Case Studies of Air Filtration at Microscales: Micro- and Nanofiber Media

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ABSTRACT

In this work, 3-D fibrous geometries are developed to resemble the microstructure of spun-bonded and electrospun filters media and used here to simulate their filtration efficiency and pressure drop. For the sake of simplicity, a continuum flow theory was considered to prevail for the case of spun-bonded media (microfiber media) whereas our electrospun media (nanofiber media) were assumed to be in a free molecular flow regime.

Our simulations results are in good general agreement with the experimental data. Especially, in predicting media's pressure drop, our results show better predictions when compared to some of the existing models. We also quantitatively demonstrated that by decreasing the fiber diameter, the minimum collection efficiency of the media having identical pressure drops increases. This effect is accompanied by a decrease in the particle diameter associated with these minimum efficiencies – the most penetrating particle diameter. Studying the influence of the gas temperature, we showed that filter's efficiency increases as the gas temperature increases. Conversely, the filter's pressure drop decreases by increasing the gas temperature.

INTRODUCTION

Filtration science dates back to the work of Happel [1] and Kuwabara [2]. Their works were later on continued by Stechkina and Fuchs [3], Lee and Liu [4], Henry and Ariman [5], Rao and Faghri [6], and Brown [7] among many others. In most of the previous studies the filter geometry has been simplified to rows of regularly arranged fibers, often in 2-D geometries, perpendicular to the flow direction [1-8]. To this end, our group has been the first to model aerosol filtration in 3-D geometries [9-10]. The work has generally been focused on simulating collection efficiency and pressure drop of virtual filters made up of micro- or nanofibers and comparing the results with both phenomenological and analytical models. The present paper outlines our previous studies [9-11] and discusses them in a condensed form.

Modeling Filters' Microstructure

Most of nonwovens used in filtration industries can be assumed to be 3-D layered structures. Such structures consist of a large number of fibers randomly distributed in a horizontal plane and sequentially deposited on top of each others to build up a 3-D geometry. In order to simulate a layered fiberweb (an un-bonded assembly of fibers), we considered the fibers to be circular cylinders with a given diameter. For simplicity, we assumed that fibers lie horizontally in the plane of web and do not bend at crossovers.

To generate a 3-D web, first a new fiber is generated at an altitude greater than the current thickness of the web. If there are no fibers underneath the new one, it is directly positioned on the plane $z = 0$. The next step is to lower the new fiber on the web or, in other words, to find the smallest vertical translation which will bring the new fiber in contact with the web as shown in *Figure 1*.

By repeating the above procedure for every new fiber one can produce a 3-D fibrous structure as shown in *Figure 2*. For more detailed information on this procedure, readers are referred to our previous publications [9-11]. Note that the above algorithm does not include any additional compaction, such as the one imposed by compaction rolls, for instance. Interested readers are referred to [12-13] for our work on modeling fibrous materials under compaction.

