ABSTRACT

WANG, QIQI. An Investigation of Aerosol Filtration via Fibrous Filters. (Under the direction of Hooman Vahedi Tafreshi and Behnam Pourdeyhimi.)

The most common method of removing particles from a gas stream is via fibrous filters. However, most of the previous studies have been limited to systems consisting of rows of fibers (often in two-dimensional geometries) perpendicular to the flow direction. The current work is aiming to develop an understanding of the role of filter’s microstructure and manufacturing process.

In the first part of this study, pressure drop and nanoparticle collection efficiency of lightweight spun-bonded media are simulated by solving the Navier-Stokes equations inside three-dimensional geometries resembling the microstructure of such media. These pressure drop and collection efficiencies showed a perfect agreement with experimental data.

In the second part of this work, the influences of fiber length and compaction ratio of filter media on the pressure drop are discussed. Simulation data of staple fiber media have shown good agreement with Davies’ empirical equation. Such an agreement indicates that, within the range of dimensions considered, the fiber length has no significant influence on the materials’ through-plane permeability as long as the SVF remains constant. Our simulation results for nonwovens with different compaction ratios, together with our experimental data, indicate that pressure drop of the porous media increases with increasing the compaction ratio or temperature of the calender rolls.
In the third part of this work, we presented our approach for modeling permeability of fibrous filters with bimodal fiber size distributions (referred to as bimodal filters in this context). The three-dimensional microstructures resembling bimodal filter media with random in-plane fiber orientation distribution were generated to compute their permeability constants. These results were compared with the previous analytical and numerical models as well as our experimental data. Here we concluded that there exists an area-weighted equivalent average diameter for each bimodal filter that can be used in the existing expressions for calculating the permeability of unimodal filters.

The last part of this thesis is dedicated to studying the permeability woven fabrics. Concerned with the accuracy of the homogeneous anisotropic lumped model of Gebart (1992) for predicting the permeability of multifilament fabrics, we devised a series of numerical simulations conducted in full three-dimensional geometry of idealized multifilament woven fabrics wherein the filaments were packed in Hexagonal arrangements. While a relatively good agreement was obtained, our results indicate that Gebart’s model underestimates the permeability of multifilament fabrics at high yarn’s solid volume fractions. We also simulated the pressure drop of monofilament woven fabrics under tension where we observed a logarithmic relationship between the discharge coefficient and the Reynolds number of the flow.
An Investigation of Aerosol Filtration via Fibrous Filters

by

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DEDICATION

To my beloved Mama and Baba.
BIOGRAPHY

Qiqi Wang was born on 26th Dec, 1980 in Shanghai, China. She received her Bachelor of Science degree in Textile Engineering from Donghua University (China Textile University) in June 2003. To fulfill her life long ambition for higher education, she joined the PhD program in Fiber & Polymer Science, and during this period she also worked as a research assistant with the Nonwovens Cooperative Research Center (NCSU) at North Carolina State University. She obtained her Doctor of Philosophy degree under the supervision of Dr. Hooman Vahedi Tafreshi and Dr. Behnam Pourdeyhimi in Oct 2007.
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CHAPTER 1

INTRODUCTION
1.1-Fibrous Filters

Our rapidly growing competitive industries, such as electronics, medical, pharmaceutical, and biological industry, require engineers to design aerosol filters tailored for different specific applications. The principal filter types include membrane filters, granular filters, foam filters and fibrous filters. Among them, the most common method of removing particles from a gas stream is via fibrous filters, such as nonwoven filtration media and woven filtration media, which are generally characterized by their collection efficiency and pressure drop for air filtration.

1.1.1-Nonwoven Filtration Media

Nonwoven can be defined as “a sheet, web, or mat of natural and/or man-made fibers or filaments, excluding paper, that have not been converted into yarns, and that are bonded to each other by any of several means”(INDA 1999). These media are created for specific end-uses, such as filtration, while achieving a comparatively low cost. Current filtration technology allows nonwoven medium with capability to move the particles from gas stream with efficiency greater than 99.99999 % by mass.

Nonwoven filters are classified either neutral or electrostatic filters. In this work, we only consider neutral fibrous filters. These media are assemblies of fibers with random orientation distributions. Fibers are fine, and fiber diameter \( d_f \) are normally smaller than 100 \( \mu m \). The fibers are made of cotton, fiberglass, polyester, polypropylene, ceramic, stainless steel and many other materials. The solid volume fraction \( \alpha \), which is the ratio of volume of all fibers in a filter to the total volume of the filter, is known to be in the ranged from 1 to 30 % (Kim, 2005). Figure 1.1 shows a typical microscopic image of nonwoven filtration media.
All Nonwoven processes have two general steps: web forming and web bonding. The web forming step can be done by one of five general methods: dry-laid (carded or air-laid), wet-laid, spun-bonded, melt-blown, and electro-spun. The fibers can be in either in the form of the short length (staple fibers) or in the form of the continuous length (filament) (INDA, 1999).

Nonwovens made of the Air-laying (AL), Carding (CA) and Wet-laying (WL), are typical examples of fiber-webs made of short fibers. The common characteristic among AL and WL is that in both of their short fibers (typically 1 to 20 mm long) are dispersed in either air or water and then deposited on a porous belt to form a web. CA process takes advantage of high-speed rotating drums having needles on their peripheries to tease the fibers apart and individualize them. Individualized fibers then become airborne and get deposited on a moving belt. AL, CA, and WL webs can be made of synthetic (e.g., thermoplastic) or natural fibers (e.g., cotton) (INDA 1999; Maze 2007a).

Nonwovens made of the Electrospinning (ES), Meltblowing (MB), and Spun-bonding (SB), are typical examples of fibrous media made of infinitely long fibers. The common characteristic among those processes is that in all of them, a continuous polymeric filament at liquid state is being attenuated to reduce its diameter from micrometer-scale down to nanometer-scale. The
major difference between the fiber-webs made by ES, MB, and SB is the fiber diameter. Fiber diameters obtainable from ES, MB, and SB processes are averagely about 0.5 um, 5 um and 20 um, respectively (INDA 1999; Maze 2007a).

1.1.2-Woven Filtration Media

Both multi-filament woven fabric and mono-filament woven fabric have been used in filtration. Woven filtration media are usually characterized by geometrical parameters, such as mesh count, mesh opening, yarn size and weave pattern. The mesh count or thread count of a fabric can be defined as the number of threads per inch or centimeter. The mesh count and yarn diameter affects the amount of open area in a particular cloth, which in turn determines the permeability and collection efficiency of woven filtration media (Cheremisinoff, 1998).

Cotton cloths, glass cloths and synthetic fiber cloths are some samples of popular types of the woven filtration media. Cotton woven filters is one kind of the most widely used filter media. The different pattern of the cotton woven fabrics, such as plain, twill, canton flannel, are used for different applications. One of the cotton filters, called Nitro-filter (Nitrated cotton cloth), is claimed that the cake is easily detached and clogging is rare due to its harder surface (Cheremisinoff, 1998). Glass cloths are made from glass fibers. Because of their high thermal resistance, high corrosion resistance, high tensile strength and wide range of fiber diameter and fiber composition, glass fiber fabric been widely used in industrial filtration. However the disadvantage of the woven fabrics are the lack of flexibility (Cheremisinoff, 1998). Woven filters from synthetic fibers are superior to most of the natural cloths. Synthetic woven filters do not swell, are inert to many acid, alkaline and solvent solution. Some synthetic filters resist relative high temperature, which can serve in the high temperature condition. The most widely used
synthetic woven filter media include nylon, Saran, Dacron, Dynel, Vinyon, Orlon and Acrilian (Cheremisinoff, 1998).

1.2-Virtual Filtration Media

For the purpose of modeling, many researchers have attempted to develop virtual structures that resemble a nonwoven fiber mat. Figure 1.2 shows an example of a virtual nonwoven medium represented by cylindrical fibers distributed randomly in 1, 2, or 3 coordinate directions (Tomadakis and Roberston, 2005). In one-dimensional random structure, like Cell model and Arrays model, the fibers have their axes parallel to each other. Two-dimensional random structure, which can represent most of the nonwoven fabrics, has layered geometry; in each plane, the fibers are randomly distributed. Three-dimensional random webs, the cylindrical fibers have their axes randomly positioned and oriented in the 3D space. Only few nonwoven, such as special air-laid, have 3D random webs.

![Illustration of random structures in one-, two-, three-dimensions](image)

**Figure 1.2:** Illustration of random structures in one-, two-, three-dimensions (Tomadakis and Roberston, 2005).

Most of nonwovens can be treated as 3-D layered structures (See 2D random web in Figure 1.2). There other attempts in generating 3-D fibrous structures in the literature such as the works of Koponen et al., (1998); and Faessel et al., (2005). The work of Koponen et al (1998) was
successful in constructing structures that realistic in terms of fiber bending (see Figure 1.3). However, their model was composed of fibers which were placed either in the Machine Direction (MD) or Cross Machine Direction (CMD).

![Figure 1.3: A fiber-web sample constructed by using the model of Koponen et al. (1998)](image)

Another interesting model in the literature is the one developed by Fassel et al (2005) who considered a 3-D probabilistic random model. In their model, the fibers are generated in a unit cell corresponding to a periodic elementary volume. The information about the fibers, such as fiber length, fiber diameter, position (x, y, z –coordinates), orientation and curvature, is randomly extracted from the statistical distribution, obtained from morphological properties of real fabric based on image analysis. Figure 1.4 shows typical simulating structures based on Fassel et al’s modeling approach.

![Figure 1.4: Faessel et al’s 3D random structures: a) random; b) semi-random; c) oriented. (2005)](image)
Over the past few years NCRC has developed a software program for simulating virtual mats of un-bonded fibers in 2-D and 3-D space (Pourdeyhimi et al. 1996a, Pourdeyhimi et al. 1996b, Maze et al. 2007a). In these virtual structures, fibers lie horizontally in the plane of web according to a given fiber orientation distribution and length. There are two approaches to generate 2-D random structures: $\mu$-randomness method for generating a web of continuous fibers and $I$-randomness method for generating a web of staple fibers. These methods have been fully detailed and their use is justified elsewhere (Pourdeyhimi et. al 1996a; Pourdeyhimi et al. 1996b; Pourdeyhimi et al. 1997). For more details reader are refereed to the recent work of Maze et al. (2007a).

In the current research, we used the above-mentioned software for generating virtual structures (Maze et al 2007a). The software allows the user to generate 3-D fiber-webs of different diameters with different web basis weights. Figure 1.5a shows a virtual lightweight spun-bonded web, and Figure 1.5b shows a virtual wetlaid glass fiber mat (Maze et al 2007a).

![Figure 1.5: Virtual Nonwoven Media generated in Nonwoven Cooperative Research Center: a) Virtual Spunbonded filter; b) Virtual wet-laid staple fiber media](image)

Recently, Fraunhofer Institut Techno-und Wirtschaftsmathematik (ITWM), Germany has developed a new software program, GeoDict, dedicated to modeling transport phenomena in
fibrous structures. GeoDict allows the users to create random 3-D fiber geometry with given average properties, such as SVF, fiber length, and fiber diameter or fiber cross-section (GeoDict Manual, 2006). Using GeoDict, we will create structures with bimodal fiber diameters for a certain Solid Volume Fraction and fiber length. Figure 1.6a shows a bimodal filter and Figure 1.6b shows a fibrous filter having Z-orientations distribution generated by applying GeoDict.

Figure 1.6: Virtual Nonwoven Media generated by using Geodict Software: a) Virtual bi-modal media; b) Nonowoven media with fibers oriented in Z-direction.

A fiber-web obtained from typical web-forming processes has normally little or no strength. Such fiber-webs require further processing to make the individual fibers or filaments bond together. Bonding can be thermal, mechanical and chemical. In this study we pay a special attention to thermally bonded webs via a process called calendering. NCRC has developed a software program for simulating virtual mats of bonded fibers in 3-D space (Maze et al. 2007b). In order to simulate a spun-bonded nonwoven web suitable for compaction, the fibers are considered to have a square cross section and lay horizontally in the plane of the web and only in the x or y directions. In this software, the orientation of this fiber is chosen randomly but according to a given proportion, which allows the user to generate anisotropic fiber-webs where the number of fibers in the x-direction, for instance, is greater than those in the y-direction. Figure 1.7 shows the SEM images of a spun-bonded fabric made of Polypropylene fibers with an average diameter of
15 µm after calendering by smooth heated calender rolls with the simulating calendered fabrics. Note the similarities between the way fabrics appears to be densified at the top and bottom layers and left somewhat fluffy in the middle in the real fabric and the virtual model.

In Chapter 2, 3, and 4, the work of modelling air filtration by applying the virtual nonwoven media generated by NCRC virtual Nonwoven generator, NCRC calendered Nonwoven generator, and Geodict Porous Media software will be presented. The algorithm to generate virtual woven filtration media together with the air flow simulation will be discussed in Chapter 5.

1.3 – Aerosol Filtration

Various processes that occur on land or water surface or in the atmosphere itself can produce aerosols. Aerosol filtration, unsurprisingly, refer to the removal of solid and liquid particles suspended in air. Assuming a spherical shape, the size of aerosol particle is usually given as the diameter of the particle. Figure 1.8 shows particle size of common air contaminants.
Compared with hydrosol filtration, which is only influenced by interception, aerosol filtration is complicated, as shown in Table 1.1. There are four basic mechanisms by which an aerosol particle can deposit on a neutral fiber in aerosol filtration. These are interception, inertial impaction, Brownian diffusion, and gravitational settling (negligible in the case of nanoparticles).

