3-D simulation of particle filtration in electrospun nanofibrous filters

S.A. Hosseini, H. Vahedi Tafreshi
Mechanical Engineering Department, Virginia Commonwealth University, Richmond, VA 23284-3015, United States

A R T I C L E   I N F O

Article history: Received 13 August 2009 Received in revised form 25 February 2010 Accepted 19 March 2010 Available online 30 March 2010

Keywords: CFD simulation Slip velocity Fibrous media Particle interception Particle diffusion

A B S T R A C T

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.

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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.
from Fluent Inc. Section 5 reports on our collection efficiency and pressure drop results obtained for nanofibrous media, and it is followed by our conclusions presented in Section 6.

2. Virtual nanofiber media

To generate 3-D fibrous geometries resembling the microstructure of a fibrous medium, a C++ computer program was developed to produce fibrous structures of different fiber diameters, porosities, thicknesses, and orientations. The media generation process is based on the randomness algorithm, and has been fully described elsewhere [19,20]. To mimic the microstructure of electrospun mats, we generated fibrous structures with fibers positioned in horizontal planes, stacked on top of one another to form a 3-D structure. Here, unlike our previous work, we allowed the fibers to inter-penetrate, as this does not affect the pressure drop or collection efficiency of the media, as long as the exact porosity is calculated correctly. The thickness of each layer is considered to be an input parameter that can be used, among other parameters, to control the SVF of the media, and was set to 1.4 mm. An example of our 3-D virtual media with a fiber diameter of 100 nm, a thickness of 1.96 µm, and an SVF of 7.5%.

3. Flow field calculations

The air flow through our virtual fibrous media is assumed to be laminar and at steady state. We have previously shown that for the range of fiber size and flow conditions considered here (Reynolds number smaller than unity), there is a linear relationship between the flow velocity and pressure drop, indicating that inertial effects are negligible [21]. The finite volume method [22] implemented in the Fluent code is used to solve the continuity and momentum equations in the absence of inertial effects:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0
\]

\[
\frac{\partial p}{\partial x} = \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)
\]

\[
\frac{\partial p}{\partial y} = \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right)
\]

\[
\frac{\partial p}{\partial z} = \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right)
\]

The boundary conditions considered for the simulations are shown in Fig. 2. Air is assumed to flow into the simulation domain through a velocity-inlet and leaves it from a pressure-outlet boundary condition. Note that our uniform flow inlet and outlet boundary conditions are placed far from the regions where strong velocity and/or pressure gradients are expected. The inlet and outlet boundary conditions are placed at distances of 20d and 5d upstream and downstream of the medium, respectively, where d is the fiber diameter. As can be seen from Fig. 2, we have used symmetry boundary conditions for the sides of the computational box, even though there is no plane of symmetry in a disordered medium. This is because if the in-plane size of the simulation domain is large, choice of lateral boundary conditions will not affect the simulation results, as the flow is mainly in the through-plane direction.

As the media generation process involves random processes, it is always necessary to repeat each simulation a number of times and average the results. It is also important to ensure that the domain size considered for the simulations is sufficiently large such that the results are not affected by any size-related artifact. Here, we used the Brinkman screening length criterion, which is given by \( \sqrt{k} \) where k is the permeability of the medium being simulated [23,24]. According to Clague and Phillips [23], a domain size about 14 times larger than the Brinkman’s length is sufficient to smooth out statistical uncertainty in the results. The larger the domain size, the fewer the number of repetitions that will be required. To obtain an estimate of the

![Image](image1.png)

**Fig. 1.** An example of our 3-D virtual media with a fiber diameter of 100 nm, a thickness of 1.96 µm, and an SVF of 7.5%.
relevant domain size to begin with, the expression of Davies [25] has been used here.

