International Journal of Chemical, Materials and Biomolecular Sciences
ISSN: 2415-6620
Vol:4, No:4, 2010

Optimizing Electrospinning Parameters for Finest diameter of Nano Fibers

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***Abstract*—**Nano fibers produced by electrospinning are of industrial and scientific attention due to their special characteristics such as long length, small diameter and high surface area. Applications of electrospun structures in nanotechnology are included tissue scaffolds, fibers for drug delivery, composite reinforcement, chemical sensing, enzyme immobilization, membrane-based filtration, protective clothing, catalysis, solar cells, electronic devices and others. Many polymer and ceramic precursor nano fibers have been successfully electrospun with diameters in the range from 1 nm to several microns.

The process is complex so that fiber diameter is influenced by various material, design and operating parameters. The objective of this work is to apply genetic algorithm on the parameters of electrospinning which have the most significant effect on the nano fiber diameter to determine the optimum parameter values before doing experimental set up. Effective factors including initial polymer concentration, initial jet radius, electrical potential, relaxation time, initial elongation, viscosity and distance between nozzle and collector are considered to determine finest diameter which is selected by user.

***Keywords*—**Electrospinning, Genetic Algorithm, Nano Fiber Diameter, Optimization

I. INTRODUCTION

A. Electrospinning

ELECTROSPINNING is a simple and versatile process offering unique capabilities for making fibers from polymer solutions and melts with diameters ranging from nano to micro scale. A variety of polymeric, ceramic and composite nano fibrous materials have been successfully prepared by electrospinning, which created interesting applications in fields of filtration, protective clothing, self cleaning, drug delivery, tissue engineering, electronic and photonic devices, etc [1].

Interest in electrospinning for real world applications is due to three aspects of the final production. Firstly, the size of the produced fiber can be in nano scale or it has a nano scale surface texture, leading to different modes of interaction with other materials compared with macro scale materials. Secondly, due to the high draw ratio, it is expected that the produced fiber will have a highly orientated molecular structure with a low number of defects, and will hence approach theoretical maximum strength. Thirdly, the produced fiber has an inherently high surface area to volume ratio [2]. These properties make nano fibers desirable for different applications. Therefore characterize of electrospinning process is essential due to produced nano fibers end uses.

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B. Electrospinning Process

Electrical fields are used to form fibers from material solutions or melts in the electrospinning process. Studies on electrically driven liquid jets were initially started in 19th century, and electrospinning of polymer fibers was first patented by Formhals in 1934 [3].

The typical electrospinning apparatus consists of three major components: a high-voltage power supply, a spinneret (or a metallic needle) and a grounded collector (figure 1) [1].

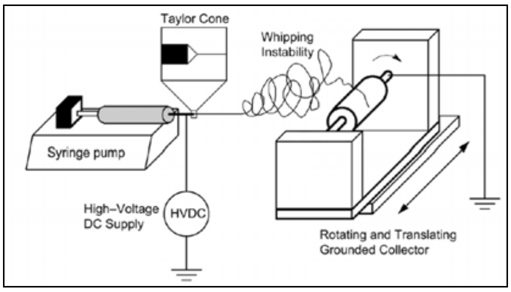

Fig.1 Schematic of a typical electrospinning system [2]

Electrospinning uses a high voltage source to inject the charge of a certain polarity into a polymer solution or melt, which is then accelerated toward a collector of opposite polarity. As the electrostatic attraction between the oppositely charged liquid and collector and the electrostatic repulsions between like charges in the liquid become stronger the leading edge of the solution changes from a rounded meniscus to a cone (Taylor cone). A polymer jet is eventually ejected from the Taylor cone as the electric field strength exceeds the surface tension of the liquid. The polymer jet travels through the atmosphere allowing the solvent to evaporate, thus leading to the deposition of solid polymer fibers on the collector [4].

C. Processing Parameters

A typical electrospinning apparatus can be used to form fibers, droplets, or a beaded structure depending on the various processing parameters. Despite electrospinning's relative ease of use, there is a number of processing parameters that can greatly affect fiber formation and structure [4]. Furthermore, the resultant fiber diameter determines properties of the electrospun fiber mats such as mechanical, electrical, and optical features [3]. As a result regulating these parameters due to having the precise nano fiber diameter is crucial.

The processing parameters include three broad categories: (i) properties of the solution used as the feedstock (solution parameters), (ii) parameters associated with the design, geometry and operation of the electrospinning apparatus (processing parameters), and (iii) atmospheric and other local processing conditions (environmental parameters) [2].