**Table 1.1:** Capture Mechanisms of aerosol filtration and hydrosol filtration

<table>
<thead>
<tr>
<th></th>
<th>Flow Phase</th>
<th>Particle Phase</th>
<th>Capture Mechanisms</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aerosol</td>
<td>gas</td>
<td>solid/liquid</td>
<td>Interception</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Inertial impaction</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Diffusion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gravitational settling</td>
</tr>
<tr>
<td>Hydrosol</td>
<td>liquid</td>
<td>solid</td>
<td>Interception</td>
</tr>
</tbody>
</table>

The only real collection mechanism is interception. The interception of a homogenous spherical particle by a cylindrical fiber can be defined as (Lastow and Podgorski, 1998) “a particle is intercepted by a fiber when the distance from the center of mass of the particle to the fiber surface is equal or less than the radius of the particle”, as shown in Figure 1.9.
For aerosol filtration, the particles will derivate from their original streamline when they pass through a fibrous filter. The derivation is caused by the combination of particle inertia impaction and diffusion due to Brownian motion. Inertial impaction, as shown in Figure 1.10 can be defined as (Hinds, 1999) as “a particle, because of its inertia, is unable to adjust quickly enough to the abruptly changing streamlines near the fiber and crosses those streamlines to hit the fiber”.

**Figure 1.10:** Inertial impaction in air filter media [NOISH 2003]

Derivation of Brownian motion governs the particle trajectory when the particle is extremely small compared to the fiber size. During diffusion, particles do not follow their original streamline, and the erratic movement causes them to be contact with the fibers inside filter structures, as shown in Figure 1.11.

**Figure 1.11:** Brownian diffusion in air filter media [NOISH 2003]

The collection efficiency of a fibrous fiber can be defined as the fraction of entering particles that are retained by the filter, either based on particle count or mass. Figure 1.12 shows the collection efficiency curve of a fibrous filter with thickness $t = \text{mm}$, SVF $\alpha = 5\%$, fiber diameter $d_f = 2 \, \mu \text{m}$ and flow face velocity $V = 0.1 \, \text{m/s}$ (Hinds 1999). The combined effects of interception, inertial impaction and diffusion leads to a typical $V$–shape in the collection efficiency curve. This is because interception and initial impaction are the dominant for big particles while diffusion is dominant for small particles. The bottom point in the efficiency curve is referred to as the Most Penetrating Particle Size (MPPS), and ranges from 0.1 to 0.3 $\mu \text{m}$ for neural filters.
Figure 1.12: A typical fraction collection efficiency curve for filter media [Hinds, 1999]

The typical $V$-shape efficiency curve shifts based upon the type of filter and flow velocity. Generally speaking, when the fiber diameter decreases, the efficiency curve will shift to left and size of the $V$-shape will decrease and vise versa. For nanoparticle filtration, which diffusion is the dominant mechanism, the residual time for the particles and fibers to interact is extended with decreasing flow velocity (Kim, 2005) and collection efficiency increases. Inertial impaction increases when flow velocity increases.

1.4 – Evaluation of Filtration Performance

Fibrous filters are normally described and rated based on their collection efficiency $E$ and pressure drop $\Delta P$ (or permeability $k$). According to their end-use, filters have different requirements for their collection efficiency. Some filters are designed to have high collection efficiency (e.g., HEPA), while others are not. A good filter is the one that has minimum pressure drop (maximum permeability) for desired collection efficiency.
Collection efficiency can be defined as the fraction of entering particles that are retained by the filter based on either particle count or particle mass. Generally, count efficiency is lower than mass efficiency:

\[ E = \frac{N_{in} - N_{out}}{N_{in}} \quad 1-1 \]

\[ E_m = \frac{C_{in} - C_{out}}{C_{in}} \quad 1-2 \]

where \( N \) and \( C \) refer to the number and mass concentration, respectively of particles at inlet and outlet of the filters.

Another term, which characterized the ability of filter to capture particles, is its penetration \( P \). Penetration is defined as the fraction of entering particles that exist or penetrate the filter based on either particle count or particle mass.

\[ P = \frac{N_{out}}{N_{in}} \quad 1-3 \]

\[ P_m = \frac{C_{out}}{C_{in}} \quad 1-4 \]

Collection efficiency and pressure drop are two terms widely used in filtration literature. Another two parameters to evaluate filter performance are: Quality factor \( (QF) \) and Minimum Efficiency Reporting Value (MERV).

\( QF \) has been used in industrial as the indicator of filters performance considering both collection efficiency and pressure drop. \( QF \) is defined as:
\[ QF = -\ln[(1 - E)\times100]/\Delta P \]

We know that most of neutral fibrous filters become more efficient as they load with dirt. MERV is a number from 1 to 20 to evaluate lowest point of efficiency, which in most cases the moment the filter is just installed (NOISH 2003). The higher the value of MERV, the more efficient the air filters. MERV value is widely used in the industry: 1) low efficiency filters with MERV 1-4 are used to challenge particle with \( d_p > 10 \) μm; 2) filters with MERV 5-8 are used to remove particle with \( d_p \) ranging from 3 to 10 μm; 3) filters with MERV 9-12 are used to challenge particle with \( d_p \) ranging from 1 to 3 μm; 4) High efficiency filters with MERV 12-16 are used to remove particle with \( d_p \) ranging from 0.3 to 1 μm; 5) High efficiency filters with MERV 16-20 are used to remove the extremely small particle with \( d_p < 0.3 \).

There are two standard test methods currently used to evaluate the filters performance in the United States: ASHRAE 52.1-1992 (American Society of Heating, Refrigerating and Air Conditioning Engineering) and ASHRAE 52.2 –1999 (NOISH, 2003). ASHRAE 52.1-1992 measures filters ability to capture a mass fraction of coarse dust and filters ability to remove large particles. ASHRAE 52.1-1992 is suitable for low- and medium- efficiency filters. ASHRAE 52.2-1999 entitled “Method of Testing General Ventilation Air Cleaning Devices for Removal by Particle Size” is a more descriptive laboratory test method, which measures filters efficiency versus wide range of particle sizes. The sample filter, typically having face dimensions of 24” by 24”, is placed in a test dust in this newer stand test. Based on filter type, the airflow in the duct is set at a constant value ranging from 500 –3000 cfm. Aerosols in 12 sizes ranging from 0.3 to 10 μm are injected upstream of the sample filter and upstream particle number and downstream particle number are detected by particle counters. The test is capable of computing the collection efficiency for each of the 12 channels.
In this study, we use TSI 8130 and TSI 3160 to measure the filtration performance. In TSI 8130 polydisperse aerosols are pulled down through the filter by a vacuum pump. Two solid-state laser-based light scattering photometers measure the aerosol concentration upstream and downstream (TSI 8130 Manual 2000) and calculate the filter efficiency.

TSI 3160 is an automated filter tester that measures particle penetration versus particle size, as shown in Figure 1.13. TSI 3160 has the electrostatic classifier, the top right part of the machine shown in Figure 1.13, and the classifier produces particles of specific sizes. It classifies particles by their electrical mobility from the poly-disperse DOP and NaCl aerosols generated by atomizers. The particle sizes range from 15 nm to 400 nm (TSI 3160 Manual 2003).

![Figure 1.13: The model 3160 automated filter tester [TSI 3160 Manual 2003].](image)

A filter test can be initiated by installing a nonwoven media on the sample holder. Challenging flow with a known particle size is achieved by using atomizers and the electrostatic classifier. Upstream and downstream particle detection is accomplished by using two 3760A condensation particle counts (CPC), and filter penetration can be obtained. TSI 3160 is capable of measuring efficiencies better than 99.999999%. 

15
1.5 – Existing Theories of Filtration

In order to predict the filtration performance based on the structure of the filter we need to consider the flow pattern. Once the basic flow pattern is known, the pressure drop across the media can be obtained and the behavior of the injected particles inside the web can be derived, which leads to a better understanding of filtration process (Brown, 1993).

Whether the inertia or the viscosity of air dominates in filtration depends on the scale of the system and on the velocity of the air. The relatively importance can be determined by the Reynolds number, \( Re \):

\[
Re = \frac{\text{inertial force}}{\text{viscous force}} = \frac{\rho V L}{\mu}
\]

where \( \rho \) is air density and is approximately 1.20 kg/m\(^3\). \( \mu \) is coefficient of viscosity, which equals 1.81X10\(^{-5}\) at NTP. \( L \) is characteristic length and can be considered equivalent to pore diameter in this case. Reynolds number is used to identify different flow regime: very low \( Re \) indicates viscous creeping motion (inertial effects are neglected), moderate \( Re \) implies a smoothly varying laminar flow, and high \( Re \) indicates turbulent flow. For the flow velocity and the fiber diameter considered in this study, \( Re \) is low, the flow is laminar flow. For microfiber media filtration with low velocity, \( Re < 1 \), and the extreme case of laminar flow, inviscid flow is valid in which inertial influence is neglected and Reynolds number is assumed to be zero. An important property of inviscid flow is that the flow pattern does not change with the velocity (Brown, 1993).

In aerosol filtration system that a continuous fluid is valid, which means the molecular effects in airflow can be neglected, the obstacles in flow path are larger than the mean free path of air molecules (\( \lambda \)). If the flow is perpendicular to the webs are 3D layered structures, which most of nonwoven filters are, the obstacle length is actually fiber diameter (\( d_f \)). At NTP (Normal
Temperature and Pressure – air at 20°C and 1 atm), the flow is continuous when the fiber is above the sub-micrometer size. Detailed discussion will be provided later in this chapter (Brown, 1993).

After a mathematical model describing a fibrous filter is conducted, filters resistance to airflow can be calculated. Then, filter collection efficiency can be obtained after particle injection. During the past decades, there have been many pioneering studies, dealing with either a single fiber or a structured array of fibers, which have helped developing the filtration science and technology to its current level (Happel 1959; Kuwabara 1959; Stechkina and Fuchs 1965; Lee and Liu 1982; Brown 1984; Abdel-Ghani and Davies 1985; Overcamp 1985; Jackson and James 1986; Spurny 1986; Rao and Faghri 1988; Rodman and Lessmann 1988; El-Shoboskshy et. al, 1994; Ramarao et. al, 1994; Li and Park 1997; Termonia 1998; Dhaniyala and Liu 1999; ; Zhu et. Al, 2000; Thomas et. al, 2001; Lisowski et. al, 2001; Kirsh 2003). However, most of the previous studies have been limited to systems consisting of rows of fibers (often in two-dimensional geometries) perpendicular to the flow direction. To our knowledge, there has been no attempt in realistically simulating the filter’s disordered structure in a three-dimensional geometry. Moreover, the role of the filter structure and its relationship with performance of the media has not yet been established.

1.5.1 - Single Fiber Theory

It is difficult to analytically describe the flow field around fibers in the real fiber. Therefore, idealized flow fields have been applied. Knowledge about how particles deposit on single-fibers is of fundamental importance to deeply understand the filtration process (Lastow and Podgorski, 1998). This is because the single fiber is the smallest element in fibrous filter, and results of single fiber are always be extrapolated to describe the whole filter.
In single fiber theory, collection efficiency of the filter $E$ could be obtained by the single fiber efficiency $\eta$ by the following equation (Hinds 1999):

$$E = 1 - \exp(-\frac{4\alpha\eta t}{\pi d_f})$$  \hspace{1cm} (1-7)

in which $t$ is the thickness of the filter and $d_f$ is the fiber diameter.

As we mentioned in Section 1.3, among all the mechanisms, interception, inertial impaction and Brownian diffusion are three of the most importance for pure aerosol filtration of nanoparticle. The mechanical single fiber efficiencies can be calculated as long as each mechanism acts independently and less then 1.0:

$$E = 1 - (1 - \eta_R)(1 - \eta_D)(1 - \eta_I)$$  \hspace{1cm} (1-8)

in which $\eta_R$, $\eta_D$ and $\eta_I$ are the single fiber efficiency due to the interception, diffusion and inertial impaction, respectively (Hinds, 1999).

The arithmetic sum of efficiencies for these mechanisms $\eta = \eta_R + \eta_D + \eta_I$ can also be considered as an approximation of efficiency for the single fiber although it is not theoretically correct (Hinds, 1999). The arithmetic sum agrees with Eq.8 within 5% when there is only one dominant mechanism, which means none of other mechanism causes collection efficiency more than 1.

**1.5.2- Cell Model**

The neighboring fiber interference was first adequately taken into account by Kuwabara (1959) and Happel (1959). By setting different boundary conditions, Kuwabara (1959) and Happel (1959), independently, calculated the flow field in an ordered matrix of fibers in a so-called cell.
Both theories differ from the earlier isolated fiber models, since they consider the fiber in a finite space instead of an infinite space. For this reason, the effects of other fibers at the outlet are taken into account (Brown, 1993).

The cell model is based on the assumption that all fibers in the filter experience the same flow field and all fibers are perfectly perpendicular to the main flow direction. In spite of the restricting assumptions considered in their development, cell models have been widely used in the literature (Davies 1973; Lee and Liu 1982; Brown 1984; Brown 1989; Brown 1998). This is because simulating a fibrous structure and solving its flow field is difficult, which makes the cell models attractive for the users.

Kuwabara model has been proved to be a better representation of the flow around fibrous filter than Happel model by a lot of studies (Lee and Liu, 1982; Stechkina and Fuchs 1965; Pich 1965; Davies 1973; Lee and Liu 1982). The concept of Kuwabara of flow cells can be described as a filter consists of parallel fibers, spaced randomly traverse to the flow. Kuwabara solved the two dimensional viscous flow equations and obtained the velocity contour around a fiber. He assumed each fiber of radius $R_f$, shown in gray (Figure 1.14), was surrounded by an imaginary co-axial cylinder of radius $b$, shown in blue (Figure 1.14).

**Figure 1.14:** Cell model considers a fiber in a finite space
The imaginary cylinders touch each other. The areas outside imaginary cylinders are neglected, and SVF can be calculated as:

\[
SVF = \frac{R_f^2}{b^2}
\]

1-9

In Kuwabara cell model, the fibers are packed in a hexagonal arrangement, as shown in Figure 1.15. The stream function, \( \psi \) with in this region can be obtained by directly solving the biharmonic equation in cylindrical polar coordinate (Davies 1973):

\[
\nabla^4 \psi = 0
\]

1-10

The simplest solution is:

\[
\psi = (Ar + \frac{B}{r} + Cr \ln r + Dr^3) \sin \theta
\]

1-11

Where \( A, B, C, D \) are constants, which fixed by the boundary conditions.