Depending on the fiber diameter and the gas thermal conditions, continuum flow regime ($Kn_f<10^{-3}$), slip-flow regime ($10^{-3}<Kn_f<0.25$), transient regime ($0.25<Kn_f<10$), or free molecule regime ($Kn_f>10$) can prevail inside a fibrous medium. Here $Kn_f=2λ_f/d_f$ is the fiber Knudsen number where $λ_f = RT / (\sqrt{2N_fπd_f^2p})$ is the mean free path of the gas molecules. Air flow around most electrospun nanofibers is typically in the slip or transition flow regimes. Slip velocity is permitted to occur at the fiber surface, as expected for flows with non-zero Knudsen numbers. This has been done by defining the wall shear stress using the Maxwell first order model [26,27]:

$$u_w = \frac{2-\sigma_v}{\alpha_v} μ \frac{\partial u}{\partial n} |_w.$$  \hspace{1cm} (5)

We have developed a C++ subroutine that works in Fluent environment, and enables it to handle the slip velocity at the fiber surface. To allow slip to occur, we modified the shear stress at the wall by using Eq. (5):

$$τ_w = \frac{μ}{\alpha_v} \frac{\partial u}{\partial n} |_w.$$

Our virtual structures are meshed using tetrahedral elements, refined close to the fiber surfaces. In an irregular structure, such as nonwoven media, there are regions where fiber-to-fiber distance is very small, at the crossovers for instance, and regions where fibers are relatively far from each other. The grid size required to mesh such a medium is often too small. The computational grid used for Computational Fluid Dynamics (CFD) simulations needs to be fine enough to resolve the flow field in the narrow gaps, and at the same time, coarse enough to cover the whole domain without requiring infinite computational power. To ensure that the results presented in this paper are independent of the number of grid points considered for the simulations, we considered one of our fibrous structures and meshed it with different mesh densities. This was done by adjusting the grid interval size in such a way as to result in 6, 10, 15, 20, and 25 grid points around the circular cross-section of the fibers. The results of our mesh-independence study are presented in Fig. 3, where pressure drop is plotted versus the number of grid points around the circular cross-section of the fibers. It can be seen that by increasing the mesh density, pressure drop increases up to reach a plateau. In the simulations presented in this work, the number of grid points on the circular cross-section of fibers was at least 15. The results shown in Fig. 3 are obtained for a medium with $d_f=400$ nm, $SVF=4.95\%$, and in the absence of slip effect.

4. Modeling particle capture in a fibrous medium

There are three basic mechanisms that lead to the capture of an aerosol particle in a neutral filter medium. These are interception, inertial impaction, and Brownian diffusion. Brownian diffusion is only important for small particles (about 200 nm or less). Interception is important when the size of the particle and fiber are comparable, and inertial impaction becomes considerable only when the particle's momentum is not negligible, either because of its large mass or high velocity. Note that van der Waals forces are ignored in this study.

Here, we considered a convective–diffusive equation for the concentration of the small particles based on the Eulerian approach [28]:

$$u \frac{\partial N}{\partial x} + v \frac{\partial N}{\partial y} + w \frac{\partial N}{\partial z} = D \left( \frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial y^2} + \frac{\partial^2 N}{\partial z^2} \right).$$  \hspace{1cm} (7)

To define Eq. (7) for Fluent’s PDE solver, we developed a C++ subroutine that was executed during the simulations. The diffusion coefficient in Eq. (7) is defined as $D = αC_T/3πd_p$, in which $C_T = 1 + Kn_p(1.257 + 0.4e^{-1/11/σ_m})$ is the empirical factor of Cunningham for slip correction at the surface of nanoparticles. It is assumed here that particles that come in contact with the fibers will be captured and vanish from the domain. Particle concentrations at the inlet and fiber surfaces are assumed to be $N=N=0$, respectively. At the outlet, we considered $\partial N/\partial z=0$ indicating that there is no change in the nanoparticle concentration flux at the outlet (flow is in the z-direction).

Fig. 4 is an example of our simulation results, where the particle concentration contour plots are shown in a plane slicing through a
medium with a fiber diameter of 1000 nm and an SVF of 7.5. In this figure, red to blue represents normalized particle concentration from 1 to zero (the blue color on the outlet plane is not part of the concentration contour plot, and is shown for better 3-D visualization only). Note that the particle concentration close to the fibers is almost zero, indicating particle deposition.

