Optimization of Electrospinning Parameter by Employing Genetic Algorithm in Order to Produce Desired Nanofiber Diameter

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***Abstract*—**A numerical simulation of optimization all of electrospinning processing parameters to obtain smallest nanofiber diameter have been performed by employing genetic algorithm (GA). Fitness function in genetic algorithm methods, which was different for each parameter, was determined by simulation approach based on the Reneker's model. Moreover, others genetic algorithm parameter, namely length of population, crossover and mutation were applied to get the optimum electrospinning processing parameters. In addition, minimum fiber diameter, 32 nm, was achieved from a simulation by applied the optimum parameters of electrospinning. This finding may be useful for process control and prediction of electrospun fiber production. In this paper, it is also compared between predicted parameters with some experimental results.

***Keywords*—**Diameter, Electrospinning, GA, Nanofiber.

I. Introduction

ELECTROSPINNING is a method of producing fiber from polymer solutions and melts with diameter ranging from nano to micro scale [1]. Due to its properties such as very small diameter, large surface area per mass ratios, high porosity along with small pores sizes, flexibility and superior mechanical properties, electrospun nanofiber have numerous application in diverse areas [2]. Nanofibers have plays significant role in biomedical field [3], [4], protective clothing [5], filtration technology [6], reinforcement materials [7], and microelectronics [8].

Processing parameter of electrospinning was divided into three broad categories, namely: (1) solution parameters (solution viscosity, solution concentration, and surface tension), (2) processing parameters (applied voltage, spinning distance, and nozzle radius), and (3) environmental parameter (temperature, humidity, and atmosphere pressure) [2]. These parameters greatly affect fiber formation and structure. Additionally, the resultant fiber diameter determines properties of the electrospun fiber mat for example mechanical, electrical, and optical features. Numerous applications require nanofibers with desired diameter, suggesting the importance of the process control.

Fiber diameter is one of the most important structural characteristics in electrospun nanofiber mats. Some experiments have been showed the importance of small diameter in its applications. Podgorski et al. [9] have proved that higher filtration efficiencies can be obtained with smaller diameter of fiber. It was also shows that sensitivity of sensors also increased with decreasing of fiber diameter [10]. Moreover, higher ionic conductivity of the polymer batteries can be producing of lower fiber diameter. In addition, Moroni et al. [11] found that fiber diameter of electrospun polyethylene oxide terephtalate (PEOT) scaffold effecting cell seeding, attachment, and proliferation. Therefore, predicted and optimizing of fiber diameter was expected to such special uses.

Optimizing of nanofiber diameter in electrospinning process actually has been performed by several experiment [2], [12]-[14] and theory studies [1], [15], [16]. In experiment, electrospinning apparatus, such collector, has been modified to minimized fiber radius and make it align. Moreover, electrospinning parameter, such as: solution concentration, surface tension, voltage, distance between nozzle-collector were investigated in certain range to obtain smaller diameter. On the other hand, some theories have been developed to investigate influence of electrospinning parameter to nanofiber diameter. Furthermore, some theories also established to predict distribution of electrospun fiber and make diameter of fiber reduced. Our previous study [17]-[20] also done by trial and error methods but it is less effective and time-consuming. However, optimizing methods with high-accuracy, such genetic algorithm, are required to find optimum parameter to produce smaller fiber diameter.

In this paper, genetic algorithm was employed to optimize all of electrospinning parameters and it was used in simulation to produce minimum nanofiber diameter. Although, Maleki et al. [16] very recently have also used genetic algorithm to obtain optimum fiber diameter, however, our results can produce smaller optimum diameter of fiber. In addition, we successfully predicted optimum conditions for all electrospinning parameters.

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II. Theoretical Study

A. Modeling of Electrospinning Parameters

Modeling of electrospinning process has been established by Reneker et al. [21], [22], with three main equations, namely viscoelastic, mass, and momentum conservation. Theoretical simulation by using this model can be performed to predicted fiber diameter [15]. Because of relation between electrospinning parameter and fiber diameter have not been existed, thus regressions approaches were applied to fit the data and then it use as fitness function. Relation between each electrospinning parameters and fiber diameter was obtained by applied Reneker model as listed in Table I.

B. Genetic Algorithm

Genetic algorithms, which were imitating the genetic evolution of species in nature, have three component of algorithm, namely initialization, reproduction, and selection [23]. In genetic algorithm, initial population was selected and the fitness of each individual in this population was evaluated for finding optimum parameters. The generation is repeated until stop condition happen. The selection is based on the percent of every operator to reproduce. The approximation of every solution is based on fitness function. Finally, least fit population is replaced with new individuals until termination condition take places [16], [24]-[27].