Two of the boundary conditions are the radical and tangential velocities vanish at the fiber surface. The third condition is given by the fixed velocity at the \( r = b \) and \( \theta = \frac{\pi}{2} \). The fourth boundary condition used by Kuwabara was zero vorticity on the cylinder surface. Kuwabara assumed the positive vorticity on the upper side of the cell is canceled the negative vorticity on the bottom side of the cell, as shown in Figure 1.15 (Davies 1973).

![Diagram](image)

**Figure 1.15:** In Kuwabara flow cell, fibers are packed in a hexagonal arrangement and vorticity is assumed to be zero on the cell bounding lines [Kuwabara, 1959]
The stream functions $\psi$ of above-mentioned model:

$$\psi = \frac{vr}{2Ku} \left\{ 2 \ln \frac{r}{R_f} - 1 + \alpha + \frac{R_f^2}{r^2} \left( 1 - \frac{\alpha}{2} \right) - \frac{\alpha^2}{2 R^2} \right\} \sin \theta$$  \hspace{1cm} 1-12

where $v = \frac{V}{1-\alpha}$ is the mean velocity inside the filter and $Ku = -\frac{1}{2} \ln \alpha - \frac{3}{4} + \alpha - \frac{\alpha^2}{4}$ is Kuwabara hydrodynamic factor. On the cell bounding lines, where $r = b$, Equation 1-12 can be simplified as $\psi = vb \sin \theta = vy$. Figure 1.16 shows the streamline a filter with SVF of 0.05 based on this model (Davies 1973).

**Figure 1.16:** Flow pattern calculated according to Kuwabara cell model [Kuwabara, 1959]

### 1.5.2.1- Interception

The interception of a homogenous spherical particle by a cylindrical fiber can be illustrated in Figure 1.17: A particle, in green, is intercepted by a fiber, in gray, when the distance from the center of the particle to the center of the fiber is equal or less than the sum of the radius of the particle and the radius of the fiber. The values of $\theta$ and $r$ of limiting streamlines at the interception point, as shown in Figure 1.17, are equal to $\pi/2$ and $R_f + R_p$, respectively (Davies 1973).
As we discussed in 1.5.1, the flow through a fibrous filter structure is nearly always laminar. For this reason, the interception of single fiber efficiency is equal to the ratio of the distance between two limiting streamlines of the flow, $2y$, to the fiber diameter, $2R_f$.

$$\eta_R = \frac{y}{R_f} \quad 1-13$$

For any point on the cell surface in the cell model, as discussed before, we have $\psi = vy$. Hence, the single fiber efficiency due to interception can be expressed as (Davies 1973):

$$\eta_R = \frac{\psi}{vR_f} \quad 1-14$$

Let $\theta = \frac{\pi}{2}$ and $r = R_f + R_p$ in the stream function, we obtain

$$\eta_R = \frac{1+R}{2Ku} \left[ 2 \ln(1+R) - 1 + \alpha + \left(\frac{1}{1+R}\right)^2 \left(1 - \frac{\alpha}{2}\right) - \frac{\alpha}{2} (1+R)^2 \right] \quad 1-15$$

In which $R = \frac{R_p}{R_f}$, is a dimensionless function, called interception function.
There exist several approximate forms of Equation 1.15 (Lee and Liu 1982a; Natanson 1957), yet small discrepancies between those approximate forms and the original expression cannot be avoided. The most widely used approximation of the single fiber efficiency due to the interception nowadays is the simplified form obtained by Lee and Liu (1982a):

$$\eta_R = \frac{1 - \alpha}{Ku} \frac{R^2}{1 + R}$$  

1-16

1.5.2.2 - Inertial Impaction

For the aerosol filtration, the particles will derivate from their original streamline when they pass through a fibrous filter. One of the mechanisms to cause the derivation is particle inertia. The deviation happens when the particle, because of its inertia, is not able to adjust quickly enough to the changing streamlines near the fiber.

The influence of inertial impaction is determined by the Stokes number, which is defined as the ratio of the stopping distance of a particle to a characteristic dimension of the obstacle $Stk = \frac{\tau V}{d_c}$,

where $\tau$ is the relaxation time of the particle, which equals to $\frac{\rho_p d_p^2 c_c}{18 \mu}$, and $d_c$ is the characteristic dimension of the obstacle, which in the case of filtration is the fiber diameter $d_f$.

$C_c = 1 + Kn_p (1.257 + 0.4e^{-1.1/Kn_p})$ is an empirical correction factor called Cunningham slip correction factor and is used only for nanoparticles where the no slip condition on the wall is invalid (Hinds 1999). Here $Kn_p = \frac{2\lambda}{d_p}$ is the particle Knudsen number and

$$\lambda = \frac{RT}{\sqrt{2}N_a \pi d_m^2 p}$$ is the mean free path of the air molecules, where $d_m = 3.7 \times 10^{-10}$ m is the
The single fiber efficiency for inertial impaction will increase the \( Stk \) number by one of the following approaches: 1) increase the particle inertial; 2) increase the face velocity; (Hinds, 1999). The single fiber efficiency for impaction is given by following equation as (Lee and Liu, 1982a):

\[
\eta_i = \left( \frac{Stk}{2Ku^2} \right)^{1-17}
\]

Where \( J = (29.6 - 28\alpha^{0.62})R^2 - 27.5R^{2.8} \) for \( R < 0.4 \). There is no simple equation for \( J \).

For \( R > 0.4 \), \( J = 2 \) has been used as an approximation by Hinds (1999).

### 1.5.2.3 – Brownian Diffusion

As we discussed before, for the aerosol filtration, the particles will derivate from their original streamline when they pass through a fibrous filter. Besides inertial impaction, the derivation is also caused by diffusion due to Brownian motion. Derivation of Brownian motion governs the particle trajectory when the particle is extremely small compared to the fiber size. Stechkina and Fuchs (1965) are the first to use cell model to deal with the efficiency caused by Brownian motion. They tried to get the particle trajectory due to the Brownian motion by solving convective diffusion in the dimensionless coordinates. The single-fiber efficiency for this mechanism \( (\eta_d) \) achieved by the method mentioned above, can be presented as follows:

\[
\eta_d = 2.9K^{-1/3}Pe^{-2/3} + 0.624Pe^{-1}
\]
In which $Pe$ is the Peclet number, which equals to $\frac{\mu d_f}{D}$.

By using the method of boundary layer theory, Lee and Liu (1982a) shows another prediction of diffusion $\eta_d$ by using Kuwabara cell model:

$$\eta_d = 2.6\left(\frac{1-\alpha}{Ku}\right)^{1/3} Pe^{-2/3}$$

Lee and Liu claimed with the inclusion of the factor $1-\alpha$ in the theoretical expression, the results can be applied over a wider range of the condition, especially for the case when $\alpha$ is high. Actually, the dependence of $\eta_d$ on $1-\alpha$ is almost negligible since the under most circumstances, the solid volume fraction is very low for fibrous filter.

**1.5.2.4 – Corrections of Cell Theory**

It is obvious to see that collection efficiency of a fibrous filter is a function of a number of parameters of flow, particle and filter and can be easily calculated based on the equations by using cell model. However, a precise prediction of the collection efficiency requires the particle trajectory based on the flow to be solved for each fiber in the filtration medium, and to characterize the efficiency for single fiber by using the average result; Yet in the cell model the fibers inside the filter are treated the same way, even though there exist big difference among fibers (Brown, 1998).

Fibrous filter is actually an irregular structure. The inhomogeneities inside a fibrous filter cover several issues, such as the fibers inside the fiber are not necessarily perpendicular to the flow direction, solidity of the filter verifies with the location, there may exist a wide range of fiber
diameter distribution and etc (Brown, 1998). The correlations for the single fiber theory have been studied extensively for last decades.

The simplest method of the first categories of refinement is to introduce the inhomogeneity factor $\varepsilon$, which is normally the ratio of experiment data for some parameter to the prediction value, into the original prediction. For example, due to the non-uniform structure of fibrous filter, the single fiber efficiency of Brownian motion has discrepancy with the experimental data. In order to overcome the discrepancy, the theoretical prediction of $\eta_d$ can be corrected by dividing by the inhomogeneity factor (Lee and Liu 1982b; Dhaniyala and Liu 2001). The theoretical correlation based on Lee and Liu’s prediction is:

$$
\eta_d = \frac{2.6}{\varepsilon} \left(\frac{1-\alpha}{Ku}\right)^{1/3} Pe^{-2/3} \alpha
$$

where $\varepsilon = \frac{\Delta P_{\text{experiment}}}{\Delta P_{\text{theory}}}$. Theoretical prediction of pressure drop will be introduced in the later part of this chapter.

Lee and Liu did another interesting work of experiment-based correlation in 1982. Since collection efficiency due to inertial impaction is relatively small when compared with two other mechanisms and thus is neglected, Lee and Liu combined the $\eta_R$ and $\eta_d$ by arithmetic adding the single fiber efficiencies obtained from Eq.16 and Eq.19 respectively (Lee and Liu 1982b). They obtained the following equation:

$$
\eta = 2.6\left(\frac{1-\alpha}{Ku}\right)^{1/3} Pe^{-2/3} + \left(\frac{1-\alpha}{Ku}\right) \frac{R^2}{1+R}
$$

They used the experiment to determine the empirical factor $\beta_1$ and $\beta_2$ from the following relationship to take inhomogeneity into account:
\[ \eta = \beta_1 \left( \frac{1-\alpha}{Ku} \right)^{1/3} Pe^{-2/3} + \beta_2 \left( \frac{1-\alpha}{Ku} \right) \frac{R^2}{1+R} \]  

Based on the experimental results, \( \beta_1 \) and \( \beta_2 \) are found to be 1.6 and 0.6 respectively when the \( \varepsilon = 1.67 \).

Abovementioned approaches obtained an empirical or semi-empirical factor, such as inhomogeneity factor and empirical factor, however these methods did not identify the influences of different inhomogeneity issues. There have been several efforts to correct the collection efficiency by solving the discrepancy owning to a certain inhomogeneity issue. Currently, the different inhomogeneities in a filter media can be considered as: 1) three dimensionality of the structure or z-direction distribution of the fiber; 2) packing density variation; 3) poly-modal of the fiber diameter distribution (Dhaniyala and Liu, 2001).

In cell model, the fluid flow around the cylindrical fiber is assumed to be a two-dimensional filed. In this respect, then angle between the fiber axis and main flow direction (z-axis) is assumed to be 90 degree. However, this assumption is not necessary to be accurate since the individual fibers may have different z-orientation, and this may cause the discrepancy in the theoretical and experimental values of collection efficiency. In order to study to z - direction fiber distribution, Schweers and Loffler (1994) subdivided a filter into a series of elements with different structural characteristics, defined by local directionally dependent permeabilities and resulting three-dimensional flow is calculated. By using collection efficiency predictions from cell mode, local particle collection can be obtained. However, this adapted model has not been strongly supported by its experimental work.
Nonwoven media have significant variation in local Solid Volume Fraction. These variations affect the flow field inside a filter structure. Clarenburg and Wal (1966) measured the media performance based on the distribution of the pore size. Lajos (1985) numerically solved the flow field inside a filter with different local solid volume fraction, and calculated the average velocity. The results show that the average velocity increases when media inhomogeneity increases. Lucke and Adam (1994) studied the relationship with inhomogeneity and the most penetrating particle size of the media.

None of the above mentioned work systematically describes how the Solid Volume Fraction of fibrous filter influences the collection efficiency. Dhaniyala and Liu (2001) introduced a simplistic theoretical modeling approach to account for the variation in Solid Volume Fraction of the fibrous filters and to estimate their effect on the collection efficiency. In their study, the fibrous filters are assumed to be consisted of cells having varying solid volume fraction, which having a log-normal probability density function \( g(\alpha, \sigma_g) \). The collection efficiency of each cell \( E(\alpha) \) is obtained by:

\[
E(\alpha) = 1 - \exp\left(-4\frac{\alpha \eta(\alpha)t}{\pi d_f}\right)
\]

in which single fiber efficiency \( \eta(\alpha) \) is calculated by applying cell model. The total collection efficiency \( E_{\text{total}} \) is then can be obtained from cell efficiency \( E(\alpha) \), local flow rate \( U(\alpha) \), average flow rate \( \bar{U}(\alpha) \):

\[
E_{\text{total}} = 1 - \frac{\int U(\alpha)}{U(\alpha)} [1 - E(\alpha)] g(\alpha, \sigma_g) d\alpha
\]
The values of $U(\alpha)$ and $\bar{U}(\alpha)$ can be calculated from pressure drop. The adapted model seems to fit the experimental data for some specific fibrous filters under certain operating conditions (Dhaniyala and Liu, 2001).

Most filtration theories deal with filter consisted of fibers with certain diameter. In real world, staple-fiber filters, such as carded, air-laid and wet-laid fabrics, are with a range of distribution in fiber diameter. Several works on theoretical and numerical modeling have been done to refine the cell model to be applied to the filters of poly-modal distribution of fiber size (Dhaniyala and Liu, 2001; Kirsch and Stechkina, 1973; Brown 1984; Brown and Thorpe 2001). In Kirsch and Stechkina’s work (1973), they modeled the poly-modal filter by using rows of parallel cylinders with different diameters arranged perpendicular to the flow section. From their study, it seems the pressure drop and the particle deposition of Brownian diffusion can be calculated from the mean cylinder radius even if there exits big difference in fiber diameters.