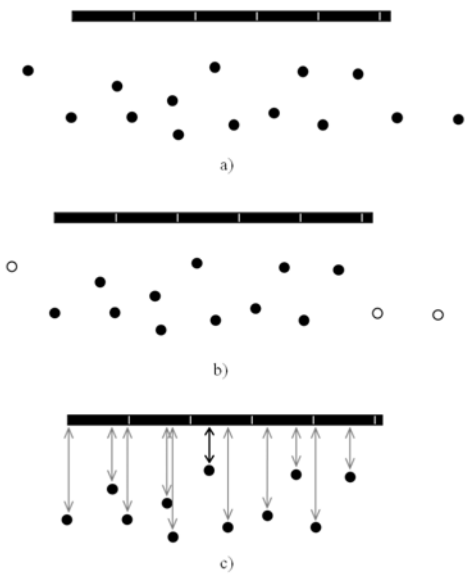

FIGURE 1. Fiber deposition procedure

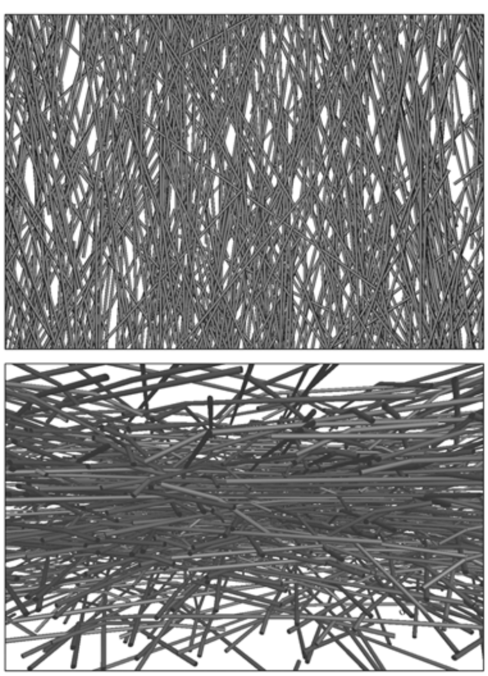

FIGURE 2. A 3-D fibrous structure generated by sequentially depositing horizontal fibers from top and side views.

Once the filter's microstructure is generated, one can consider solving fluid flow equations in the pore space between the fibers and obtain the flow field, for instance. Such information can be then used to determine the pressure drop of the filter media. Moreover, the air flow field can also be used to calculate the instantaneous drag force on airborne particles and help in predicting the trajectory of aerosol particles as the go through the filter media.

In the next section we outline our attempts to use the above 3-D microstructures in simulating nanoparticle filtration via nano- and microfiber filters.

Filtration via Microfiber Media

A steady state laminar incompressible model has been adopted for the flow regime inside our virtual filter. Gambit, a preprocessor for Fluent code, is used in this work for meshing the filter structures. The coordinate of the fibers in the virtual filter are exported to Gambit via a journal file. The imported geometry is then meshed using tetrahedral elements, refined close to the fiber surfaces. Air is assumed to flow into the simulation domain through a velocity-inlet and leaves it from a pressure-outlet boundary condition.

We have used symmetry boundary conditions for the sides of the computational box as no significant lateral air flow is expected inside a filter media. For the air flow on the fiber surfaces, we assumed a no-slip boundary condition. This is because for the air thermal condition and the fiber diameter considered in this paper, the continuum flow prevails, i.e., $Kn_f = 2\lambda / d_f << 1$, where Kn_f is the fiber Knudsen number, λ is the mean free path of the air molecules (about 60 nm).

Figure 3 shows the velocity field inside a filter medium with a SVF of about 3% and a fiber diameter of 17µm.

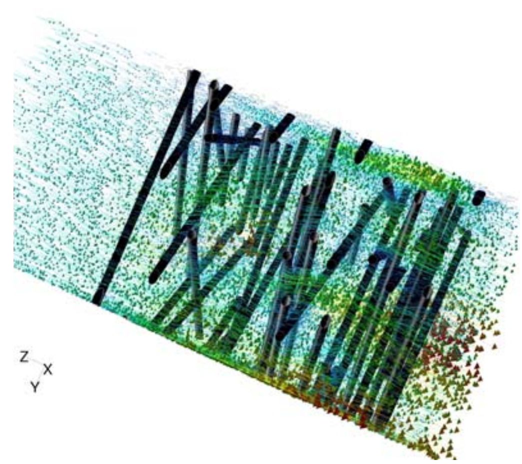

FIGURE 3. Flow field inside a filter medium [9]

Having the velocity field, one can calculate the drag force on each fiber and obtain the pressure drop of the media.