A considerable part of electrospinning information comes from empirical observations which are time and energy consuming processes. Moreover, the complexity of the electrospinning process makes the empirical determination of the parameters very difficult. Predicting the optimum parameters affected on nano fiber diameter could be useful for process control and the investigation of nano fiber production. The optimum numeric value of parameters can be evaluated by using a well-designed genetic algorithm.

II. Procedure

A. Electrospinning Model

Thompson et al. [5] applied their model for electrospinning, accounting for the large nonlinear perturbations, viscoelasticity, evaporation and solidification, to determine the effects of the parameters on the fiber diameter. They considered input parameters are volumetric charge density (C/L), distance from nozzle to collector (cm), initial polymer concentration (wt%), density (gm/cm3), electric potential (kV), relative humidity of solvent vapor in air (%), initial jet radius (cm), perturbation frequency (s-1), relaxation time (s), surface tension (dyne/cm), vapor diffusivity (cm2/s), solvent vapor pressure (mbar), initial elongation viscosity (P). The parameters were evaluated on a relative basis to determine a strong/moderate/minor rating for the influence of the parameters on the nano fiber diameter. It should be noted that in their model each parameter was independent from the other one. It should be noted that in their model each parameter was considered independently from the other one.

Linear regressions were applied to fit the data. Some of the parameters did not have a linear relationship and were fitted with a power-law expression to determine the range in the slopes. In these fitting lines the y-axis represented the normalized final cross-sectional radius of the jet and the x-axis was the normalized input parameter which had been varied in each case.

In this work, six factors from these thirteen parameters were selected based on their utmost regression factor. The slope of the fitted lines was used for rating how strongly each parameter affected the final jet radius; the greater the magnitude of the line slope the stronger the effect on the final cross-sectional radius. Afterward, genetic algorithms (GAs) were used to optimize these electrospinning parameters to have user defined nano fiber diameter.

Therefore, influenced factors including initial polymer concentration, initial jet radius, electrical potential, relaxation time, initial elongation viscosity and distance from nozzle to collector were considered as genes to optimize to determine user defined possible diameter. The fitness function and regression factor of the parameters are listed in table I.

B. Genetic Algorithm

Genetic algorithms simulate the genetic evolution of species in nature according to the principles of natural selection and "survival of the fittest", stated by Darwin. The basic algorithm consists of three components: initialization, reproduction and selection. The algorithm is repeated with reproduction and selection until a certain number of generations or the best individual (global optimum) is met [6].

In genetic algorithm for finding optimum factors, first initial population is chosen and the fitness of each individual in this population is evaluated. The generation is repeated until termination condition takes place. Selection is based on the percent of every operator to reproduce. The estimation of every solution is based on fitness function. Finally, least fit population is replaced with new individuals until termination condition happens.

C. Initialization

The first step in the implementation of any genetic algorithm is to generate an initial population. The evolution procedure begins by randomly generating an initial population of integer strings (chromosome) [7]. In this work, to generate initial population, data were selected from the input range (Table I). For each input parameter (chromosome), ranges were selected based on literature experimental data and step changes initially varied by a small amount around the base value to establish a general and real trend. In choosing reasonable step change values, some parameters are limited at the onset of electrospinning such as polymer concentration, numerically 0 to 100%, but actual electrospun solutions usually fall in the range of 5 to 30% depending on the polymer and solvent type. Similarly the electric potential is limited by the dielectric breakdown in air at about 300 kV/m. Given a nozzle collector separation distance of 20 cm, breakdown occurs at about 60 kV electric potential. The parameter ranges to generate population are listed in the Table I. The initial population size is 100 which its chromosomes are selected randomly and each chromosome has six genes based on possible variables. The possible solutions according the range of each parameter would be 1,048,576 ways which the initial population size would be 0.0095% of the total feasible solutions.

D. Fitness evaluation

In Genetic algorithms, a function is defined to measure the fitness of each individual chromosome to determine which one is fit to reproduce and survive 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 [6]. In this work, fitness function is the multiple of each of six parameters fitness function and selection would be based on the inverse of fitness value divided by sum of total fitness values.

E. Selection

During each successive generation, a proportion of the existing population is selected to breed a new generation. Individual solutions are selected through a fitness-based process, where fitter solutions (as measured by a fitness function) are more likely 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 [8].

