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3-D simulation of particle filtration in electrospun nanofibrous filters

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ABSTRACT

Virtual 3-D geometries resembling the internal microstructure of electrospun fibrous materials are generated in this work to simulate the pressure drop and collection efficiency of nanofibrous media when challenged with aerosol particles in the size range of 25 to 1000 nm. In particular, we solved the air flow field in the void space between the fibers in a series of 3-D fibrous geometries with a fiber diameter in the range of 100 to 1000 nm and a Solid Volume Fraction (SVF) in the range of 2.5 to 7.5%, using the Fluent CFD code, and simulated the flow of large and fine particles through these media using Lagrangian and Eulerian methods, respectively. Particle collection due to interception and Brownian diffusion, as well as the slip effect at the surface of nanofibers, has been incorporated in the CFD calculations by developing customized C++ subroutines that run in the Fluent environment. Particle collection efficiency and pressure drop of the above fibrous media are calculated and compared with analytical/empirical results from the literature. The numerical simulations presented here are believed to be the most complete and realistic filter modeling published to date. Our simulation technique, unlike previous studies based on oversimplified 2-D geometries, does not need any empirical correction factors, and can be used to directly simulate pressure drop and efficiency of any fibrous media.

1. Introduction

The adverse health effects and corresponding medical costs associated with particulate air pollution are well-documented, and include increased risk of cancer, respiratory and cardiovascular disease and decreased life expectancy. Fiber-based filters represent the single largest mediator of particulate air pollution in commercial and residential environments.

Recently, nanofiber filtration media have been produced by using a technique known as electrospinning (the term "nanofiber" is often used in practice for fibers with a fiber diameter smaller than about 500 nm). It is well-documented that significant "slip" occurs when a gas flows around a nanofiber [1]. This is because when the fiber diameter is close to the mean free path of the gas molecules (e.g., 65 nm for air in Normal Temperatures and Pressures), the flow field around the fiber can no longer be assumed to be in a continuum regime, and the no-slip boundary condition at the fiber surface is invalid. Because nanofibers can cause the so-called "slip effect", they cause less resistance against air flow, leading to a smaller pressure drop across the media. To the knowledge of the authors, there is no study in the literature devised to simulate the collection efficiency and pressure drop of a nanofiber filter medium in realistic 3-D domains. As will be discussed later in this paper, almost all existing models, starting with the work of [2], are developed using oversimplified 2-D geometries, wherein fibers are neatly placed in square or hexagonal arrangements (e.g., [3–18]). The predictions of such unrealistic models were then corrected using a variety of empirical coefficients, each valid for a given range of fiber diameters, particle diameters, or flow hydrodynamic/thermal regimes. In a previous work we simulated the performance of a fibrous filter medium using 3-D fibrous geometries with no empirical correction factors [19]. That work, however, was limited to the case of microfiber media as the slip effect was not included in the simulations. Moreover, particle capture via interception was neglected for simplicity which restricted our simulations to filtration regimes with small particle-to-fiber diameter ratios (i.e., particle diameters smaller than 500 nm). In a recent work by Maze et al. [20], we simulated the deposition of nanoparticles on nanofiber media. In this work, however, the air velocity field was assumed to be constant throughout the media regardless of the presence of fibers, which can only be justified in the case of nanofibers under reduced operating pressures, or elevated gas temperatures. In the current work, on the other hand, there are no restrictions on the range of fiber diameters, particle diameters, or hydrodynamic/thermal conditions of the gas. The simulation scheme presented here can be used to model the collection efficiency and pressure drop of any fibrous media challenged with any aerosol flows.

The next section presents our algorithm for generating virtual 3-D fibrous media. In Section 3, we describe the governing equations and the boundary conditions. In Section 4, we describe the Lagrangian and Eulerian particle tracking methods together with our C++ subroutines developed to enhance the capabilities of the CFD code

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