1.5.3 – Arrays Model

Single fiber theory is the simplest credible quantitative approach to describe the filtration process in fibrous filters. However, nonwoven media has an irregular structure that cell theory cannot describe. Even though a lot of studies have been done to refine this model, there is no theory exists give a good account for all the problems (Brown 1998). A regular array of parallel fibers is another theoretical approach to describe the filtration process. Among array structures having various arrangements, channel array and stag array structures, as shown in Figure 1.18 are two of the most importance in filtration modeling (Brown 1998).
Cell model needs two parameters to define a structure, fiber diameter \( d_f \) and Solid Volume Fraction \( \alpha \). The bi-harmonic equation \( \nabla^4 \psi = 0 \) for cell model was comparatively easy to solve because the boundary conditions were set at either fiber radius or the cell radius. Simplest array models, such as channel array and staggered array, require three parameters for a full description: fiber diameter \( d_f \), solid volume fraction \( \alpha \) and the ratio of the inter-fiber spacing \( Y \) to interlayer spacing \( X \) (Brown 1998). Figure 1.19 shows the solution domain of the channel array model.

As we just mentioned, array models have three parameters and need to have a higher – order stream function to satisfy five boundary conditions instead of four in the cell model. The work of Sangani and Acrivos (1982), gave the new stream function by solving series bi-harmonic
equations for Stokes Flow, and obtained the hydrodynamic factor for both channel arrays model and stag arrays model, respectively:

\[ K_{\text{channel}} = -\frac{1}{2} \ln \alpha - 0.738 + \alpha - 0.887\alpha^2 + 2.038^3 \]  

\[ K_{\text{stag}} = -\frac{1}{2} \ln \alpha - 0.745 + \alpha - \frac{1}{4}\alpha^2 \]

Another work solved the flow field of arrays model by using extension of cell model approach was done by Drummond and Tahir (1984),

Variational method approach is to directly use of Helmholtz’s principle, by finding flow pattern which gives rise to the lowest rate of energy dissipation by viscous drag. The advantage of this approach is that a continuous stream function throughout the solution domain can be obtained in a simple analytical form (Brown 1993). Figure 1.20 shows the streamlines calculated by Brown for channel arrays model and stag arrays model, respectively.

Figure 1.20: Streamline calculated by variational method for channel arrays model and stag arrays model, respectively. [Brown, 1993]

The most popular approaches for solving the flow through an array of fibers are based on numerical methods. The flow pattern through channel arrays and stag arrays can be solved by finite element, finite difference or finite volume methods. In these numerical methods, a mesh is set up and the solution of the flow equations is carried out at each point (finite element and finite
difference) or each volume (finite volume). The advantage of this approach is that the flow pattern in the solution domain is realistic without any arbitrary boundary condition (Brown, 1998). Henry and Ariman (1983) numerically solved flow field inside the stag array model and Rao and Faghri (1988) obtained the flow pattern of the channel array model by numerically solving the full Navier-Stokes equations.

1.5.4 – Pressure Drop and Slipping Effect

The important assumption in the above-mentioned studies is that the relative velocity of the gas at the surface of the fibers is zero, which is not met for small fibers at NTP. Slipping effect must be considered for small fibers whose size is comparable with the mean free path of air molecules (Davies, 1973).

Four different regimes can be distinguished in the gas flow based on the value of the Knudsen number $\frac{2\lambda}{d_f}$: 1) free molecule regime ($Kn > 10$); 2) Transient regime ($10 > Kn > 0.25$); 3) Slip flow regime ($0.25 > Kn > 0.001$); 4) Continuum regime ($Kn < 0.001$). Several studies have been carried to predicting the collection efficiency and pressure drop of these regimes (Pich, 1966; Dawson, 1969, Pich, 1972). Most of these works were carried out with paper filters used with high flow rates and may not obey the Darcy’s law. Problems with high Knudsen number still include the calculation of the particle motion through the lower atmosphere or higher temperature condition (Davies, 1973).
For a continuous flow, a filter’s pressure drop is a function of air viscosity, filter thickness, face velocity, fiber diameter, and a parameter, \( f(\alpha) \), being only a function of the filter Solid Volume Fraction (SVF) (Hinds, 1999).

\[
\Delta p = f(\alpha) \frac{\eta U}{d_f^2}
\]

\( f(\alpha) \) has different forms according to different theories. For example, for the Kuwabrara’s cell model, \( f(\alpha) \), can be represented by (Hinds, 1999):

\[
f(\alpha) = \frac{16\alpha}{Ku}
\]

For the channel arrays model, \( f(\alpha) \) based on Rao and Faghri (1988) numerically solution is expressed as:

\[
f(\alpha) = 10.54\alpha + 157.36\alpha^2 + 578\alpha^3
\]

By solving series of bi-harmonic equations for Stokes flow, Sangani and Acrivos (1982) obtained another expression for the channel arrays model:

\[
f(\alpha) = \frac{16\alpha}{K_{\text{channel}}} = \frac{16\alpha}{-\frac{1}{2}\ln \alpha - 0.738 + \alpha - 0.887\alpha^2 + 2.038^3}
\]

For the staggered arrays model, \( f(\alpha) \) based on the numerical study conducted by Henry and Ariman (1983) is:

\[
f(\alpha) = 9.784\alpha + 152.64\alpha^2 + 555.6\alpha^3
\]

Sangani and Acrivos (1982) obtained another expression for the stag arrays model:
\[ f(\alpha) = \frac{16}{K_{stag}} = \frac{16}{-\frac{1}{2} \ln \alpha - 0.745 + \alpha - \frac{1}{4} \alpha^2} \]

Even though attempts are often made to justify the good correlations by theoretical models, yet some of the most successful permeability models are based on pure empiricism (Davies 1973, Brown 1993, Hinds 1999). Davies’s experimental correlation is obtained to calculate the pressure drop of a variety of filter media with SVF ranging from 0.6% to 30% (Davies 1973). Dimensionless pressure drop based on Davies’ correlation is:

\[ f(\alpha) = 64\alpha^{3/2}(1 + 56\alpha^3) \]

Pich (1971) summarized theoretical findings for pressure drop over all values of Knudsen number. One of the most important relationships is that the pressure drop across the filters, \( \Delta P \), is dependent on the pressure drop across the filter when \( Kn = 0, \Delta P_0 \). For \( Kn < 0.001 \),

\[
\frac{\Delta P_0}{\Delta P} = 1
\]

For 0.25 > \( Kn > 0.001 \),

\[
\frac{\Delta P}{\Delta P_0} = \frac{1 + \frac{0.998Kn_0}{-0.75 - 0.5\ln\alpha}}{1 + \frac{0.998Kn}{-0.75 - 0.5\ln\alpha}}
\]

where \( Kn_0 \) is the Knudsen number of the fibers at maximum pressure, which is usually one atmosphere.

For \( Kn > 10 \),

\[
\frac{\Delta P}{\Delta P_0} = 1
\]
\[
\frac{\Delta P}{\Delta P_0} = \frac{0.57}{Kn} \left( -0.75 - 0.5 \ln \alpha + 0.998 Kn_0 \right)
\]

No theory exists for the transition regime for \( 10 > Kn > 0.25 \), and the schematic dependence is shown in Figure 1.21, which X-coordinate is the operating pressure and Y-coordinate is the pressure drop, \( \Delta P \).

![Figure 1.21](image)

**Figure 1.21:** A schematically dependence of the pressure drop across the filters on the operating pressure of fibrous filter with low solid volume fraction [Pich 1971].

The slip effect influence on single fiber efficiency in slip flow region can be accounted by correlating the diffusion and interceptions term by slip correction factors \( C_d \) and \( C_R \), respectively (Dhaniyala and Liu 1999)

\[
\eta = \beta_1 \left( \frac{1 - \alpha}{Ku} \right)^{1/3} Pe^{-2/3} C_d + \beta_2 \left( \frac{1 - \alpha}{Ku} \right) \frac{R^2}{1 + R} C_R
\]

where \( C_d = 1 + 0.388 Kn \left( \frac{1 - \alpha}{Ku} \right)^{1/3} \) and \( C_R = 1 + \frac{1.996 Kn}{R} \).
Another two terms to describe the pressure drop across a fibrous fiber is air resistance and permeability. The term air resistance is often used for the pressure drop across a filter at some arbitrary flow rate. Hence, the resistance, $W$, is

$$W = \frac{\Delta P}{Q}$$

Where $Q = \frac{U}{A}$ is the flow rate. $A$ is the area of the cross-section of the sample.

The second term is permeability. Based on Darcy’s law (only valid for slow, viscous flow), permeability, $k$, is inversely proportional to the pressure drop:

$$k = \frac{U \mu}{\Delta P}$$

1.6-Thesis Overview

During the past decades, there have been many pioneering studies, dealing with either a single fiber or a structured array of fibers, which have helped developing the filtration science and technology to its current level. However, most of the previous studies have been limited to systems consisting of rows of fibers (often in two-dimensional geometries) perpendicular to the flow direction. To our knowledge, there has been no attempt in realistically simulating the filter’s disordered structure in a three-dimensional geometry. Moreover, the role of the filter structure and its relationship with performance of the media has not yet been established.

The current study is the first step in developing an understanding of the role of filter geometry and fiber type as well as manufacturing process in the efficiency of filter media. According to Brown (1998), there has been no theory so far which takes the above parameters into account.
when predicting the performance of a filter. A Case Study of Simulating Submicron Aerosol Filtration via Spun-bonded Filter Media was reported in Chapter 2. In this study, for the first time, a virtual 3-D web is generated based on the fiber orientation information obtained from analyzing microscopic images of lightweight spun-bonded filter media. Pressure drop and collection efficiency of our virtual filters are simulated and had excellent agreement with experiment.

Filters have been used in different applications, and for this reason, there are different requirements of the collection efficiency for filters. For example, HEPA filters need to have high collection efficiency for small particles while filters using in the swimming pool are fine with low collection efficiency for small particles. However, low pressure drop is always a critical requirement. Chapter 3, Chapter 4 and Chapter 5 focus on developing the understanding of the role of filter geometry on the pressure drop of uni-modal nonwoven media, bi-modal nonwoven media and woven filters, respectively.
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CHAPTER 2

AEROSOL FILTRATION VIA LONG-FIBER FILTER MEDIA

(SPUNBONDED NONWOVEN)

This chapter is modified from a manuscript entitled “A Case Study of Simulating Submicron Aerosol Filtration via Spun-bonded Filter Media”, by Q. Wang, B. Maze, H. Vahedi Tafreshi, and B. Pourdeyhimi, and has been published in Chemical Engineering Science, 61, 4871-4883 (2006).
2.1-Introduction

The rising awareness of environmental agencies and the general public for a clean environment together with demands of many advanced industries, such as electronics, medical, pharmaceutical, and biological research, have urged the filtration industry to investigate on ways to improve the indoor air quality for the past decades (Maynard and Kuempel 2005). The most common method of removing particles from a gas stream is via fibrous filters which are generally characterized by two basic parameters: collection efficiency and pressure drop. During the past decades, there have been many pioneering studies, dealing with either a single fiber or a structured array of fibers, which have helped developing the filtration science and technology to its current level (Happel 1959; Kuwabara 1959; Stechkina and Fuchs 1965; Lee and Liu 1982; Brown 1984; Abdel-Ghani and Davies 1985; Overcamp 1985; Jackson and James 1986; Spurny 1986; Rao and Faghri 1988; Rodman and Lessmann 1988; El-Shoboskhy et. al, 1994; Ramarao et. al, 1994; Li and Park 1997; Termonia 1998; Dhaniyala and Liu 1999; Zhu et. Al, 2000; Thomas et. al, 2001; Lisowski et. al, 2001; Kirsh 2003). However, most of the previous studies have been limited to systems consisting of rows of fibers (often in two-dimensional geometries) perpendicular to the flow direction. To our knowledge, there has been no attempt in realistically simulating the filter’s disordered structure in a three-dimensional geometry. Moreover, the role of the filter structure and its relationship with performance of the media has not yet been established. This is probably because of the difficulties involved in generating 3-D structures similar to that of a filter media as well as calculating the particle capture efficiency when the geometry is too complex. The current study is the first step in developing an understanding of the role of filter geometry (e.g., non-uniformity and fiber orientation distribution) and fiber type (length and diameter) as well as manufacturing process in the efficiency of filter media. According to Brown (1998), there has been no theory so far which takes the above parameters
into account when predicting the performance of a filter. In this work, we simulated the filter collection efficiency and pressure drop in a series of three-dimensional virtual spun-bonded nonwovens generated based on our nonwovens characterization techniques (Pourdeyhimi et. al 1996a; Pourdeyhimi et. al 1996b; Pourdeyhimi et. al 1997).

Spun-bonding is a manufacturing technique, which offers a one-step process for producing nonwovens from the raw materials (thermoplastic polymers) as the fiber and fabric production are combined. In spun-bonding, filaments are extruded from multiple banks of spinnerets. These filaments are then drawn to their final diameters (about 20 micrometer) by two high-speed air-jets and laid down onto a porous substrate, as shown in Figure 2.1. Because of their sticky surface, fibers tend to form weak bonds with each other at the crossovers in a spun-bonded web. However, these webs, normally, need to undergo a compaction process (hot or cold compaction rolls) before they can be winded. The basis weight, $W_b$, (defined as the mass per unit of area) and thickness of the spun-bonded fabrics typically range lie between 10 to 200 g/m$^2$ and 0.1 to 2 mm, respectively. Spun-bonded fabrics are known for having continuous fibers (infinite length) as the filaments do not break up during the attenuation process.

![Figure 2.1: Schematic drawing of the spun-bonding process](image)
In this chapter, we first study the structure of spun-bonded Nonwovens and then investigate on their submicron efficiency and pressure drop. We compare our study with the well-known available 2-D models and experimental data, and effect of calendaring on the permeability.

