Journal of Applied Polymer Science

Empirical model to simulate morphology of electrospun polycaprolactone mats

S. H. Yousefi,[1] C. Tang,[2] H. Vahedi Tafreshi,[1] B. Pourdeyhimi[3]

[1]Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, Richmond, Virginia 23284-3015

[2]Department of Chemical and Life Sciences, Virginia Commonwealth University, Richmond, Virginia 23284-3015

[3]The Nonwovens Institute, NC State University, Raleigh, North Carolina 27695-8301

Correspondence to: H. V. Tafreshi (E-mail: htafreshi@vcu.edu)

ABSTRACT: This work is the first to report a study aimed at generating 3D virtual geometries that represent the microstructure of an electrospun fibrous mat comprised curly fibers. Polycaprolactone (PCL) mats are considered in our study as an example of such fibrous structures. We started with simulating the formation of PCL filaments and observed good agreement between the predicted and measured fiber diameters. In the absence of quantitative information about the shape of a curly PCL fiber, we treated these fibers as arrays of beads arranged on epitrochoid profiles. We then used the fiber deposition diameter and velocity in a mass-spring-damper (MSD) model to generate 3D fibrous geometries comprised hundreds of such curly fibers. The damping and spring constants in the MSD model were obtained through calibration with experimental data reported for single electrospun PCL nanofibers. The size of the epitrochoid-like fibers was obtained empirically through matching the average thickness of the resulting mats with those measured experimentally. With the calibrated code, we studied the effects of electrospinning conditions on the porosity of PCL nanofiber mats. It was found that increasing the voltage or decreasing the needle-to-collector distance results in PCL mats with thicker fibers, and consequently, lower porosities. © 2019 Wiley Periodicals, Inc. J. Appl. Polym. Sci. **2019**, *136*, 48242.

KEYWORDS: electrospinning; modeling; nanofibers; PCL

Received 29 March 2019; accepted 11 June 2019

DOI: 10.1002/app.48242

INTRODUCTION

Electrospinning is a low-capital-cost method of producing micro- or nano-fibers for applications such as tissue engineering, particle filtration, membrane desalination, catalysis, self-cleaning, drug delivery, and sensing among many others.[1–10] A major challenge in fiber electrospinning is the lack of control over fiber orientation or position in the resulting electrospun mats. This makes it very difficult to design and produce an electrospun mat with a desired porosity or pore size. It is also quite difficult to accurately measure the thickness, porosity, or surface roughness of electrospun fibrous mats as they are often very thin and soft.[6] Structural simulation can generally be of great help in such conditions, but unfortunately, the complex nature of the electrospinning process makes it very difficult to develop an accurate model to describe and predict the outcome of an electrospinning experiment. Yarin and Reneker were the first to develop a mathematical model to simulate the trajectory of an electrospun filament as it leaves the needle until it reaches the collector.[11–13] Their model incorporates the contribution of solution flow rate, solution viscosity, relaxation time, and electrical potential in fiber attenuation. The work of Renekar *et al.*[11] and Yarin and Zussman[12] was later used to develop subsequent numerical models to include the effects of air drag force or the effects of embedded nanoparticles on filament trajectory during electrospinning.[14–17] Our group also used the work of Refs. 11–13 to simulate the formation of a polystyrene (PS) filament in an electrospinning setup and use the resulting information in an in-house mass-spring-damper (MSD) model to study the effects of electrospinning conditions [e.g., voltage or needle-to-collector distance (NCD)] on mat thickness or porosity.[18] In this article, we improved our MSD algorithm by allowing the fibers to have an in-plane curvature (needed for simulating mats consisting of curly fibers) and also used single-fiber mechanical properties for calibration. This article presents the simulation of electrospun PCL fiber-mats as an example of fibrous mats made up of curly fibers. In this article, we also discuss challenges involved in modeling a mat comprised randomly distributed curly fibers.

The remainder of this article is structured as follows. We discuss our experimental and numerical procedures in sections "Experiment" and "Numerical Simulation," respectively. In section Results and Discussion, we first obtain fibers' deposition diameters (and