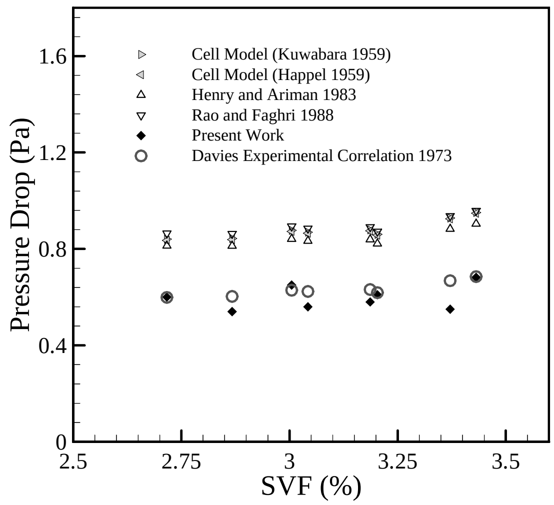

FIGURE 4. Pressure drop of our modeled microstructure in comparison with existing 2-D models. I good agreement with empirical data is evident [9].

Figure 4, shows the filter pressure drop obtained from simulating the structures shown in *Figure 3* along with the predictions of previous analytical and numerical models in the literature. The empirical correlation obtained by Davies [14] is also presented for comparison. It can be seen that there is a perfectly good agreement between our CFD simulations and the Davies's equation. Pressure drop based the traditional 2-D models resulted in higher predictions [9].

Once the particle-free flow field is obtained, the airborne particulates can be released in the solution domain. The rational for this method is the dilution of the suspension, which leads to negligible perturbations of the continuum field by the presence of the particulate phase. Particle trajectories are then tracked via the Lagrangian method and their positions are monitored. For more information on this see our previous work [9].

Figure 5 shows the average collection efficiency of the filter shown in *Figure 3* versus particle diameter along with the predictions of the Kuwabara's cell model. It can be seen that the filter collection efficiency decreases by increasing the particle size in the range of 50nm to 500 nm. Particles are assumed to be Diethylhexyl Phthalate (DOP) with a density of 1000 kg/m3.

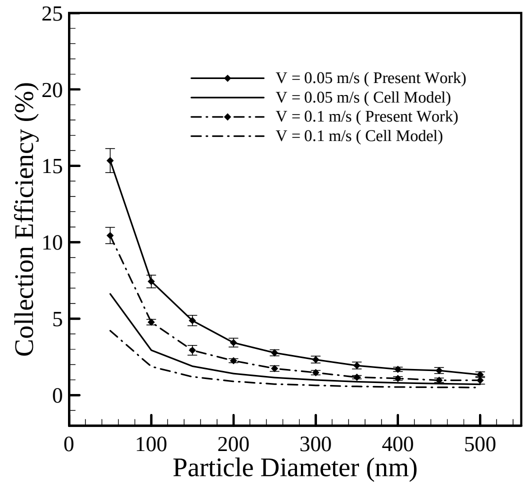

FIGURE 5. Collection efficiency vs. particle diameter [9].

Filtration via Nanofiber Media

Depending on the fiber diameter and the air thermal conditions, there are four different regimes of flow around a fiber. These are continuum regime ($Kn_f < 10^{-3}$), slip-flow regime ($10^{-3} < Kn_f < 0.25$), free molecule regime ($Kn_f > 10$), and a transient regime ($0.25 < Kn_f < 10$). The flow field about an electrospun nanofiber ($d_f \cong 100$) is not in continuum regime. The no-slip boundary condition at the fiber surface is no longer valid and this makes the calculations more complicated. The modeling approach discussed in the previous chapter cannot be directly applied in here. To simplify the problem, we assumed the nanofiber filters to operate at low pressures. This will cause the hydrodynamic condition to shift to the free molecular flow regime $Kn_f > 10$. At such a high Knudsen numbers, one can consider ignoring the presence of the fibers in the flow field. This is, of course, a very rough approximation, but can help reducing the complexity of the modeling task. For more discussion on this approximation see our previous work [10].

There are two basic mechanisms by which an aerosol nanoparticle can deposit on a neutral nanofiber. These are interception and Brownian diffusion. While there are available expressions for calculating the SFE via modified cell models in slip-flow, there is no expression available for the free molecular regime.

Collection efficiency of a filter is determined by the number of particles it can remove from an aerosol flow. In our simulations, we introduced a certain number of particles upstream of the filter and follow their trajectories as they flow through the medium. If they collide with a fiber, they are removed from the stream.

