



A mathematical model to predict the effect of electrospinning processing parameters on the morphological characteristic of nano-fibrous web and associated filtration efficiency

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ABSTRACT

A robust simplified method was developed to study the effect of electrospinning processing parameters on the morphological properties of electrospun nano-fibrous web, its air permeability, and filtration efficiency against aerosol particles. The developed predictive model related the electrospinning processing parameters to the nano-fibrous web properties. The model was validated experimentally and then is used to study the effect of each electrospinning processing parameters (flow rate, electric field, concentration, and time of electrospinning) on the nano-fibrous web properties. For example, it is shown that only 20 min of electrospinning is able to reduce the air permeability by 66% while one hour of electrospinning coating time is able to increase the filtration efficiency to reach 100% for a range of aerosol particle diameters from 300 to 1000 nm. The validated systematic model is used for developing design charts that allow the determination of the desired air permeability and the filtration performance of the nano-fibrous web from the electrospinning parameters and vice versa within a wide range of feasible processing parameters and fiber diameters.

1. Introduction

Over the last two decades, the rapid development of the nanotechnology resulted in great progress, not only in the preparation of nanofibers, but also in their functional applications (Fang, Wang, & Li, 2011). Currently, the most interesting applications are identified in the following functional areas: biomedical, energy harvest and storage, and environmental protection (Fang et al., 2011). The environmental protection is considered of great importance since current environmental problems have serious negative impacts on human health (Haines, Kovats, Campbell-Lendrum, & Corvalan, 2006). Nanofibers are expected to be used in the filtration of pollutant substances from air or liquid due to their high specific surface area (Barhate & Ramakrishna, 2007). Furthermore, the high porosity, the low basis weight, and the small pore size make the nanofibers appropriate to be used in garments for protective clothing (Lee & Obendorf, 2007). Another important feature of nanofibers in protective garment is its high air permeability compared to most conventional protective clothing material currently available (Lee & Obendorf, 2007).

A number of processing techniques have been used to prepare polymeric nanofibers (Huang, Zhang, Kotaki, & Ramakrishna, 2003). Among these techniques is the electrospinning process which is a simple and convenient technique for production of

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Nomenclature		v_f	length of fiber deposited per time (m/s)
AP	air permeability (m/s)	w	basis weight (g/m ²)
C	polymer concentration	\bar{z}	thickness (m)
C_r	correction factor	<i>Greek symbols</i>	
C_c	Cunningham slip correction factor	α	solidity
C_d	downward concentration of the aerosol particles	μ	viscosity (N s/m ²)
C_u	upward concentration of the aerosol particles	η	filter collection efficiency
d_f	fiber diameter (m)	η_Σ	total single fiber efficiency
E	electric field (V/m)	η_D	single fiber efficiency by diffusion
I	electric current (A)	η_{DR}	single fiber efficiency by enhanced interception-diffusion
k_b	Boltzman constant	η_R	single fiber efficiency by interception
kn	Knudsen number	γ	surface tension coefficient (N/m)
ku	Kuwabura number	λ	mean free path of air molecules (m)
m_f	mass deposition rate of fibers (kg/s)	χ	characteristic length
N_f	number of fibers	ΔP	standard pressure drop for testing fabric (124.5 Pa)
p	porosity	ρ	density of the solution (kg/m ³)
pe	Peclet number	ρ_b	bulk density of the nano-fibrous web (kg/m ³)
Q	volumetric mass flow rate (m ³ /s)	ρ_f	density of the fiber (kg/m ³)
R	interception number	ρ_p	density of the aerosol particle (kg/m ³)
R_c	radius of collector (m)	χ	characteristic length
Stk	particle Stokes number	ω	rotation rate (rd./s)
T	temperature (K)	$\bar{\epsilon}$	permittivity of air
t_e	time of electrospinning (s)		
u_0	face velocity (m/s)		
v_T	deposition velocity (m/s)		

polymeric nanofibers and nanocomposites (Lee & Obendorf, 2007). It is based on accelerating a polymer solution in an electric field between a charged nozzle and a ground collector (Shin, Hohman, Brenner, & Rutledge, 2001). The electrospun nanofibers are usually deposited on a high permeable and porous substrate covering the collector of the electrospinning device (Lee & Obendorf, 2007). The result is a nano-fibrous web of high porosity, large surface-to-volume ratio, light weight, relatively high air permeability and small pore size.

The small pore size characteristic of the nano-fibrous web results in improved air filtration performance. Chattopadhyay, Hatton, and Rutledge (2015) studied the aerosol filtration of electrospun cellulose acetate filters with different mean fiber diameters and compared the results with two conventional filters (glass fiber and microfiber filters). Kuo, Bruno, and Wang (2014) investigated the performance of ultrafine nanofibers against nanoparticles and showed that this type of filter is advantageous especially when high filtration efficiency is required at low weight. Indeed, the air filtration performance of the electrospun nano-fibrous web is related to the electrospinning processing parameters, the air face velocity, and the aerosol particle diameter. The properties of electrospun fibers can be manipulated by varying the processing parameters of electrospinning such as the polymer concentration, the electric field, the time of electrospinning, and the volumetric flow rate (Leung, Hung, and Yuen (2010); Pai, Boyce, and Rutledge (2011)). In addition, the fiber diameter, the fiber thickness, and the porosity affect the filtration performance of the filter as well as its air permeability at different air face velocity (Abuzade, Zadhoush, & Gharehaghaji, 2012; Leung et al., 2010).

The electrospun nano-fibrous web used in protective garments is recommended to have a desirable rate of air permeability to improve clothing breathability which can be achieved by optimizing the electrospinning process (Abuzade et al., 2012). Usually, the optimization method to set electrospinning process parameters reported in literature has been dependent on empirical methods (Faccini, Vaquero, & Amantia, 2012). However, the use of a modeling approach of electrospinning process to predict nano-fibrous web morphology (fiber diameter, porosity, thickness), air permeability and filtration efficiency would serve as an important design tool in such processes.

Many researchers have developed models that estimate the fiber diameter based on the polymer solution properties and the electrospinning effective parameters (Taylor, 1969; Feng, 2002; Hohman, Shin, Rutledge, & Brenner, 2001; Yarin, 2011). Some of these models were limited to a single electrospinning stage and did not model the whole electrospinning process (Taylor 1969; Feng 2002). Other models were complex and necessitated a high computational cost (Yarin, 2011). Fridrikh, Jian, Brenner, and Rutledge (2003) derived a simplified model that related the processing parameters to the final fiber diameter. This model was recently used by Ismail, Maksoud, Ghaddar, Ghali, and Tehrani (2016) who developed a combined accurate mathematical model that covers both the stable and the unstable stages of electrospinning to predict the fiber diameter.

The porosity of the nano-fibrous web, which is a function of the fiber diameter and the web thickness, can also be estimated by a direct measurement or a theoretical model. The bulk density and porosity of the nano-fibrous web can be measured by a number of techniques such as the Scanning Electron Microscope (SEM) and the weighting technique (Ma, Kotaki, Yong, He, & Ramakrishna, 2005). By considering the mat as quantized planes of overlapping fibers and creating a randomly oriented fibers grid, one can estimate the porosity of the web by a theoretical model (Lowery, 2009).

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