We also used the Lagrangian method, where each individual particle is tracked throughout the solution domain, to calculate particle capture view interception and inertial impaction. In the Lagrangian method, the force balance on a particle is integrated to obtain the particle’s position in time. The dominant force acting on a particle is the air drag force. For particle Reynolds number smaller than unity, we have [29]:

\[
\frac{du_p}{dt} = \frac{18 \mu}{d_p^2 \rho_p c} (u - u_p) \quad (8)
\]

\[
\frac{dv_p}{dt} = \frac{18 \mu}{d_p^2 \rho_p c} (v - v_p) \quad (9)
\]

\[
\frac{dw_p}{dt} = \frac{18 \mu}{d_p^2 \rho_p c} (w - w_p) \quad (10)
\]

where the subscript \(p\) denotes the particle properties. Particles in both Lagrangian and Eulerian simulations were introduced to the simulation domain from the inlet boundary condition with uniform velocity and concentration profiles.

The Standard Discrete Phase Model (DPM) in Fluent code treats the particles as point masses, and therefore cannot calculate particle deposition due to interception. In this work, we developed a C++ subroutine that modifies Fluent’s standard DPM module to include the particle deposition via interception. This has been done by continuously monitoring the distance between the particles’ center of mass and the fibers’ surface during the trajectory tracking in a loop. If a particle’s center of mass reaches a distance of one particles’ radius from any fiber surface, our subroutine then eliminates it from the domain and considers it captured.

Fig. 5 illustrates an example of the particle tracking exercise reported in this study. For the sake of clarity, only a few particle trajectories are shown. For illustration purposes, particles are released from 100 injection points located on the same plain, as was shown in Fig. 4. To generate this figure, spherical objects are placed at the center of mass of each particle as they travel through the medium. The size of the spherical symbols in the figure is graphically chosen to be close to that of the actual particles (500 nm) for illustration, i.e., the actual particle size is used only in the calculations, not in the graphical presentation. It can be seen that our interception subroutine eliminates the trajectories that are intercepted by fibers (see the magnified view of two intercepted trajectories in Fig. 5b). Note that particles do not interact with each other. Therefore, one can (and must) release a large number of particles to correctly predict the particle capture.

5. Results and discussions

Kuwabara [2] was the first to develop a mathematical theory (cell model) for predicting the collection efficiency of fibrous filters in the continuum flow regime. Other researchers later improved the work of Kuwabara by considering the so-called “fiber array” models, and obtained different expressions for pressure drop and particle collection efficiency of fibrous media (see [30] for a review). A filter’s pressure drop is a function of air viscosity, filter thickness, face velocity, fiber diameter, and material’s SVF, as:

\[
\frac{\Delta p}{h} = f(\alpha) \frac{\mu V}{d_f^2}.
\]

Here \(f(\alpha)\) is a function of SVF only, and has different forms based on different theories. The most popular correlation for calculating the pressure drop of a fibrous medium is the empirical correlation of Davies [25], given as:

\[
f_{\text{Dav}}(\alpha) = 64\alpha^{3/2} (1 + 56\alpha^3).
\]
Our pressure drop per unit thickness results for fibrous media with fiber diameters ranging from 100 nm to 1000 nm, and different SVFs from 2.5% to 7.5%, are shown in Fig. 6. It can be seen that pressure drop increases with increasing SVF, as expected. Predictions of Davies’ equation are also added to this figure for comparison. It can be seen that the Davies correlation over-predicts the pressure drop of nanofiber media. This is because the media used in Davies’ experiments comprised of fibers with a diameter ranging from 1.6 μm to 80 μm, and so his correlation is inaccurate in predicting the pressure drop of nanofiber media, where a significant slip takes place. Note that in our previous studies, we demonstrated perfect agreement between the predictions of Davies’ correlation and our CFD simulations conducted for microfiber media [19,31–33].