1. Initialization

Generate an initial population was first step in the implementation of any genetic algorithm. It was begun by generating an initial population of integer strings (chromosome) at random [28], [29]. In this paper, initial populations were generated by selecting from the input interval (Table I). For every input parameter (chromosome), interval was selected based on literature experimental data [15] and step changes initially varied by a small amount near the base value to determine a general and real trend. The parameter ranges to generate population are listed in the Table I. The initial population size is 100 which its chromosomes are selected randomly.

2. Fitness Evaluation

The fitness function is defined to establish the fitness of each individual chromosome to control which one is fit to reproduce and continue for the next generation. Thus, given a particular chromosome, a fitness function returns a single numerical score, “fitness”, which is proportional to the “ability” of the individual that the chromosome represents [28], [29]. In this paper, fitness function is different for of each parameter fitness function and selection would be based on the inverse of fitness value as listed in Table I.

3. Selection

The proportion of the existing population is selected to breed a new generation in each successive generation. Individual solutions are selected during a fitness-based process, where fitter solutions (as calculated by a fitness function) are more possible to be selected. Certain selection methods rate the fitness of each chromosome and preferentially select the best one based on the problem and each operator [15].

4. Reproduction

In this paper, two operators were used including crossover and mutation. Crossover and mutation are the two most important genetic operators to offer genetic variations to the population by bringing in chromosomal changes in GA. Crossover is exchanges gene between chromosomes, and mutation changes some genes in chromosomes at random. In this study, we set the percentage of mutation operation more than other operators to have the best possible selection in the search space. These processes finally resulted in the next generation population of chromosomes that were different from the initial generation.

5. Termination

This generational process is repeated until a termination condition is reached. The termination condition was derived from convergence of population or stopped by user.

III. Procedures

A program used to optimize the electrospinning parameter was created by implementing the flowchart given in Fig. 1. It was shown that there were three important operators in GA, namely initiation, crossover, and mutation.

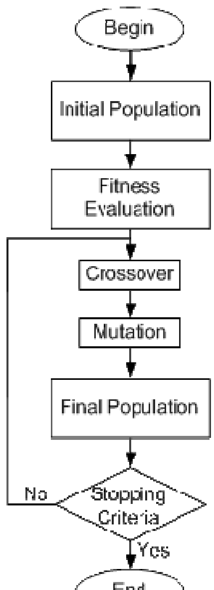

Fig. 1 Flowchart of optimizing electrospinning parameters using genetic algorithm

Fig. 1 depicted that the GA was begun by initializing a population at random. These chromosomes are then evaluated by the fitness function, which returns a measure of chromosome goodness in minimalization problems [29]. This fitness function represents the quantity optimized by the GA. After initialization, the population is iteratively subjected to

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the three genetic operators: selection, cross over, and mutation. Each iteration of these operators in sequence (including the preceding or consequent evaluation step) is termed a generation.

The application of selection results in a new population of N_p chromosomes that has better fitness function values than the original population. The fitness function and interval of parameter in this study was given in Table I.

TABLE I
INTERVAL AND FITNESS FUNCTION FOR EACH ELECTROSPINNING PARAMETER

Parameter	Interval	Fitness Function
Volume charge density (C/L)	[0.65, 3]	$y = (1.13x^3 - 7.28x^2 + 14.72x - 7.37)\ 10^{-5}$
Polymer concentration (%)	[0,25]	$y = (-0.5x^2 + 2.4x + 678.8)\ 10^{-9}$
Initial jet radius (mm)	[0.1,3]	$y= (21.95x^3 - 34.32x^2 + 26.99x - 0.63)\ 10^{-6}$
Applied voltage (kV)	[1,60]	$y = (0.1x^2 + 2.5x + 592.2)\ 10^{-9}$
Distance nozzle-collector (cm)	[5,25]	$y = (0.13x^3 - 6.44x^2 + 84.31x - 84.28)\ 10^{-8}$
Viscosity (kP)	[1,11]	$y = (0.07x + 87.36)\ 10^{-8}$
Solution density (gr/cm^3)	[0.7,1.3]	$y = (6.25x^3 - 19.49x^2 + 4.94x + 19.59)\ 10^{-7}$
Time relaxation (ms)	[10,20]	$y = (734.62x^3 - 36.86x^2 + 0.60x)\ 10^{-2}$
Vapor difusity (mm^2/s)	[0,52]	$y = (-0.40x + 15.20)\ 10^{-7}$
Relative humidity (%)	[0.5,50]	$y = (-0.02x^3 + 0.31x^2 - 0.05x + 67.91)\ 10^{-5}$
Air temperature (°F)	[60,150]	$y = (0.01x^2 - 1.41x + 71.69)10^{-7}$
Perturbation frequency (kHz)	[9,100]	$y = (0.01x - 30.14)\ 10^{-8}$

