



Modeling electrospun fibrous structures with embedded spacer particles: Application to aerosol filtration

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ABSTRACT

This work presents a physics-based modeling technique to simulate the 3-D microstructure of electrospun fibrous media with embedded spacer particles. The model accepts inputs like diameter, basis weight, deposition velocity, and bending properties for the fibers as well as diameter and basis weight for the spacer particles. The model then predicts morphological parameters like filter porosity and filter thickness, among many others. The work presented in this paper is the first to report the effects of spacer particles with different diameters or basis weights on the thickness and solid volume fraction of spacer-embedded fibrous media. Such morphological information is then used for collection efficiency and pressure drop predictions when challenged with aerosol particles in the particle diameter range of 20 nm to 5 μm at a face velocity of 10 cm/s. Our results indicate that adding spacer particles to a fibrous filter can lower its collection efficiency and pressure drop, but the reduction in the pressure drop will be at a higher rate resulting in better filters, i.e., filters with better quality factors.

1. Introduction

Electrospinning is a one-step method to produce a fibrous material by simply dissolving a polymer in a chemical solvent and electrifying the resulting solution through a needle [1,2]. An intriguing attribute of the electrospinning process is the possibility of varying the spinning conditions or the concentration of the polymer solution to produce a combination of fibers and beads through promoting or preventing the breakup of the electrified polymer jet (e.g., [3–10]). More specifically, one can often go from a fiber-only morphology to a fibers-and-beads or to a beads-only morphology by varying the polymer concentration, DC voltage, needle-to-collector distance (NCD), and/or polymer flow rate (see e.g., [3–10]). Electrospinning can also be used to embed external particles inside (e.g., [11–14]) or between (e.g., [15,16]) the fibers to incorporate additional functionalities in a fibrous material (the latter is often achieved via simultaneous electrospinning–electrospraying). The particles trapped between the fibers can also provide structural benefits to a fibrous material. These particles, for instance, can serve as “spacers” between the fibers and help to increase the porosity of an electrospun material, and thereby improve its performance in applications like tissue engineering [17], particle or droplet filtration/separation [18], or water desalination [19] among many others.

Generating virtual fibrous geometries that resemble the 3-D microstructure of a fibrous material has proven to be valuable in design

and development of nonwoven media for applications like aerosol filtration [20–22], fluid transport [23–25], heat insulation [26,27], or modern textiles in general [28–30]. The current paper is the first to report simulation of fibrous structures in presence of spacer particles. As will be discussed later in the paper, this can only be accomplished with a simulation algorithm that allows a fiber to adjust its shape to the shape of the 3-D objects (e.g., fibers or particles) to which it comes into contact, and in doing so, respects the fiber mechanical properties (e.g., stiffness). Needless to say that, the algorithm should detect and prevent any solid–solid interpenetration (obviously non-physical) to occur for the simulations to realistically and accurately represent the morphology of the material.

The remainder of this paper is structured as follows. We first present our experimental work on electrospinning fibers and beads in Section 2, and then move on to discuss our numerical simulations in Section 3. In Section 4, we present a set of analytical equations that can be used to estimate the collection efficiency and pressure drop of a filtration media comprised of fibers and spacer particles. Our results and discussion are given in Section 5, where we present an example for the practical applications of the structure simulation algorithm developed in this work in the field of aerosol filtration. This is followed by our conclusions in Section 6.

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