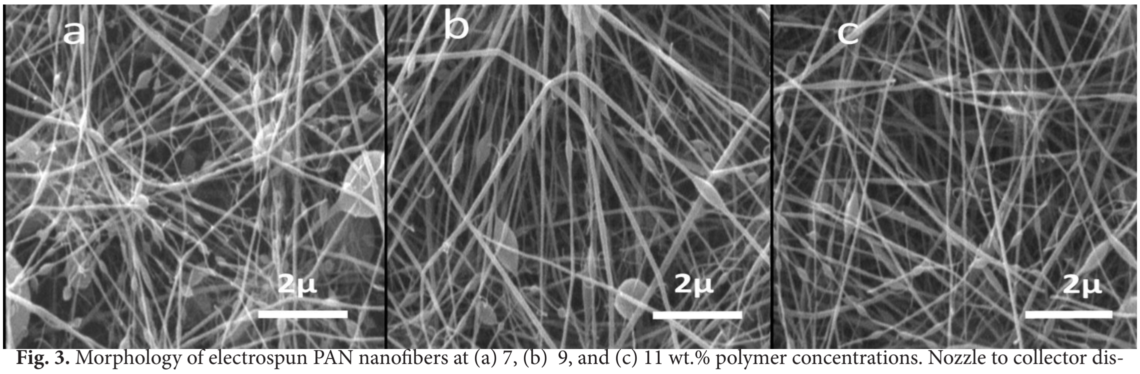

Fig. 3. Morphology of electrospun PAN nanofibers at (a) 7, (b) 9, and (c) 11 wt.% polymer concentrations. Nozzle to collector distance and applied voltage were 10 cm and 20 kV,

between nanofibers diameter and polymer solution concentration (24-26). Polymer solution concentration controls the polymer chains mobility and entanglement via viscosity. In a low viscosity polymer solution, the polymer chins are more flexible and the polymer chains entanglement is low resulting in more flexibility of polymer under interaction with the electric field in electrospinning process and production of thin nanofibers(27, 28). Moreover, continuous, bead free, and smooth fibers cannot be formed in a very low viscosity polymer solution, whereas the hard ejection of jets from nozzle and polymer solution is the result of very high viscosity. In other word, an optimum value of viscosity is required for suitable electrospinning and nanofibers. The surface tension is the dominant factor in a low viscosity solution and only micro/nanoparticles and beaded fiber can be formed. The viscosity simply can be adjusted via polymer solution concentration.

Applied voltage is the other important parameters in electrospinning systems that influence the nanofibers formation and morphology. A high voltage higher than the critical value is required to form jets/fibers at the surface of the nozzle. The critical value was 11 kV, which jets/filaments cannot be formed below these values.

Fig. 4(b) and Fig. 5 are shown the effect of applied voltage on PAN nanofibers diameter and morphology where the PAN solution concentration was 7 wt% and the applied voltage was increased from 15 to 25 kV, while the other parameters were constant. Increasing the applied voltage from 15 to 25 kV resulted in the formation of nanofibers with the mean diameter of 60.96 ±25.11 to 79.91 ± 29.94, respectively. This increase in nanofibers diameter can be attributed to the acceleration of polymer movement from the nozzle to collector surface and faster stretching of polymer jet which led to the formation of nanofibers with the bigger diameter (29, 30).

In addition to the electrospinning process, applied voltage influenced the morphology of nanofibers. Fig. 5 shows the morphology of nanofibers electrospun from 7wt.% PAN solution under different applied voltages.

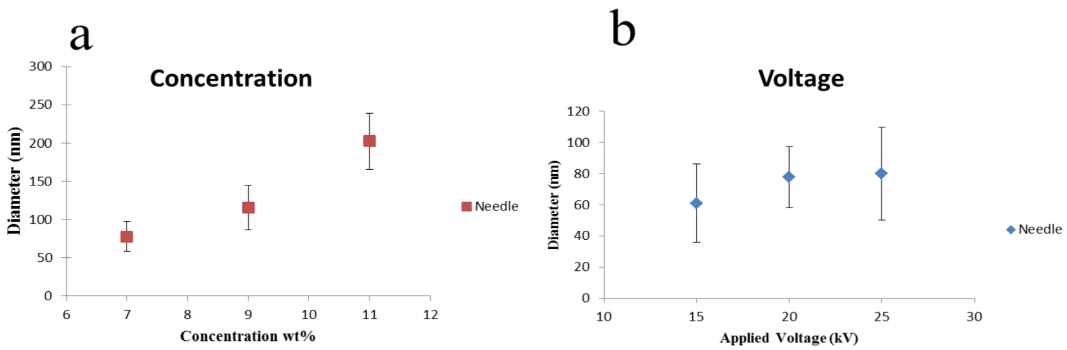

Fig. 4. Diameter of PAN nanofibers electrospun via needle system at different concentration (a) and applied voltage (b).

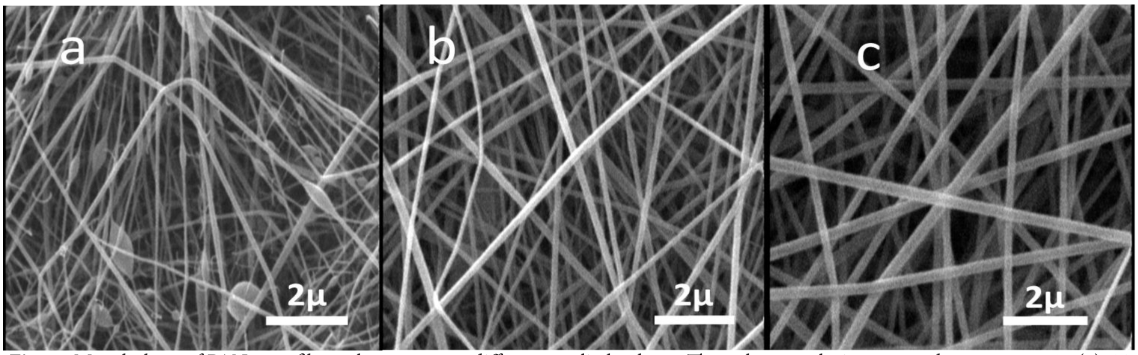

Fig. 5. Morphology of PAN nanofibers electrospun at different applied voltage. The polymer solutions were electrospun at 15 (a), 20 (b) and 25 kV (c) applied voltage, the polymer concentration and nozzle to collector distance were 7.0 wt.% and 10 cm respectively.

As shown in Fig. 5, increasing applied voltage from 15 to 25 kV resulted in the formation of uniform nanofibers and reduction of beads along the nanofibers.

CONCLUSIONS

To the best of our knowledge, the electrospinning parameters and the electric field profile play a significant role on electrospinning system, morphology and diameter of PAN nanofibers. The electric field modeling demonstrated that in electrospinning direction, the surface of the nozzle has the maximum concentration of electric field lines which decayed rapidly in the direction of spinning toward the collector surface. Critical voltage for needle electrospinning system was 11kV, which below this applied voltage nanofibers did not produce. Our experimental results showed that raising PAN polymer solution concentration increased the diameter of nanofibers and decreased beads along. PAN nanofibers can be transformed to carbon nanofibers via heat treatments. Carbon nanofibers have various applications in biomedicine such as biosensing, tissue engineering, filtration, and electro conductive composites.

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CONFLICTS OF INTEREST

The authors declare that they have no conflict of interest.

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