In the next section, the analytical models from the literature will be briefly introduced. Section 2.3 describes the numerical scheme used for solving Navier-Stokes equations and particle tracking inside the filter. Simulation results and experimental data of un-bonded spun-bonded media are presented in section 2.4 followed by the further discussion of the calendaring effect on spun-bonded fabric in section 2.5. The conclusions are presented in section 2.6. Note that our algorithm for generating spun-bonded webs has been briefly presented in Chapter 1

### 2.2- Analytical Models

There are four basic mechanisms by which an aerosol particle can deposit on a neutral fiber. These are interception, inertial impaction, Brownian diffusion, and gravitational settling (negligible in the case of nanoparticles, Lee and Liu 1982, Rao & Faghri 1988, Kirsh 2003, Maynard and Kuempel 2005). The total particle collection efficiency of a filter is the result of a combination of all these mechanisms. To predict collection efficiency of fibrous filters, efficiency of a single fiber has been extensively investigated during the last decades. The influence of the neighboring fibers in calculating Single Fiber Efficiency (SFE) was first taken into account by Kuwabara (1959) and Happle (1959). By setting different boundary conditions, Kuwabara (1959) and Happle (1959), independently, calculated the flow field in an ordered matrix of fibers in a so-called cell. The cell model is based on the assumption that all fibers in the filter experience the same flow field (no fiber falls into the wake of the others) and all fibers are
perfectly perpendicular to the main flow direction. In spite of the restricting assumptions considered in their development, cell models have been widely used in the literature (Davies 1973; Lee and Liu 1982; Brown 1984; Brown 1989; Brown 1998; Boulaud and Renoux 1998). This is because simulating a fibrous structure and solving its flow field is difficult, which makes the cell models attractive for the users.

Based on the Kuwabara’s cell model if the flow pattern and web structure are known, the filter efficiency \( E \), can be calculated from SFE, \( E_\Sigma \) (Hinds 1999).

\[
E = 1 - \exp\left(-\frac{4 \alpha E_\Sigma t}{\pi d_f}\right)
\]

where \( \alpha \) is the Solid Volume Fraction (SVF), \( t \) is the thickness of the filter, and \( d_f \) is the fiber diameter.

The total SFE, \( E_\Sigma \), can then be obtained as the sum of SFE due to interception \( E_R \), inertial impaction \( E_I \), and Brownian diffusion \( E_d \) (Hinds 1999).

\[
E_\Sigma = 1 - (1 - E_R)(1 - E_I)(1 - E_d)
\]

SFE due to the interception \( E_R \), is given as (Lee and Liu 1982):

\[
E_R = \frac{1+R}{2Ku} \left[ 2\ln(1+R) - 1 + \alpha + \left(\frac{1}{1+R}\right)^2 \left(1 - \frac{\alpha}{2}\right) - \frac{\alpha}{2}(1+R)^2 \right]
\]

in which \( Ku = -\frac{\ln \alpha}{2} - \frac{3}{4} + \alpha - \frac{\alpha^2}{4} \) is the Kuwabara’s hydrodynamic coefficient and \( R = d_p / d_f \) is the particle-to-fiber diameter ratio where \( d_p \) is the particle diameter. SFE due to inertial impaction \( E_I \), is given by (Lee and Liu 1982):

\[
E_I = \frac{(Stk)J}{2Ku^2}
\]
Where \( J = (29.6 - 28a^{0.62})R^2 - 27.5R^{2.8} \) for \( R < 0.4 \) and \( Stk = \frac{\rho_p d_f^2 CV}{18 \eta d_f} \) is the Stokes number, defined as the ratio of particle stopping distance to the fiber diameter (Hinds 1999). Here \( \rho_p \), \( \eta \), and \( V \) are particle density, air viscosity, and the flow velocity, respectively.

\( C_c = 1 + Kn_p (1.257 + 0.4e^{-1.1/Kn_p}) \) is an empirical correction factor called Cunningham slip correction factor and is used only for nanoparticles where the no slip condition on the wall is invalid (Hinds 1999). Here \( Kn_p = \frac{2 \lambda}{d_p} \) is the particle Knudsen number and \( \lambda = \frac{\bar{R} T}{\sqrt{2 N_a \pi d_m^2 p}} \) is the mean free path of the air molecules, where \( d_m = 3.7 \times 10^{-10} \) m is the collision diameter of the air molecules. \( p \) and \( T \) are the air pressure temperature, respectively. \( N_a \) and \( \bar{R} \) are the Avogadro number and the universal gas constant, respectively. The smaller the particle, the greater is the slip correction factor. Note that the higher the slip, the weaker is the coupling between the particles and the carrier gas and therefore, the trajectory of a particle is expected to have a greater deviation from its original streamline.

Using the Kuwabara cell model, Lee and Liu (1982) obtained an expression for the SFE of Brownian diffusion, \( E_d \):

\[
E_d = 2.6(1 - \frac{\alpha}{Ku})^{1/3} Pe^{-2/3}
\]

in which \( Pe = Vd_f / D \) is the Peclet number, \( D = \frac{\sigma C_c T}{3 \pi \eta d_p} \) is the diffusion coefficient, and \( \sigma = 1.38 \times 10^{-23} \) m\(^2\)s\(^{-2}\)K\(^{-1}\) is the Boltzmann constant. It is worth mentioning that Stechkina and Fuchs (Spurny 1986; Rao and Faghri 1988) derived a similar expression independent of the based on Kuwabara’s model. Their expression however, predicts almost the same collection efficiency as that of Lee and Liu (1982). Note that there are various expressions for each capture
mechanism in the literature. Here we considered only the most recent and well-known theoretical expressions based on Kuwabara flow field.

As mentioned before, pressure drop is another important parameter used to characterize a filter. In the literature, the filter’s pressure drop is a function of air viscosity, filter thickness, face velocity, fiber diameter and dimensionless pressure drop \( f(\alpha) \) (Rao and Faghri 1988).

\[
\Delta p = f(\alpha) \frac{\eta V}{d_f^2}
\]  \hspace{1cm} 2-6

Dimensionless pressure drop is only a function of SVF, \( \alpha \), and has different forms based on different theories. The Happel’s cell model (1959) results the following expression for the dimensionless pressure drop:

\[
f(\alpha) = \frac{16\alpha}{-0.5\ln\alpha - 0.5 \frac{1 - \alpha^2}{1 + \alpha^2}}
\]  \hspace{1cm} 2-7

For the Kuwabara’s cell model (1959), \( f(\alpha) \) can be represented by:

\[
f(\alpha) = \frac{16\alpha}{Ku}
\]  \hspace{1cm} 2-8

Henry and Ariman (1983) numerically solved the flow field around a staggered array of parallel cylinders to model the fibrous filter. Their dimensionless pressure drop is expressed as:

\[
f(\alpha) = 2.446\alpha + 38.16\alpha^2 + 138.9\alpha^3
\]  \hspace{1cm} 2-9
Another numerical study was conducted by Rao and Faghri (1988). The dimensionless pressure drop based on their work is:

\[ f(\alpha) = 2.653\alpha + 39.34\alpha^2 + 144.5\alpha^3 \]

2-10

Davies’s experimental correlation is obtained to calculate the pressure drop of the filter media and is proven to be accurate for a SVF range of 0.6% - 30%. Dimensionless pressure drop based on Davies’s correlation can be represented by (Davies 1973):

\[ f(\alpha) = 64\alpha^{3/2}(1 + 56\alpha^3) \]

2-11

In this study, we use well-known traditional 2-D models for comparison with our data obtained from simulation of 3-D virtual filter media. The following chapter describes our algorithm for generating virtual media.

2.3 -Aerosol Flow Modeling

As has been mentioned in Chapter 1, we know that SVFs of NCRC virtual Nonwoven media are only a function of the size of the sample being generated. Increasing the width of the box in our algorithm can cause a reduction in the SVF. In order to find the sample size that can resemble a real spun-bond fabric of a given basis weight (here 14.6 g/m²) and SVF (here 2.8%), we generated spun-bonded webs of 14.6-g/m² in square boxes with different size. The fiber diameter is kept constant at 16 micron (see Figure 2.2). The rapid decrease in the SVF with increasing sample size is evident. From Figure 2.2, one can see that the relevant sample size for simulating a spun-bonded media with a SVF of 2.8% is about 0.5 mm. As will be discussed soon in this section, the above dimensions are foreseen to simulate a real spun-bonded filter nonwoven having
a fiber diameter of 17 micron, a basis weight of 16.3 g/m², SVF of 3.05% and a thickness of 0.55mm (see Figure 2.3).

**Figure 2.2**: SVF and thickness of the media is shown versus the sample size. Fiber diameter is 16 micron.

**Figure 2.3**: A microscopic image of the spun-bonded media considered in this study. Average fiber diameter, web thickness, and basis weight are found to be 17 micron, 0.55mm, and 15.3 g/m², respectively. SVF is calculated to be 3.05%
A steady state laminar incompressible model has been adopted for the flow regime inside our virtual filter. The finite volume method (Patankar 1980) implemented in Fluent code is exploited to solve the airflow field. The governing equations: continuity, conservation of linear momentum, and energy written in vectorial form are as follow:

\[
\frac{D \rho}{Dt} + \rho \nabla \cdot V = 0 \tag{2-12}
\]

\[
\rho \frac{DV}{Dt} = -\nabla p - \eta \nabla \times (\nabla \times V) + \frac{4}{3} \eta \nabla (\nabla \cdot V) \tag{2-12}
\]

\[
\rho c_p \frac{DT}{Dt} = -\frac{DP}{Dt} + \Phi + \kappa \nabla^2 T \tag{2-13}
\]

In the above equations, \(\Phi\), \(k\), and \(c_p\) represent, viscous dissipation (negligible at low speeds), thermal conductivity, and the specific heat of air. Gambit, a preprocessor for Fluent code, is used in this work for meshing the aforementioned filter structures. The coordinate of the cylindrical objects (fibers) in the virtual filter are exported to Gambit via a journal file. The journal file describes all the operations needed to reconstruct the 3-D nonwoven structure in Gambit. The imported geometry is then meshed using tetrahedral elements, refined close to the fiber surfaces.

Note that for a given \(W_b\), thickness of the web, \(t\), increases by increasing the size of the box. To further check on the algorithm, we plotted the SVF of these webs versus their thickness, \(t\) in Figure 2.4 in a log-log scale. As expected, product of SVF and thickness is a constant \((a \times t \times \rho_f = W_b = 14.6g \, m^2)\). Results shown in Figure 2.2 and 2.4 are averaged over an ensemble of 10 webs.
Irregular structures, such as nonwoven media, have a wide range of pore sizes. 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 the gap between two fibers around their crossover point is often too small. The computational grid used for CFD 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 an infinite computational power. The smaller the relative angle between two fibers, the harder is meshing their contact areas if the total number of cells is to be kept constant (less than about 3,200,000 here). In order to circumvent these meshing issues, the diameter of the fibers was slightly increased, while maintaining their positions. This caused the fibers to interpenetrate, thus changing their contact points (or lines) to contact areas, which reduces the skewness of the cells. Increasing the fiber diameter, however, increases the SVF of the structure. By trial and error, a compromise was reached at a 6% increase in the fiber

Figure 2.4: The relation between the thickness and SVF of filter media having a basis weight of 14.6 g/m² and a fiber diameter of 16 micron.
diameter, for an increase of 12% in the SVF, which brings it to 3.1%. This is the reason why we considered a fiber diameter of 16 micrometer while our targeted real media has an average fiber diameter of 17 micrometer.

Boundary conditions considered for the simulations are shown in Figure 2.5. Air is assumed to flow into the simulation domain through a velocity-inlet and leaves it from a pressure-outlet boundary condition. The inlet boundary condition is placed at a distance $L$ upstream of the filter to insure the particles are not released in an area affected by the flow field about the fibers. We used a distance of $L = 20d_f$ based on the study reported by Wang and Jaroszczyk (1991), which indicates that at such a distance upstream of a fiber, the particles can be assumed to be in an undisturbed flow field.

![Figure 2.5: The simulation domain and boundary conditions are shown.](image)

As can be seen from Figure 2.5, we have used symmetry boundary condition for the sides of the computational box, even though there is no plane of symmetry in a disordered fibrous structure. This boundary condition is considered for the simulations because we did not have any
information regarding the flow velocity and/or pressure inside of the structure prior to the simulations. Considering symmetry boundary conditions should be acceptable 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., \( Kn_f = \frac{2\lambda}{d_f} \ll 1 \), where \( Kn_f \) is the fiber Knudsen number, \( \lambda \) is the mean free path of the air molecules (about 60 nm).

Fluent stores the results of discrete calculations at the cell centers. The values for the cell faces should be obtained by interpolation between the cell center values. To help the solution reach the convergence, we started with a first-order upwind scheme for the above-mentioned interpolation. Once the solution approached a stable condition, we switched to the second order upwind to increase the accuracy.

Once the particle-free flow field is obtained, the airborne particulates, modeled by rigid spheres of uniform density \( \rho_p = 1000 \text{kg/m}^3 \) (unit-density) are then introduced into 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.

In the Lagrangian method, the force balance on a particle is integrated to obtain the particle position in time. The dominant forces acting on the nanoparticles are drag force exerted by the flow and the Brownian force:
\[
\frac{dv_{i_p}}{dt} = F_d(v_i - v_{i_p}) + F_b
\]

where \( v_i \) and \( v_{i_p} \) are the field and particle velocity in the \( x \), \( y \), or \( z \) direction. \( F_d \) and \( F_b \) are amplitudes of the drag (for \( \text{Re}_p = \frac{\rho d_p V_d}{\eta} < 1 \)) and Brownian force given as:

\[
F_d = \frac{18\eta}{d_p^2 \rho_p C_c}
\]

and

\[
F_b = \frac{18 \mu \zeta_i}{d_p^2 \rho_p C_c} \sqrt{\frac{2\nu}{\Delta t Sc}}
\]

where \( Sc \) is the Schmidt number defined as \( Sc = \frac{3\pi d_p \eta \nu}{C_c \sigma T} \), \( \zeta_i \) are zero-mean, unit-variance independent Gaussian random numbers. The nanoparticle trajectory calculation implemented in Fluent code is originally developed by Ahmadi and his co-workers (Ounis et al. 1991; Li and Ahmadi 1992; Ounis and Ahmadi 1990).