After the application of selection, the crossover operator is applied. Crossover works to hybridize the chromosomes that survive selection by combining their genetic material. Finally, the mutation operator is applied to randomly alter the chromosomes and prevent premature convergence to a suboptimal result [23]. After mutation, the population is reevaluated, and a new generation begins. The procedure is continued until a design goal is met, no improvement is noticed in the population, or a fixed number of generations have passed.

IV. OPTIMIZATION RESULTS AND DISCUSSION

The optimum parameters of electrospinning were determined by employed genetic algorithm and we found required quantities as listed in Table II.

Table II gives optimum values of electrospinning processing parameters. Using the optimum values, it was found that the optimum fiber diameter is 32nm. Very recently, Maleki et al. [16] have also used genetic algorithm to obtain optimum fiber diameter. However, our results can produce smaller optimum diameter. In addition, we also successfully predicted optimum conditions for all electrospinning parameters. This finding implies that genetic algorithm is an appropriate method to find out optimum parameters in electrospinning.

A brief comparison of the predicted results with recently reported literature data is given in the following.

TABLE II
INTERVAL AND FITNESS FUNCTION FOR EACH ELECTROSPINNING PARAMETER

Parameter	Value	Diameter
Volume charge density (C/L)	0.78	32 nm
Polymer concentration (%)	2	
Initial jet radius (mm)	2.5	
Applied voltage (kV)	2	
Distance nozzle-collector (cm)	14.25	
Viscosity (kP)	7.66	
Solution density (gr/cm^3)	1	
Time relaxation (ms)	0.01	
Vapor difusity (mm^2/s)	0.002	
Relative humidity (%)	1	
Air temperature (°F)	68	
Perturbation frequency (kHz)	10	

1. Volumetric of Charge Density

Volume charge density was amount of electrical charges distributed through the whole body of the jet [30]. Relation between charge density and polymer type, concentration, molecular weight, volumetric flow rate, solvent, applied voltage and nozzle to collector distance have been investigated by Theron et al. [12]. Moreover, Falahi et al. [30] shows that increasing voltage, volume charge density is decreased and fiber diameter is increased. It may cause by charge interaction and bending instability on the jet [17], [20]-[22], [31]. In this study, the optimum parameter of volume charge density was found by applying genetic algorithm. This finding consistent with the experiment results [12], [15], [30].

2. Initial Jet Radius

The initial jet radius is related to the orifice size of the pipette supplying the polymer solution to the droplet shaped as the Taylor Cone [15]. The fiber radius decrease with decreasing of initial jet radius was reported by Kati et al. [32]. The optimum initial fiber was 2.5 μm which was determined in this study agreed with Kati et al. result [32].

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3. Distance Nozzle-Collector

Distance between nozzle-collector (d) shows the strength of electric field (E) in electrospinning process (E=V/d), where V is voltage. In electrospinning process, longer spinning distance will give more time for the jet to stretch in the electric field before it is deposited on the collector. Moreover, solvents will have more time to evaporate. Therefore, the fiber diameter will be decreased. On the other hand, increasing the spinning distance, the electric field strength will decrease, resulting in less acceleration, hence stretching of the jet which leads to thicker fiber formation. Effect of distance nozzle-collector on fiber diameter has been reported in some literature [33], [34]. Finding optimum of distance nozzle-collector is very important because it has strong effect on fiber radius [15]. To get optimum value of distance nozzle-collector in 5 cm to 25 cm ranges, in this study, we employ genetic algorithm to get desired radius. By applying GA method, 14.25 cm of distance between nozzle-collector was found. Our finding is consistent with the trend observed by Thompson et al. [15].

4. Relaxation Time

Relaxation time determine a material's ability to relax given some outside disturbance or condition, and for polymer solutions depends on polymer type and viscosity, concentration, molecular weight, solvent type and molecular structure of the polymer. Novel methods to measure this parameter have been developed by Stelter et al. [35]. Relaxation parameter related with viscosity force which was it decrease with elastic modulus [15]. In this study, optimum time relaxation was investigated in 10 ms to 20 ms in range. Optimum time relaxation of 9 μs was found by applying genetic algorithm and it agree with Thompson et al. [15].