It is well-known that the smaller the fiber diameter, the higher is the collection efficiency of the media having identical weights. This is because the available surface area increases by decreasing the fiber diameter. However, the increased surface area causes the pressure drop to increase too. To simulate the collection efficiency of nanofiber media having different fiber diameters, we generated virtual fiberwebs of 50nm, 100nm, and 200nm diameters having a thickness of 3.1 µm. To have a meaningful comparison, the SVF of these media were chosen in such a way that they would cause identical pressure drops when operating at a reduced operating temperature and pressure of 300 K and 13.6 kPa, respectively.

Figure 6 shows these three fiberwebs from top view. Note that the scale bars have different lengths in these figures. These structures are challenged monodisperse particles. The diameters in each batch range from 50 nm to 500 nm and the resulting collection efficiencies are plotted in *Figure 7*. It can be seen in *Figure 7* that while all these three filter media have identical pressure drops, their collection efficiencies are very different. The medium with thinner fibers have higher efficiency. The most penetrating particle size is found to be about 100nm to 200nm and it moves towards smaller diameters by reducing the fiber diameter.

Figure 8 shows the influence of air temperature on capture efficiency. Here, the abovementioned fiberweb with 100nm fibers is challenged with nanoparticles airborne in hot air with different temperatures of 300, 650 and 1000 Kelvin. It can be seen that by increasing the air temperature, the medium's particle capture efficiency increases especially at small particle diameters. As shown by the dashed lines in *Figure 8*, by increasing the air temperature the diameter associated with the most penetrating particles moves towards greater values. Note that the pressure drop decreases by increasing the air temperature.

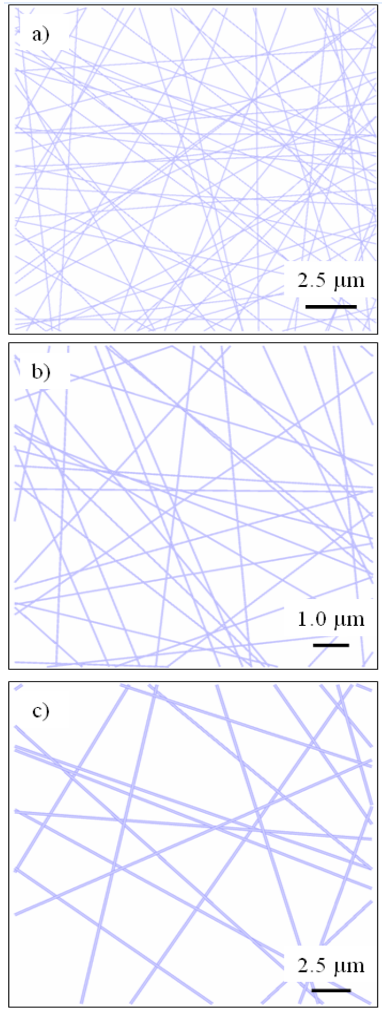

FIGURE 6. Top view of three virtual webs made of fibers with a diameter of 50, 100, and 200 nanometers, respectively. Note that the size of the scale bar is different in (a) and (c).

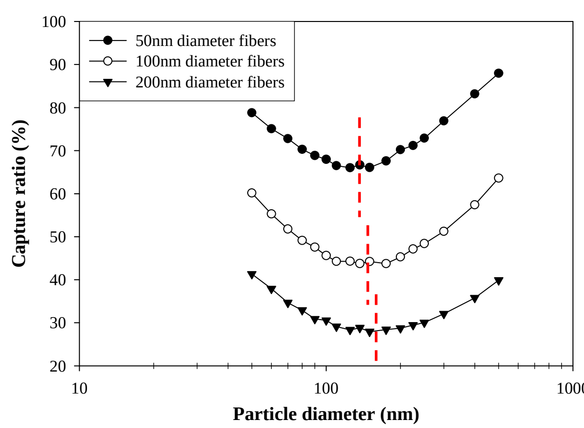

FIGURE 7**.** Collection efficiency of filter media made of fibers of 50, 100, and 200 nanometers diameters. All the three webs have identical thickness and pressure drops but different SVFs.