At the atmospheric temperature and pressure, inertial impaction can be ignored for nanoparticles at low and moderate air filtration velocities. Moreover, interception plays a significant role in the filtration process, only if \( d_p \) and \( d_f \) are comparable. When \( d_p / d_f << 1 \), the interception can be always ignored; this is the case in the present work, since in the range of particles considered (50 to 500 nm), \( d_p / d_f \) is always much smaller than unity. However, in the case of nanofiber-filters, interception is an important capture mechanism which greatly improves the filter efficiency. The influence of interception and inertial impaction in total filtration efficiency is shown in Figure 2.6 for a filter having a SVF of 3.1%, thickness of 0.57 mm, and a fiber diameter of 17 micrometer using the Kuwabara’s cell model presented in section 2.2. It can be seen that the collection efficiency is only due to the influence of the Brownian diffusion.
Figure 2.6: Collection efficiency of one of the filter media considered in this study based on cell model predictions. A comparison is shown between the three capture mechanisms of Brownian diffusion, inertial impaction and interception showing the dominance of the Brownian diffusion. $d_f = 17$ micron, $t = 0.57$ mm, SVF = 3.1%.

2.4 - Results and Discussion

Efficiency of a filter is determined by the number of particles it can remove from an aerosol flow:

$$E = \frac{N_{in} - N_{out}}{N_{in}}$$  \hspace{1cm} (2-17)

where $N_{in}$ and $N_{out}$ are the number of entering and exiting particles, respectively. In our steady-state simulations, we introduce a certain number of particles upstream of the filter and follow their trajectories as they flow through the filter. We then compare $N_{in}$ and $N_{out}$ to calculate the filter efficiency.

As mentioned before, in order to simulate the aerosol flow through a filter media, the virtual structure should be meshed. Figure 2.7a shows a typical mesh on one of the symmetry planes.
Prior to making any conclusions from the CFD results, one should make sure that the results are not mesh dependent. In this respect, we considered one of our virtual media (shown in Figure 17) and studied the effect of mesh density on the capture efficiency and pressure drop. To do so, we increased the number of mesh points on the perimeter of the fibers. Starting from 6, the number of mesh points was increased up to 18 as shown in Figure 2.7b.

Figure 2.7: An example of the generated mesh on one of the symmetry boundaries is shown in (a). Note the fibers with 9 and 18 grid points on their perimeter shown in (b).
We also increased the number of mesh points on the edges of the simulation box with almost the same proportion to control the skewness of the cells. The results of mesh density analysis are presented in Figure 2.8 for collection efficiency and Figure 2.9 for pressure drop.

**Figure 2.8:** The influence of the mesh density on the filter collection efficiency (SVF=3.1%, \( t=0.57 \) mm)

**Figure 2.9:** The influence of the mesh density on the filter pressure drop (SVF=3.1%, \( t=0.57 \) mm)
As it can be seen, increasing the mesh density results in an initial reduction in the collection efficiency. However, further increase in the mesh count beyond 15 points did not show any significant changes. Similar trend is evident in the pressure drop calculation. For the present work, an 18-point mesh was used for all the structures to insure the accuracy of the calculations even though 15-point mesh could be also acceptable.

We also studied the influence of particle concentration of the incoming aerosol flow on the collection efficiency calculations. We challenged the abovementioned filter with different particle concentrations of $N_{in} = 800$, 8000, 80,000, and 240,000 particles/cm$^3$. To do so, we injected certain number of particles at the box inlet (0.5 mm × 0.5 mm) calculated according to the number of particles that may encounter the filter in the unit of time if the filter is challenged with an aerosol flow having a concentration of $N_{in}$ and a face velocity of $V = 0.05$ m/s.

![Figure 2.10: The influence of the inlet aerosol concentration on the filter collection efficiency (SVF=3.1%, $r=0.57$ mm)](image)

Figure 2.10: The influence of the inlet aerosol concentration on the filter collection efficiency (SVF=3.1%, $r=0.57$ mm)
Figure 2.10 shows the filter collection efficiency versus the particle size for the above inlet concentrations. It can be seen that concentration of the aerosol does not have any significant influence on the results beyond a concentration of $N_{in} = 8000$ particles/cm$^3$. We used a concentration of $N_{in} = 80,000$ particles/cm$^3$ for the simulations reported in this study.

Figure 2.11: Top view of the media subsections considered in our CFD simulations (a to h) along with an image taken from the real filter media (i). SVF of each subsection is shown for comparison.
We generated a series of eight 0.5 mm × 0.5 mm spun-bonded virtual fiber webs having a SVF close to the targeted value of 3.1% and fiber a diameter of 17 micrometer. Figure 2.11 shows the top view of these media together with an image taken randomly from the real media.

Each of the structures is challenged with different monodisperse aerosols having a particle size ranging from 50 nm to 500 nm. Two different face velocities of 0.05 and 0.10 m/s have been considered. Note that for such a face velocity and the range of particles considered, the particle Reynolds numbers, $Re_p$, are always smaller than unity.

Velocity vectors colored by the velocity magnitude in Figure 2.12a show the airflow field inside one of the above structures. Fibrous filters are inhomogeneous structures and this leads to the variation of the flow field inside the filter. Figure 2.12b is an example of particle trajectories in the filter media. Here for the illustration purposes we injected 100 particles of 100 nm diameter all from a straight line.

**Figure 2.12a:** Velocity filed shown with velocity vectors inside a 3-D virtual filter.
Figure 2.12b: Trajectory of particles released from a line through the structure.

Figure 2.13 shows the average collection efficiency of the filter versus particle diameter along with the predictions of the Kuwabara’s cell model. It can be seen that the filter collection efficiency is decreased by increasing the particle size in the range of 50nm to 500 nm.

Figure 2.13: Collection efficiencies for two different face velocities of 0.1 and 0.05 m/s are shown. Kuwabara’s cell model predictions are also presented for comparison.
The collection efficiency predicted by our simulations follow a trend very similar to that of the Kuwabara’s cell model. However, there seems to be a slight difference between the two predictions. Experimental verifications, therefore, are needed to judge the accuracy of the models. To this end, we used a filter tester, TSI 8130, from TSI Inc. to verify the collection efficiencies obtained from the modeling. In TSI 8130 poly-disperse aerosols are pulled down through the filter by a vacuum pump. Two solid-state laser-based light scattering photometers measure the aerosol concentration upstream and downstream (TSI Manual) and calculate the filter efficiency.

Ten replicates of the medium discussed in this paper (see Figure 2.11) have been exposed to aerosol flow at two different flow rates corresponding to the targeted face velocities. TSI 8130 uses Diethylhexyl Phthalate (DOP) aerosols with a size distribution shown in Figure 2.14 (TSI Manual).

![Figure 2.14: Particle size distribution of the aerosol used in TSI 8130](image)
Individual efficiencies for each particle size, ranging from 50 to 500 nm, are multiplied by their corresponding probability functions from Figure 2.14. Such information is gathered from the eight structures shown in Figure 2.12 and their average value is compared with the experimental data from TSI 8130 (see Table 2.1). We followed an identical procedure to calculate the filter efficiency from the Kuwabara’s cell model and reported the average value in Table 2.1 for comparison. Experimental data seem to fall between our CFD simulations and the cell model predictions with a closer agreement with the CFD results. Note that in our simulations, as well as the Kuwabara’s cell model, particle rebound from the fiber surface is not considered. This assumption, of course, is not entirely true for the experiments. The over-prediction of the CFD results shown here can also be attributed to this assumption. It should be noted that the results presented here are only valid for the SVF, filter thickness, and the fiber diameter considered and are not meant to be generalized.

Table 2.1: Comparison between the collection efficiencies of the present work, Kuwabara’s cell model, and TSI 8130. Modeling inputs: \( df = 17 \) micron, \( t = 0.57 \) mm, SVF = 3.1\%. Real media: \( df = 17 \) micron, \( t = 0.55 \) mm, SVF = 3.05\%.

<table>
<thead>
<tr>
<th></th>
<th>( V = 0.05 ) m/s</th>
<th>( V = 0.1 ) m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment</td>
<td>3.23</td>
<td>2.52</td>
</tr>
<tr>
<td>Present Work</td>
<td>4.93</td>
<td>3.31</td>
</tr>
<tr>
<td>Cell Model</td>
<td>1.64</td>
<td>1.05</td>
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In Figure 2.15, we presented the filter pressure drop obtained from simulating the structures shown in Figure 2.11 along with the predictions of previous analytical and numerical models. The empirical correlation obtained by Davies (1973) is also presented for comparison using exactly the same SVF, thickness, and fiber diameter. 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 (Brown 1984; Davies 1973; Dhaniyala and
Liu 1999). The pressure sensors in the TSI 8130 are not sensitive enough to detect tiny pressure drops when the filter media is very thin and so are not taken into account in this work.

**Figure 2.15:** Pressure drop calculation from our CFD simulations compared with the Kuwabara’s cell model and the empirical equation’s of Davis (1973), a) $V=0.05\text{m/s}$, b) $V=0.1\text{m/s}$
2.5 - Conclusions

In this work, we presented a case study of simulating filtration of nanoparticles via thin spun-bonded filters. The ultimate goal of a study like the one reported here is to build a relation between the properties of the media (fiber type, manufacturing process, and filter structure) and its filtration efficiency, and the current work is only the first step toward this goal.

The numerical simulations presented were obtained by solving the Navier-Stokes equations inside a virtual 3-D filter media constructed in accordance with the real features of spun-bond nonwovens. Pressure drop of our CFD simulations are in a perfect agreement with the Davies’s empirical correlation unlike the previously published models based on 2-D fiber arrangement. Our simulations, in agreement with the Kuwabara’s cell model, showed that the collection efficiency of a spun-bonded filter having a fiber diameter of 17 micron, an average SVF of 3.1%, and an average basis weight of 14.6 g/m² is higher for smaller particles in the range of 50 nm to 500nm. We also demonstrated that the collection efficiencies are higher for smaller face velocities. Our simulated collection efficiencies were compared with the predictions of the Kuwabara’s cell model and TSI 8130 filter tester. Experimental data were found to be between the predictions of the cell model and our simulations with a closer agreement with the CFD results for the particular SVF, thickness, and the range of particles and fiber diameters considered in this case.

The current work builds a platform for conducting further virtual experiments on filter media. Future works will be simulating multi-layer media, each layer consisting of fibers with different diameters and/or length.
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CHAPTER 3

INVESTIGATION OF UNI-MODAL FILTER PRESSURE DROP:

FIBER LENGTH & COMPACTION RATIO

This chapter are take from a manuscript entitled “Simulating Through-plane Permeability of Fibrous Materials Having Different Fiber Lengths”, by Q. Wang, H. Vahedi Tafreshi, and B. Pourdeyhimi, and has been published in Modeling and Simulation in Materials Science and Technology, 15(8), 2007, and a manuscript entitled “Simulating Permeability of 3-D Calendered Fibrous Structures” by S. Zobel, B. Maze, Q. Wang, H. Vahedi Tafreshi, and B. Pourdeyhimi, and has been published in Chemical Engineering Science, 62(22), 6285-6296 (2007).
3.1-Through-plane Permeability of Fibrous Materials Having Different Fiber Lengths

Assuming that fibers can be represented as straight cylinders, an algorithm for generating virtual 3-D layered fibrous media made up of fibers having identical diameters but different lengths is presented. It is shown that for a given basis weight and computational box (sample size), reducing the fiber length causes the Solid Volume Fraction (SVF) to increase as the fibers pack next to one another more efficiently. The air permeability of these media is numerically simulated and discussed in detail with respect to the available 2-D and 3-D studies in the literature. Our permeability calculations show an excellent agreement with the predictions of the empirical equation of Davies (1973) as well as the analytical model of Spielmann and Goren (1968). Such an agreement indicates that, within the range of dimensions considered, the fiber length has no significant influence on the materials’ through-plane permeability as long as the SVF remains constant. While this concept has been empirically observed in the past, our work is the 1st numerical simulation devised to confirm it.

3.1.1-Introduction

Nonwoven fibrous materials such as filters, papers, wipes, insulators, etc. have enormous industrial applications. For many applications, nonwovens’ through-plane permeability is an important property. Nonwovens are made by assembling short or infinitely long fibers (continuous filaments) on top of one another and bonding the same by mechanical, thermal, or chemical means. Manufacturing nonwovens typically consist of three major steps; fiber production, fiber-web (fiber assembly) formation, and fiber bonding. The fiber-web structure has a major role in determining the final properties of the end product. Generally speaking, one can produce nonwovens having different properties by using fibers with different diameters, lengths, or cross-sectional shapes. Nonwoven materials can be engineered to efficiently serve their
specific application if realistic models are used to predict their properties prior to the manufacturing process. Numerical simulation offers attractive opportunities for exploring structure-property-relationships and identifying dominant structural features that control the material’s behavior.

There are a number of attempts in the literature dealing with the 3-D simulation of the structure of disordered fibrous materials for the purpose of studying their properties. The works of Rodman and Lessmann (1988), Zhu et al. (1997), Clague and Phillips (1997), Tomadakis and Robertson (2005), Faessel et al (2005) are among those dedicated to the modeling of the 3-D structure of nonwovens and paper boards. In the above 3-D models fibers were allowed to penetrate into one another at their crossovers. Fiber interpenetration can serve as a controlling parameter that allows one to generate fibrous media structure with relatively high SVFs. To the knowledge of the authors, the first published work to report fiber-to-fiber contact and bending without fiber interpenetration is that of Niskinen and Alava (1994). These authors focused on short fiber assemblies, as in the case of paper boards, and assumed the fibers to be randomly distributed in the domain but only oriented in two orthogonal directions of \( x \) and \( y \). Their fibers, being designed for Lattice-Boltzmann simulations (same as that the work of Qi and Uesaka, 1995), were made up of large numbers of cubes placed next to one another resulting in fibers with rectangular cross-sections. Note that without fiber interpenetration or bending the generated 3-D fiber-webs will have relatively low SVFs.