In Fig. 6, we have also included the predictions obtained via the empirical correlation of Ogorodnikov obtained for slip and transition regime [34]:

\[
f_{\text{ogo}}(\alpha) = \frac{16\alpha}{(-0.5 - 0.5 \ln \alpha + 1.15 \ln(1-\alpha)^4)} \tag{13}
\]

It can be seen that very good agreement exists between our simulation results and the empirical correlation of Ogorodnikov, especially for fibers with very small diameters. As the slip effect reduces for fibers with larger diameters (e.g., 1000 nm), Ogorodnikov loses its accuracy.

Efficiency of a filter medium can be obtained in terms of its thickness, SVF, and fiber diameter if the total Single Fiber Efficiency (SFE), \(E_{\Sigma}\), is available. Efficiency of a fibrous filter is given as [35]:

\[
E = 1 - \exp\left(\frac{-4\alpha E_k - t}{16d(1-\alpha)}\right). \tag{14}
\]

The total SFE, \(E_{\Sigma}\), is the sum of SFEs due to interception, inertial impaction, and Brownian diffusion [35]. Inertial impaction for low-speed submicron particles is quite negligible, and will not be included in our discussion here. Total SFE is given as:

\[
E_{\Sigma} = 1 - (1 - E_k)(1 - E_d) \tag{15}
\]

where \(E_k\) and \(E_d\) are single fiber efficiency due to interception and Brownian diffusion, respectively.

Different formulas are suggested for calculating the interception efficiency. Table 1 presents some commonly used SFE expressions for particle capture due to interception. For comparison purposes, we plotted the efficiency of one of our virtual filter media due to interception, as predicted by these expressions in Fig. 7. It can be observed that the existing expressions do not perfectly agree with one another. This is simply because each expression is empirically adjusted for a given range of particles, fibers, and/or flow regime, and so are not accurate for a wide range of parameters. Our particle capture results due to interception are also shown in the figure for comparison.

<table>
<thead>
<tr>
<th>Investigator(s)</th>
<th>SFE expressions for interception</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lee and Gieseke [36]</td>
<td>(E_k = \frac{1}{(1 + \frac{R}{C_1})^{2}})</td>
</tr>
<tr>
<td>Pich [6]</td>
<td>(E_k = \frac{1}{(1 + \frac{R}{C_1})^{2}})</td>
</tr>
<tr>
<td>Liu and Rubow [12]</td>
<td>(E_k = \frac{1}{(1 + \frac{R}{C_1})^{2}})</td>
</tr>
<tr>
<td>Lee and Liu [8]</td>
<td>(E_k = \frac{1}{(1 + \frac{R}{C_1})^{2}})</td>
</tr>
</tbody>
</table>

Table 1

Some of the popular Single Fiber Efficiency semi-empirical expressions obtained for capture via interception.

Fig. 6. Pressure drop per unit thickness of different media with different SVFs and fiber diameters are compared with the predictions of Davies (black lines) and Ogorodnikov (red line) empirical correlations. Dashed–dotted line (–·–), long-dashed line (–––), solid line (–), dotted line (–·–), dashed line (––), and dashed–double-dotted line (·–·–), represent fiber diameters of 1000 to 100 nm, respectively.

Fig. 7. Existing semi-empirical correlations for particle capture due to interception are compared with one another and our simulation results for a filter with a fiber diameter of 100 nm and an SVF of 2.5.
When the capture via diffusion are compared with one another and our simulation results for a particle with a diameter smaller than 75 m, it can be seen that FOM increases by decreasing the particle diameter. It is also demonstrated that the existing empirical/semi-empirical expressions obtained for particle capture due to Brownian diffusion are not always perfectly match, our CFD results are in close agreement with the predictions of the above semi-empirical correlations.

Some of the popular Single Fiber Efficiency (SFE) due to interception correlations are compared with one another and our simulation results for a filter with a fiber diameter of 100 nm and an SVF of 2.5.