5. Initial Elongational Viscosity

The experimental data show a strong dependence on viscosity for fiber morphology [36]. The higher initial elongation viscosity means a stronger stretching which might be related to a higher applied voltage. As a result of the latter the final cross-sectional fiber radius decreases at higher initial elongational viscosities. Our optimation result shows that the 7.66 kP was an optimum elongational viscosity. This result agrees with Thompson et al. [15].

6. Initial Polymer Concentration

It is well known that polymer concentration is principal parameters in the electrospinning process because it is strongly related to the viscosity of the solution. Fabrication and morphology of nanofibers are dependent on solution viscosity [37]. Lower polymer concentration produces many beads or many microspheres in electrospinning products, moreover, electrospraying occur when the concentration became low enough. On the other hand, increase of the initial polymer concentration can decrease the numbers and sizes of beads, and reduce beads completely in some cases. Reference [15] examined concentration ranging from 1-40%. In this study, optimation of initial polymer concentration was performed in 1% to 25% and the optimum parameter of 2% was found. This finding may cause fiber with more beads.

7. Applied Voltage

In electrospinning, there are two main different effects in applying voltage on fiber radius. Firstly, increasing the applied voltage will increase the electric field strength and larger electrostatic stretching force causes the jet to accelerate more in the electric field, so supporting fiber formation. Secondly, because charge transport is only carried out by the flow of polymer in the electrospinning process [38], increasing the voltage would induce more surface charges on the jet. Then, the mass flow rate from the needle tip to the collector will increase, so the solution will be drawn more quickly from the tip of the needle causing fiber diameter to increase. This optimizing was performed on voltage ranging from 1 kV to 60 kV. The optimum voltage was found on 2 kV. This finding was agreed with Thompson et al. [15].

8. Solution Density

The diameters of electrospun polystyrene (PS) fibers to decreased with increasing density of the solvents [39]. This optimizing was performed on solution density ranging from 0.7 to 1.3 gr/cm^3. The optimum solution density was found on 1 gr/cm^3. It was also agreed with Thompson et al. [15].

9. Perturbation Frequency

The model identifies the perturbation frequency as a typical frequency (100 kHz) of noise in a laboratory that triggers the bending instability by introducing small initial perturbations, namely, causing some segment to move out of alignment with the rest of the jet [21], [40]. Until now, there has not been studied perturbation frequency as related to the electrospinning process. This optimizing was performed on perturbation frequency ranging from 9 kHz to 100 kHz. The optimum perturbation frequency was found on 10 kHz. This finding was agreed with Thompson et al. [15].

10. Vapour Diffusivity

In general, vapor diffusivities in air of most of the typical solvents used in electrospinning do not differ too much, and different solvents lead to different fiber diameters (holding the other parameters constant) primarily because of their different evaporation rates. The lower evaporating solvent allowing for longer stretching process before jet solidification taking place, and thus for thinner fibers. This optimizing was performed on vapour difusity ranging from 0 mm^2/s to 52 mm^2/s. The optimum vapour diffusity was found on 0.002 mm^2/s. This finding was agreed with Thompson et al. [15].

11. Relative Humidity

C.L. Casper et al. [41] described the effect of humidity on fibers, but it dealt with the development of porous fibers when electrospinning under elevated humidity. No definitive comparisons with experimental data can be currently made. The effects of relative humidity are strongly coupled to other parameters and operating conditions. This parameter may be more important through the coupled effects than this current analysis indicates. This optimizing was performed on relative

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humidity ranging from 0.5% to 50 %. The optimum of relative humidity was found on 1%. This finding was agreed with Thompson et al. [15].

12. Air Temperature

Temperature has an effect on the average diameter of the nanofibers because it is related with evaporation rate of the solvent and rigidity of the polymer chain [42]. According to Mit-Uppatham et al. [43] the fiber diameter decreases with increasing temperature. Their group demonstrated that an increase in temperature caused the decrease of solution viscosity, surface tension, conductivity, and resulting fiber diameter. Our optimizing which was done ranging from 60°F to 150°F also shows that optimum temperature was 68°F.

V. Conclusions

Optimization of electrospinning processing parameters to obtain optimum fiber diameter has been theoretically done. Optimum parameter of electrospinning, i.e., volume charge density, polymer concentration, initial jet radius, voltage, distance nozzle-collector, viscosity, solution density, time relaxation, vapour diffusivity, relative humidity, air temperature and perturbation frequency, was investigated by applied genetic algorithm. It was found that simulation produces the optimum fiber diameter is about 32 nm.

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