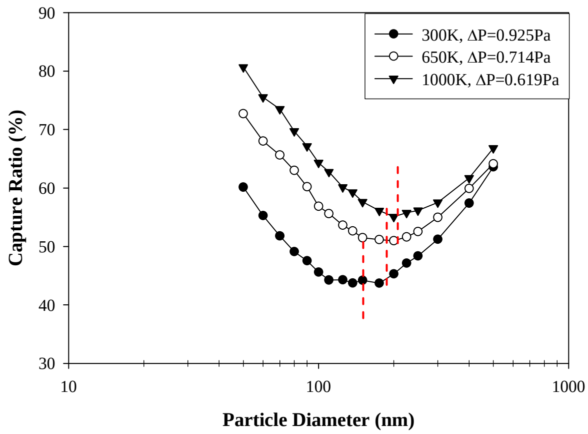

FIGURE 8. Influence of gas temperature on nanoparticle collection efficiency.

In order to simulate the caking phenomenon, we assumed that particles attach to a fiber if a collision occurs. Similarly, a new particle is assumed to deposit on an existing one if a collision occurs. We considered the particles to be taken from a log-normal size polydisperse distribution similar to that of Diethylhexy Phthalate (DOP) particles generated by the aerosol generator of TSI 8130 filter testers. *Figure 9* shows an example of a polydisperse cake at 75% filter efficiency deposited on the aforementioned filter medium with 100 nm fibers.

The above simulation demonstrates the feasibility of modeling 3-D models for emulating cake formation on nanofiber filters. The ultimate goal of such a study is to develop a relationship between the properties of the media and their filtration characteristics where there is no available analytical model.

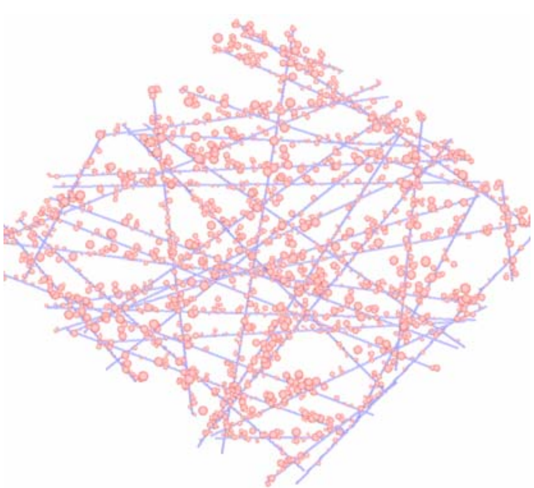

FIGURE 9. An example of a polydisperse cake made at a temperatures of 300 Kelvin at 75% filter efficiency.

CONCLUSIONS

In this paper, we briefly discussed our 3-D approach for simulating aerosol filtration at microscales. The research outlined here is aimed at building a relation between the properties of different filter media (fiber type, manufacturing process, and filter structure) and their filtration properties, and the current work is only the first step towards this goal.

In modeling microfiber filter media we solved the Navier-Stokes equations in 3-D geometries resembling spun-bonded un-calendered media. Pressure drop of our CFD simulations are in perfect agreement with the empirical correlations. In agreement with Kuwabara model, we also showed that the collection efficiency is higher for smaller particles in the range of 50 nm to 500nm. With regards to nanofiber filter, we simulated a case of nanoparticle filtration via nanofiber webs. We challenged our filters with polydisperse aerosols to simulate the caking process. A quantitative comparison between the media having identical pressure drop but different fiber diameters is presented to show that by reducing the fiber diameter, the collection efficiency of the medium increases and the diameter associated with the most penetrating particles shifts towards lower values. It was also shown that by increasing the temperature of the air, the filter's collection efficiency increases while its pressure drop decreases.

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