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Characterizing nonwoven materials via realistic microstructural modeling

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ABSTRACT

A physics-based nonwoven structure generation model is presented in this work. The model is capable of incorporating the mechanical properties of the fibers in the simulations by treating each fiber as an array of beads connected to one another via springs and dampers. Our algorithm can realistically simulate the bending of the fibers at fiber–fiber crossovers or when external forces are applied to the fibers during fiber deposition process. In fact, a unique attribute of the modeling approach presented in this work is that it can be modified to emulate, to some extent, the manufacturing process by which the nonwoven media have been produced. Unlike most previous structure generation models, our mass-spring-damper algorithm does not require the thickness or porosity of the media to be fed to the model as an input, and it is also capable of avoiding fiber–fiber overlaps. For demonstration purposes, virtual media with bimodal fiber diameter or contact angle distributions were produced and used to estimate the pressure required for water to penetrate through a hydrophobic fibrous membrane, i.e., the so-called liquid entry pressure (LEP). The LEP calculations here are based on a simplifying assumption that the air–water interface remains intact across the width of the simulation domain as it travels throughout the media. Effects of fiber diameter(s), fiber orientations, or fiber contact angle(s) on LEP are simulated and discussed in detail.

1. Introduction

Fibrous materials are unique in possessing three different attributes simultaneously: they are porous, they are flexible, and they are strong. For this reason, fibrous materials have been used in a variety of applications including, but not limited to, air or liquid filtration (see e.g., [1–5]), membrane separation (see e.g., [6–9]), and fluid absorbency (see e.g., [10–12]) to name a few. Engineering the next generation of fibrous materials for the above applications will have to rely on the ability to model the microstructure of the media and to optimize it for the specific environment of the targeted application.

In the context of particle/fluid filtration modeling, the first journal publication to report the use of 3-D fibrous structures as the simulation domain was the work of Wang et al. [13] in 2006. In this work (and a series of proceeding publications focused on particle filtration [14–21], fluid absorption [22,23], or heat insulation [24,25]), the fibrous media were treated as an un-bonded web of loose fibers, in which cylindrical objects (resembling rigid fibers) were dispersed in a 3-D domain with random in-plane and/or through-plane orientations. With the size of the computational domain held constant, the number of fibers was increased incrementally to reach the desired solid volume fraction (SVF) for the virtual media. In generating such fibrous structures, one could allow the fibers to interpenetrate into one another (unrealistic of course) or prevent that by monitoring the minimum distance between the fibers during fiber generation. Overlapping fibers are not of much concerns in simulations aimed at modeling fluid, particle, or heat transfer in the space between the fibers (e.g., [13–24]), but they should not be allowed when fiber–fiber contact plays an important role, e.g., in modeling heat conduction through fibers (e.g., [26]) or mechanical strength of the material (e.g., [27–29]).

In a recent publication, a new method to create virtual fibrous structures with reduced (but not prevented) fiber–fiber overlaps and arbitrary random curvatures has been reported in [30]. Generating non-overlapping fibrous structures using a random-walk algorithm has also been reported in [31] and used as a computational domain in some subsequent studies (e.g. [32–34]). However, resemblance of a structure created by the trajectory of a randomly moving particle to the microstructure of a real fibrous material is not immediately obvious. It is also not clear how mechanical properties of a fiber or the effects of the process by which the fibrous material is manufactured can be simulated by a random-walk-based model. It is worth mentioning that there exist some image-based approaches to obtain a realistic computational

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