F. Reproduction

In this work, four operators were used including cut copy (8%), copy (4%), crossover (36%) and mutation (52%). For cut copy operator, 8% of chromosomes which have the highest fitness values were selected and transferred to the next generation without any change. 4% of chromosomes were randomly copied from the previous generation. In GAs, crossover and mutation are the two major genetic operators to provide genetic variations to the population by bringing in chromosomal changes. Crossover, as the name implies, exchanges information (gene) among chromosomes. Mutation randomly alters some genes in chromosomes.

Here, the percentage of mutation operation was set more than other operators to have the best possible selection in the search space. These processes ultimately resulted in the next generation population of chromosomes that were different from the initial generation. Generally, the average fitness of the population was increased by this procedure, since only the best organisms from the first generation were selected for breeding, along with a small proportion of less fit solutions.

G. Termination

This generational process is repeated until a termination condition is reached. Here, a range of nano fiber diameter (minimum and maximum desirable diameter of nano fiber) was chosen as input and the output would be a chromosome with optimum values of these six effective factors. The termination condition was derived from the upper and lower diameter range of nano fiber.

III. CONCLUSIONS

The fitness of the best and average individual in each generation increased toward the global optimum. The algorithm was applied for different diameter ranges of nano fibers. For example if the range of 200-204 nano meters fiber diameter (as input) would run, The optimum diameter would be 202.372 nm which is derived by optimum parameters of 6% (Initial Polymer Concentration), 0.0195cm (Initial Jet Radius), 20kv (Electrical Potential), 0.014s (Relaxation Time), 10000 (Viscosity), 40cm (Distance from Nozzle). The trend of this process is shown in figure 2.

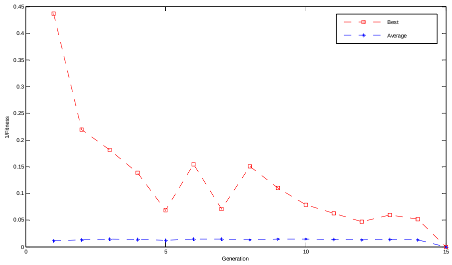

Fig. 2 A typical run for the range of 200-204 nano meters diameter of nano fibers.

Similarly, the result for the range of 600-610 nano meters of fibers is shown in figure3.

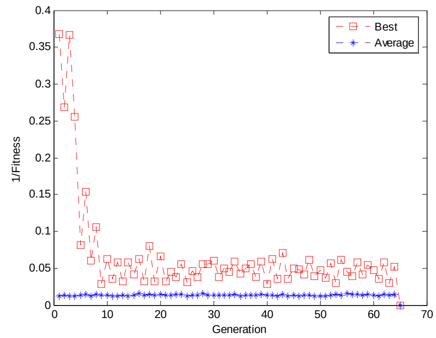

Fig. 3 A typical run for the range of 600-610 nano meters diameter of nano fibers

In this used defined range (e.g. 600-610 nm), the optimum diameter selected by genetic algorithm is 605.038 nm by 2.4% (Initial Polymer Concentration), 0.024cm (Initial Jet Radius), 8kv (Electrical Potential), 0.012s (Relaxation Time), 5000 (Viscosity), 6cm (Distance from Nozzle).

As the population converges, the average fitness will approach that of the best individual. The results show that Genetic Algorithm is a suitable method to determine optimum influenced factors in electrospinning.

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TABLE I
THE FITNESS FUNCTION AND REGRESSION FACTOR OF THE PARAMETERS

Parameter	Regression	Fitness Function	R^2	Input range (*genes*)
Initial Polymer Concentration (wt%)	Linear	$y = 0.9304x - 0.1038$	0.987	0.2,0.4,0.6,0.8,1,1.2,1.4,1.6,1.8,2,2.5,3,3.5,4,4.5,5
Initial Jet Radius(cm)	Linear	$y = 66.018x - 35.427$	0.8374	0.7,1,1.3,1.6,2,2.4,2.6,3.5
Electrical Potential(kV)	Linear	$y = 0.2029x + 0.7544$	0.9052	0.1,0.4,0.8,1,1.1,1.2,1.3,1.4,1.5,1.6,1.7,1.8,1.9,2,2.5,3
Relaxation Time(s)	Power-law	$y = 0.815x^{5.440}$	0.898	0.9,1,1.1,1.2,1.3,1.4,1.5,2
Initial Elongation Viscosity(P)	Linear	$y = -43.555x + 39.757$	0.9343	0.1,0.3,0.5,0.6,0.7,0.8,0.9,1
Distance from Nozzle to Collector(cm)	Power-law	$y = 0.7926 x^{-2.6561}$	0.7449	0.3,0.5,0.65,0.75,1,1.25,1.5,2