In our previous publications (Wang et al., 2006; Maze et al., 2007), we simulated the filter collection efficiency and pressure drop in a series of 3-D virtual fiber-webs, made up of infinitely long fibers (spunbonded and electrospun filters), generated based on our nonwovens characterization techniques (Pourdeyhimi et al., 1996a; Pourdeyhimi et al., 1996b; Pourdeyhimi
et al., 1997). In the current study, we report on our through-plane permeability simulations obtained for fibrous media consisting of short fibers with varying lengths. Wet-laid nonwovens and ordinary paper boards are typical examples of materials made up of short fibers of varying lengths. In these cases, short fibers are dispersed in water and then deposited on and compressed against a porous belt to form a web.

This section has been modified from a manuscript has been submitted to “Modeling and Simulation in Materials Science and Technology”. In section 3.2.2, we discuss the influence of the fiber length and simulation box on the Solid Volume Fraction (3-D layered fiber-web generation algorithm has been introduced in previous chapter). Section 3.2.3 describes the numerical simulation scheme considered for solving Navier-Stokes equations. Results and discussions are presented in section 3.2.4.

3.1.2- Virtual 3D Webs Having Various Fiber Lengths

The SVF of the virtual webs made by our algorithm, mentioned in Chapter 1, is independent of their basis weight (weight per unit area), as expected. In Figure 3.1a and b SVF is plotted versus basis weight for different sample sizes. Figure 3.1a presents a series of fiber-webs with a fiber length of 3 mm and diameter of 15µm while shown in Figure 3.1b is the SVF of fiber-webs made up of 20µm-fibers with a length of 0.75 mm.

As it can be seen, the SVF is invariant with the basis weight and increasing the number of fibers per unit area of the sample only increases the thickness of the web as expected. SVF, however, is a function of the size of the sample being generated when the basis weight is kept constant. Increasing the width of the box in our algorithm causes the SVF to decrease if the fiber length and basis weight are kept constant (Wang et al., 2006; Maze et al., 2007). Note that the same is not
true for the case of having a constant box width and decreasing the fiber length, as will be discussed later in this paper.

**Figure 3.1**: SVF of the samples having different basis weight for different sample sizes. It can be seen that SVF is independent of the basis weight and varies only with the size of the simulation box. a) Fiber length and diameter are 3 mm and 15µm, b) fiber length and diameter are 0.75 mm and 20µm, respectively.
It is worth mentioning that SVF of a real nonwoven fiber-web is independent of the sample size as long as the sample size is sufficiently larger than the smallest length scale in the medium. Unlike the case of infinitely long fibers (Wang et al., 2006; Maze et al., 2007; Zobel et al., 2007), webs made up of short fibers have a well-defined length scale, i.e., fiber length. For such fiber-webs sample size should not be a parameter influencing the SVF. However, same as the case of infinitely long fibers (filaments), sample size does influence the SVF of the web if the sample size is smaller or close to the fiber length. Increasing the width of the box can cause a reduction in the SVF of the web if the sample size is not sufficiently greater than the fiber length. In a previous publication we demonstrated that this dependency becomes progressively weaker by increasing the sample size while keeping the fiber length constant (Pourdeyhimi et al., 2006) In the virtual structures presented here sample size is not large enough to observe size-independent SVFs. This is solely due to the fact that conducting CFD simulations on large samples require formidable amount of computational memory.

3.1.3- Flow Field Simulation

In order to study the relationship between the media’s structural parameters (e.g., fiber length and SVF) and their through-plane permeabilities, we generated a series of 3-D virtual nonwovens with fiber diameter of 19µm. A steady state laminar incompressible model has been adopted for the flow regime inside our virtual media. Note that 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 the inertial effects are negligible. The finite volume method (Patankar, 1980) implemented in Fluent code is exploited to solve continuity and conservation of linear momentum in the absence of inertial effects:
\[ \nabla \cdot V = 0 \]
\[ \nabla p = \eta \nabla^2 V \]

where \( V \), \( p \), and \( \eta \) represent flow velocity, pressure, and viscosity, respectively. Gambit, a preprocessor for Fluent code, is used in this work for meshing the aforementioned fibrous structures. The coordinate of the cylindrical objects (fibers) are exported to Gambit via a journal file. The journal file describes all the operations needed to reconstruct a 3-D nonwoven structure in Gambit. The imported geometries are then 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 the gap between two fibers around their crossover point 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 an infinite computational power. The smaller the relative angle between two fibers, the harder is meshing their contact areas if the total number of cells is to be kept. In order to circumvent these meshing issues, the diameter of the fibers was slightly decreased, while maintaining their positions. This slightly increases the distance between the fibers at the crossovers and, thus, reduces the skewness of the computational cells. Note that, in general, reducing the fiber diameter is the best way to circumvent the meshing difficulties. This, however, causes the medium’s SVF to reduce. Increasing the fiber diameter on the other hand increase the SVF of the medium but it does not always help the meshing. Here, our fiber-webs were initially generated with fibers having a diameter of 20 \( \mu \text{m} \) but their diameters were eventually decreased to 19 \( \mu \text{m} \) in order to ease the meshing procedure. This 5% reduction in the fiber diameter cause a decrease of about 10% in the media’s SVF.
The boundary conditions considered for the simulations are shown in Figure 3.2. Air is assumed to flow into the simulation domain through a velocity-inlet and leaves it from a pressure-outlet boundary condition. Note that, in general, uniform flow inlet and outlet boundary conditions should be placed far from the regions where strong velocity and/or pressure gradients are expected. As it has been discussed in our previous work (Wang et al., 2006) placing the inlet or outlet boundary conditions too close to the media’s surface can result in inaccurate pressure drop predictions. Here inlet boundary conditions here are placed at a distance $L > 10d_f$ upstream of the media.

It is important to ensure that the sample size considered for the permeability simulations is large enough in such a way that the pressure drop values are not dependent on the size of the simulation box at a given SVF. Here we used the Brinkman screening length criterion which is given by $\sqrt{k}$ where $k$ is permeability of the medium (Clague and Phillips, 1997; Clague et al., 2000) According to Clague and Phillips (1997), a box size about 14 times larger than the Brinkman’s length is sufficient to smooth out the local heterogeneities. To obtain an estimate of the relevant sample size, Davies equation has been used.

As can be seen from Figure 3.2, we have used symmetry boundary condition for the sides of the computational box, even though there is no plane of symmetry in a disordered fibrous structure. Note that if the sample size is large enough such a boundary condition will not affect the simulation results as the flow is mainly in the through-plane direction and lateral flows are negligible. It is worth mentioning periodic boundary conditions need to be considered if sample size is not large enough to ignore the flow in the lateral directions (Koponen et al., 1998).
Figure 3.2: The simulation domain and boundary conditions are shown

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. Defining the Knudsen number based on the mean intercept length, \( Kn = \lambda / \bar{d} \), we obtained a range of \( 6 \times 10^{-5} < Kn < 4 \times 10^{-4} \) which confirms the assumption of continuum flow through the media (Tomadakis and Dupani, 2007). Here \( \bar{d} = -d_f / \ln(1-\alpha) \), \( d_f = 19 \mu m \), and the range of SVFs considered is from 0.02 to 0.11.

3.1.4- Results and Discussion

As mentioned earlier, the nonwoven media were meshed via Gambit program. Figure 3.3 shows a typical mesh on one of the symmetry planes of the simulation box. To find out about the acceptable ranges of grid size, one of our virtual media was meshed with different interval sizes
and its pressure drop was calculated accordingly. Note that we also increased the number of mesh points on the edges of the simulation box with almost identical proportion to control the skewness of the cells. These results are normalized with the mesh-independent pressure drop and shown in Figure 3.4). As it can be seen, increasing the mesh density on the perimeter of a fiber results in an insignificant change in the permeability of the medium beyond a value of about 15. The results reported in this paper are obtained with more than 15 grids points around the perimeter of each fiber.

Figure 3.3: An example of the generated mesh on one of the symmetry boundaries is shown.
To compute the permeability of nonwoven fiber-webs having different fiber lengths, we generated a series of 1 mm × 1 mm structures with a diameter of 19 µm and a basis weight of 18 g/m². Figure 3.5a shows the top view of these media. The fiber length varies from 0.1 mm to 0.75 mm. Note that keeping the simulation box (sample size) and basis weight constant, the SVF decreases by increasing the fiber length (see Figure 3.6). This is because when fibers are smaller, they pack more efficiently (the thickness of the media decreases by decreasing the fiber length).
Figure 3.5a: Top view of the media considered in our CFD simulations.

The case of $l_f = 0.1$ mm and $l_f = 0.3$ mm is shown in Figure 3.5b from two different view points.

The increase in the media’s thickness by increasing the fiber length is evident.
Figure 3.5b: The side and isometric views of fabrics with 0.1 mm (a) and 0.3 mm (b) in $l_f$ shows that the thickness of the fabrics increases with increasing the fiber length.

Figure 3.6: SVF versus $l_f$ for media with fixed box (sample) size and fiber diameter.
The media shown in Figure 3.5a are virtually exposed to air flow with a face velocity 0.05 m/s. Velocity vectors colored by the velocity magnitude in Figure 3.7 show the airflow field inside one of the above structures. Fibrous media are inhomogeneous structures and this leads to the spatial variation of the flow field. Permeability of the above structures is determined from the difference between the pressures at the inlet and outlet. In the literature, the pressure drop is considered to be a function of air viscosity and velocity as well as the medium’s thickness and fiber diameter:

\[ \Delta p = f(\alpha) \frac{\eta tV}{d_f^2} \]  

3-3

where \( t \) is the medium’s thickness. The dimensionless pressure drop, \( f(\alpha) \), is only a function of SVF, \( \alpha \), and has different forms based on different theories.

**Figure 3.7:** An example of the velocity field inside our 3-D media.
Note that the above equation is based on the assumption that \( f(\alpha) \) is strictly a function of SVF. Such an expression may be valid only if there is a good separation of scales between the thickness of generated samples and the local heterogeneities. Otherwise, a thickness-dependence may exist. To address this concern we calculated the layer-averaged SVF of all the fiber-webs considered in this study and studied the variation of these averaged SVFs across the thickness of the media (plots not shown for brevity). No strong indication of thickness-dependency was observed in the SVF profiles – as expected from the real fiber-web. We also devised two sets of simulations where five fiber-webs of identical parameters \( (l_f = 0.6 \text{ mm}, \ d_f = 19\mu\text{m}, \text{sample size} = 0.5\text{mm}) \) were generated with two different basis weights of 10 and 20 g/m\(^2\) (corresponding to thickness of 0.41 mm and 0.84 mm, respectively). Pressure drop values obtained from these simulations were observed to be different with a factor of two which indicate existing of a linear proportionality between the pressure drop and basis weight (thickness) of the media.

The most well-known expression for dimensionless pressure drop is from the experimental work of Davies (1973). His empirical correlation is proven to be accurate for a SVF range of 0.6% to 30%:

\[
f(\alpha) = 64\alpha^{3/2} (1 + 56\alpha^3)
\]

Spielman and Goren (1968) have developed a very successful analytical model capable of predicting the permeability of fibrous materials with different spatial fiber orientations. For the case of materials having fibers laid randomly in the planes perpendicular to the direction of the superficial flow, Spielman and Goren (1968) proposed the following expression for the permeability, \( k = \frac{d_f^2}{f(\alpha)} \).
where $K_0$ and $K_1$ are modified Bessel functions of the second kind, and $r_f$ is the fiber radius.

Figure 3.8 shows the results of our numerical simulations obtained for the abovementioned structures along with the predictions of the empirical correlation of Davies [1] and the analytical model of Spielman and Goren (1968). It can be seen that pressure drop increases by increasing the SVF of the material when the fiber diameter is kept constant. Moreover, it can be seen that there is a very good agreement between our CFD simulations and the previous studies. Such an agreement has also been observed for the media made up of infinitely long fibers in our previous work (Wang et al., 2006). This good agreement indicates that within the range of fiber lengths considered in this study, fiber length has no influence on the media’s permeability if the SVF is kept constant and our paper serves as the first numerical simulation to confirm this fact.

**Figure 3.8:** Pressure drop calculation from our CFD simulations compared with the Kuwabara’s cell model, and the empirical equation’s of Davis (1973), and analytical expression of Spielman and Goren (1968). Face velocity is $V=0.05m/s$
It is worth mentioning that there are several 2-D periodic models that have been developed in the past decades for the purpose of simulating an air filter’s performance, i.e., collection efficiency and pressure drop (Kuwabara, 1959; Henry and Ariman, 1983; Rao and Faghri, 1988 amongst many works) or power-law fluids (Idris et al., 2005; Lundstrom et al., 2006). For the completeness of the study, we have plotted the predictions of the Kuwabara’s famous cell model in Figure 3.8 as an example of the 2-D models for comparison. In Kuwabara’s model

\[ f(\alpha) = \frac{16\alpha}{Ku} \]

in which \( Ku = -\frac{\ln \alpha}{2} - \frac{3}{4} + \alpha - \frac{\alpha^2}{4} \). As pointed out by Rodman and Lessman (1988) and Dhaniyala and Liu (1999), all 2-D models underestimate the in-plane permeability of a fibrous medium.