### Table 2

<table>
<thead>
<tr>
<th>Investigator(s)</th>
<th>SFE expressions for diffusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stechkina &amp; Fuchs</td>
<td>$E_d = 2.98Ku^{-1/3}Pe^{-2/3} + 0.62Pe^{-1}$</td>
</tr>
<tr>
<td>Fuchs [7]</td>
<td></td>
</tr>
<tr>
<td>Liu and Rubow [12]</td>
<td>$E_d = 1.6(1 - \alpha/12Pe^{-2/3})C_3$</td>
</tr>
<tr>
<td>Payet [13]</td>
<td>$E_d = 1.6(1 - \alpha/3Pe^{-2/3})C_4 + 0.388Kn_0^{1/3} Pe^{-3/3}$</td>
</tr>
<tr>
<td>Lee and Liu [8]</td>
<td>$E_d = 1.6(1 - \alpha/3Pe^{-2/3})C_4$</td>
</tr>
<tr>
<td>Pich [5]</td>
<td>$E_d = 2.27Ku^{-1/3}Pe^{-2/3}(1 + 0.62KnPe^{1/3}Ku^{-1/3})$</td>
</tr>
</tbody>
</table>

**6. Conclusions**

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. The numerical simulations presented here are the most complete and realistic filter modeling published to date, and unlike previous studies based on oversimplified 2-D geometries, do not need any empirical correction factors. This modeling strategy can be used to directly calculate the pressure drop and collection efficiency of fibrous media with any fiber diameter when challenged with aerosols of any particle size, and can be used to study particle loading and filter lifecycle simulations.

We, in particular, demonstrated that the existing empirical/semi-empirical correlations do not agree with one another when deployed to predict collection efficiency of nanofibrous media. This is most likely due to the empirical nature of the correction factors used in their development. Particle collection due to interception and Brownian diffusion, as well as the slip effect at the surface of nanofibers, has been incorporated in our CFD calculations by developing customized C++ subroutines that run in the Fluent environment. Our results show good general agreement with the existing correlations, and can be used to examine their accuracy. We also demonstrated that the popular correlation of Davies [25] fails to accurately predict the pressure drop of nanofiber media. Closer agreements have been observed with the pressure drop correlation of Ogorodnikov [34].

#### Nomenclature

- $d_f$: fiber diameter
- $d_{cp}$: collection diameter
- $d_p$: particle diameter
- $C_d$: Cunningham slip correction factor
- $D$: diffusion coefficient
- $E_{sc}$: total SFE
- $E_d$: SFE due to diffusion
- $E_k$: SFE due to interception
- $h$: filter thickness
- $k$: permeability
- $K_n$: fiber Knudsen number
- $K_{np}$: particle Knudsen number
- $K_u$: Kuwabara hydrodynamic factor
- $n$: normal position vector
- $N$: particle concentration
- $N_A$: Avogadro’s number
- $p$: pressure
- $P$: penetration
- $r$: fiber radius
- $R$: universal gas constant
- $t$: time
- $T$: temperature
- $V$: face velocity
- $u$: fluid velocity in the x-direction
- $u_p$: particle velocity in the x-direction
- $u_w$: fluid velocity at the wall
- $v$: fluid velocity in the y-direction
- $v_p$: particle velocity in the y-direction
- $w$: fluid velocity in the z-direction
- $w_p$: particle velocity in the z-direction
- $\alpha$: Solid Volume Fraction
- $\lambda$: mean free path
- $\mu$: viscosity
- $\rho_p$: particle density
- $\sigma$: Boltzmann constant (1.38 x $10^{-23}$ m$^2$ kg s$^{-2}$ K$^{-1}$)
- $\alpha_r$: tangential momentum accommodation coefficient
- $\tau_w$: wall shear stress

**Fig. 8.** Existing semi-empirical correlations for particle capture due to Brownian diffusion are compared with one another and our simulation results for a filter with a fiber diameter of 100 nm and an SVF of 2.5.
Fig. 9. Total filter efficiency is calculated by adding our simulation results for particle capture via Brownian diffusion and direct interception, and are compared with the predictions of the expressions given by [12], as an example. Note that the SVFs of the results presented in this figure are approximate values with a 10% margin of error from the stated values in the legend (i.e., 2.5%, 5.0%, and 7.5%).
Acknowledgment

SAH acknowledges VCU School of Engineering for financial support.

References