### 3.1.5 – Conclusions

In this work an algorithm for generating virtual 3-D structure of un-bonded fiber-webs is presented. Fibers are assumed to be cylindrical and deposited on top of each other with no nonphysical interpenetration. It was shown that for a given basis weight and computational box (sample size), reducing the fiber length causes the Solid Volume Fraction (SVF) of the material to increase. This is because short fibers can more efficiently pack into a give box size. The air permeability of these media is numerically simulated and compared with the well-know experimental and analytical studies in the literature. It was shown that permeability decreases by increasing the SVF of the material when the fiber diameter is kept constant. Our permeability calculations showed a perfect agreement with the predictions of the Davies’ empirical equation (1973) and the analytical model of Spielmann and Goren (1968). This indicates that at least for a range of 0.1 mm < \( l_f < 0.75 \) mm considered in this work, the fiber length has no considerable influence on the materials’ permeability as long as SVF is kept constant. While this concept has
been empirically observed in the past, our work is the 1st numerical simulation devised to demonstrate it.

3.2 – Permeability of Media Having Different Compaction Ratio

Fibrous filters such as nonwoven materials are often consolidated by various approaches, i.e., hot compaction rolls. Hot calendering compresses the fiber assembly and can cause changes in the structure. Calendering causes a significant increase in the Solid Volume Fraction (SVF) of the media and therefore, affects the compaction ratio and thus their permeability. To our knowledge, no work in the literature has been dedicated to modeling the permeability of the calendered nonwovens. In this study, virtual nonwoven structures are generated and compressed from top and bottom to resemble the hot calendering process. The dimensionless permeability of the calendered media is computed using CFD tools and reported for different compaction ratios. Results of our simulations are compared with the experiment as well as the available empirical and/or analytical permeability models in the literature and good agreement, depending upon the SVF, is observed.

3.2.1– Experiments: Calendered Spunbonded Media

Our objective in this section is to study the permeability of the nonwoven materials before and after the calendering process. In this process, an un-bonded web is passed through the nip of two rolls pressed against each other at a desired pre-set pressure and heated internally to a desired temperature (see Figure 3.9). The nip pressure of the calendar brings the fibers together to cause fusion of filaments/fibers at their cross-over points. Bonding is accomplished through three critical steps: 1) heating the web to partially melt the crystalline regions, 2) diffusion of the newly released chain segments across the fiber-fiber interface, and 3) subsequent cooling of the web to cause its re-solidification and to trap the diffused chain segments. The degree of fiber-to-fiber
fusion in the bonding spots determines the final strength of the bond and ultimate properties of the fabric. Calendaring results in a consolidated, well-bonded sheet of fabric. Calendering is often used with nonwovens produced via spun-bonding, which has been briefly introduced in Chapter 2.

**Figure 3.9:** Schematic drawing of smooth calender bonding.

In order to study the influence of compaction ratio, we produced spun-bonded fabrics made of Polypropylene fibers with an average diameter of 15 µm with different basis weights ranging from 20 to 100 g/m². These fabrics were compacted using heated smooth calender rolls in NCRC’s pilot nonwoven laboratory. Three different temperatures of 105, 120, and 135°C and three different nip pressures of 200, 400, and 600 pounds per linear inch (pli) were considered in the experiments. Note that nip pressure is normally shown in force per unit length of the line of contact between the rolls, i.e., width. Influence of the calendering temperature and pressure is shown in Figure 3.10 where a given fabric has been calendered under different conditions. It can be seen that by increasing the nip pressure, the SVF of the fabric increases. It also shows that increase the rolls temperature leads to an increase in the SVF. Changing the rolls temperature and pressure here was only a means of increasing the SVF of the nonwoven media. The data shown in Figure 3.10 are averaged over all the basis weights considered. This is because, as discussed in section two, the SVF of a nonwoven fabric is independent of its basis weight. This is also confirmed experimentally in our preliminary experiments (not shown). It is worth mentioning that a similar argument is valid even if the fabrics have been calendered. If the calender's settings are
fixed, no matter what the basis weight (thickness), the resulting fabrics will have, within some statistical error, an identical SVF if their fiber diameters are the same. This is because in a typical calender, a feedback control system, depending on the thickness of the incoming fabric, adjusts the gap between the two rolls in such a way that the given nip pressure is achieved. Therefore, no matter what the thickness, all the fabrics are compacted with the same compaction ratio and will have an identical SVF.

Figure 3.10: Influence of the calendering temperature and pressure on the SVF of spun-bonded fabrics

Figure 3.11 shows three SEM images of a above mentioned spun-bonded fabric made of Polypropylene fibers with an average diameter of 15 µm after calendering by smooth heated calender rolls. The spun-bonded fibers were produced and calendered in the pilot spinning laboratory of the Nonwovens Cooperative Research Center at NC State University. Note the changes in the fabrics’ density across the thickness in Figure 3.11c. Fabric appears to be densified at the top and bottom layers and left somewhat fluffy in the middle. Then, the media were tested
by KES-F8-API air permeability tester, and the obtained results have been shown in Figure 3.13 together with the predicted values from both analytical and numerical studies.

**Figure 3.11:** SEM images of a spun-bonded fabric after calendering from different views.

### 3.2.2– Simulation: Calendered Spunbonded Media

In this section, we generate virtual spun-bonded nonwovens and simulate their structural changes during the calendering process at different compaction ratios (the ratio of the original to final thicknesses). The permeability of the media is then calculated at each step of compaction by computing the resistance of the fabric against a uniform laminar air flow. Note that the algorithm for generating spun-bonded nonwovens and their compaction has been introduced in chapter 1.
Note also that the numerical scheme used for solving Navier-Stokes equations inside the filter is the same as the one applied in 3.2.3.

To simulate the effect of compaction on the media’s permeability five uncompressed samples were generated, according to the aforementioned algorithm (see chapter 1). These structures were made up of 100 fibers with a length of 40 units, laid down randomly in the $x$ or $y$ directions. The thickness of these structures, being statistically a function of the fiber deposition procedure, happened to vary between 43 and 50 units. These structures were compressed to different final thickness of 25, 17, 13, 10, and 8 units. Increasing the compaction ratio, $C_r$, defined as the ratio of the final to original thicknesses here, causes SVF of the calendered media to increase. Figure 3.12 shows a fluffy structure compacted to different thicknesses. It can be seen that by increasing the compaction ratio from one to five, the SVF increases from 4.5% to 25%.

![Figure 3.12: A fluffy structure compacted to different degrees of compaction ratios. It can be seen that by increasing the compaction ratio from 1 (a), 2 (b) to 5 (c), SVF increases from 4.5% (a), 10% (b) to 25% (c).](image)

The air flow through the abovementioned nonwovens is simulated assuming that the fibers are 10µm in diameter. This means the media simulated here is 0.4 mm × 0.4 mm. The air is assumed to flow with a face velocity of 0.05 m/s. The fabrics’ permeability constants are calculated via the
Darcy’s law. These results are non-dimensionalized by the fiber radius and presented in Figure 3.12 along with the experimental results obtained. It can be seen that by increasing the SVF, the dimensionless permeability decrease, as expected. Note, however, that there is good agreement between the simulation results and the experimental data. Note also that the spun-bonded fabrics are often nonuniform (patchy). This means that the thickness may change from point to point and this can cause the experimental data to greatly scatter. To circumvent this problem we eliminated the values that were too far from the expected range. We also compared our results with the predictions of available permeability models for a better validation of our results. These are from the works of Jackson and James (1986), Davies (1973), and Spielman and Gloren (1968) as follows:

\[
\frac{k}{a^2} = \frac{3}{20\alpha}(-\ln \alpha - 0.931), \quad 3-7
\]

\[
\frac{1}{3} + \frac{5}{6}\frac{\sqrt{k}K_1\left(\frac{a}{\sqrt{k}}\right)}{aK_0\left(\frac{a}{\sqrt{k}}\right)} = \frac{1}{4\alpha} \quad 3-8
\]

\[
\frac{1}{2} + \frac{\sqrt{k}}{a}\frac{K_1\left(\frac{a}{\sqrt{k}}\right)}{K_0\left(\frac{a}{\sqrt{k}}\right)} = \frac{1}{4\alpha} \quad 3-9
\]

where \(K_0\) and \(K_1\) are the modified 2nd kind Bessel functions of orders zero and one, respectively. Here \(a\) and \(\alpha\) are fiber radius and medium’s SVF. Note that Equation 3-8 is obtained for fibrous media with fibers randomly oriented in a 3-D space while Equation 3-9 is for 3-D stacks of horizontal fibers with random in-plane orientation (layered structures).

As Figure 3.13 shows, the permeability of our uncompressesd structures (low SVF) is close to the predictions of Davies (1973), Jackson and James (1986), and the layered structure model of
Spielman and Goren (1968), Equation 3-9. At high SVFs our results are in closer agreement with the predictions of the 3-D random model of Spielman and Goren (1968), Equation 3-8. Interestingly, this indicates that our uncompressed fiberwebs are best represented by a layered structure while the compressed ones, due to the bending action and fiber curvature, behave closer to a 3-D random structure. Noted that the works of Davies (1973) and Jackson and James (1986) is only accurate for low SVFs (SVF < 25%) while that of Spielman and Goren (1968) is known to be valid for a wider range of SVF < 50%. Nevertheless, a very good agreement between our simulations, experiment, and available models in the literature is evident.

Figure 3.13: Dimensionless permeability constants from simulation, experiment and available models in the literature

3.2.3– Results and Conclusions

In this section, for the first time, an attempt has been made to model a nonwoven fiber-web and its structural changes during the thermal calendering process. To simplify this highly complex problem several assumptions were made. Fibers were assumed to have square cross sections and bend over each other according to a simple set of rules. The fibers lateral displacement during the
compaction process, requiring a series of force balance calculations over the fibers, was ignored as the current algorithm is only designed to model the geometry of a calendered fabric. The current study is a 1st step in developing more sophisticated algorithms. Nevertheless, simulation results are in good agreement with our experimental data as well as those of other existing permeability models in the literature. Our results indicate that the calendering has a very significant influence on the fabric’s SVF. We have experimentally observed such a U-shape SVF profile as shown in Figure 3.10c.

The dimensionless permeability of the calendered media was computed using CFD tools and reported for compression ratios. Our simulation results were compared with our own experiments as well as the available empirical and/or analytical models in the literature and a good agreement, depending on SVF, is observed. This is simply because highly-oriented fibers pack better and therefore, cause the SVF of the whole fiber-web to increase. Fiber-webs of identical SVF, however, exhibited almost identical permeabilities regardless of their fiber orientations.
References:


CHAPTER 4

INVESTIGATION OF BI-MODAL FIBER FILTERS:

PRESSURE DROP

This section is taken from a manuscript: Q. Wang, H. Vahedi Tafreshi, and B. Pourdeyhimi, “Note on 3D model of airflow through fibrous filter with bi-modal fiber size distribution”, has been submitted for publication in a peer reviewed journal.
4.1- Note on 3D Model of Aerosol through Fibrous Filter with Bi-Modal Fiber Size Distributions

A conventional approach for modeling permeability of fibrous fabrics with bimodal fiber size distributions is to consider the webs as arrays cylinders with different radius, either in square or hexagonal packing. In this work, for the first time, the full 3-D geometries of bi-modal filters with random fiber orientation distribution is generated to compute its permeability and compare with the previous periodical analytical and numerical models as well as experimental results (see Section 4.1.3). While a relatively good agreement is obtained for low the perturbation distance for bi-modal media with low SVF, our results indicate that the traditional 2D periodical model, such as Lundstrom and Gebart’s theories (1995), overestimated the permeability of bimodal fabrics (see Section 4.1.3). We concluded that a unimodal surface-weighted equivalent diameter of each bimodal filter can be used in the existing expressions for calculating the permeability, which is in a perfect agreement with the empirical work (Brown and Thorpe, 2001; see section 4.2)

4.1.1 -Introduction

Permeability of fibrous filters has been vastly studied in the past (Wang et al, 2006). Most of these works are limited on fabrics with unimodal fiber diameter, which is not necessary to be true for filtration media. A great portion of the fibrous filters, are made of blends of coarse fibers (for mechanical strength) and fine fibers (for filter collection efficiency) with different average diameters. The simplest approach to calculate the permeability of abovementioned structure is to assume that individual fibers contribute to the pressure drop independently and the total pressure drop is given simply as sum of pressure drops due to individual fibers (Clague and Phillips, 1997; Sakarv et al, 2000). Among few numerical and analytical works been done on the filter with more than one fiber size, most of the previous studies have been limited to systems consisting of
rows of fibers (often in two-dimensional geometries) perpendicular to the flow direction. To our knowledge, there has been only one attempt to simulating the bi-modal media in 3D simulating the permeability of bi-modal media (Clague and Philips, 1997). However, the geometries Clague and Philips used are 3D random, which is the not the normal case of fibrous filters (3D layered). In the current study, we report on our through-plane permeability simulations obtained for 3D-layered fibrous media consisting of two fiber size compared with available models and experimental results.

As we mentioned, except for the work of Clague and Philips (1997), who studied the 3D random bimodal fibrous media, almost all other available published theories are periodic models with controlled Solid Volume Fraction ($SVF\), \alpha (Lundstrom and Gebart, 1995; Papathanasiou, 2001; Brown and Thorpe, 2001; Jaganathan et. al, 2007). These models treated fibrous media as perfect quadratic or hexagonal arrangements with cylinder fibers. Lundstrom and Gebart in 1995 conducted 2-D simulation for the flow of Newtonian fluid perpendicular to and parallel with the idealized bi-modal media, shown in Figure 4.1.

![Periodical unit cell for bimodal filters used in Lundstrom and Gebart’s work (1995): quadratic packing in (a) and hexagonal packing in (b).](image_url)

**Figure 4.1:** Periodical unit cell for bimodal filters used in Lundstrom and Gebart’s work (1995): quadratic packing in (a) and hexagonal packing in (b).
Based on the unit cell in Figure 4.1, Lundstrom and Gebart (1995) obtained the following permeabilities. Permeability for bi-modal filters with quadratic packing shown in Figure 4.1a:

\[
K_{\text{quadratic}} = \frac{16}{9\sqrt{2\pi}} \left( \frac{\Delta}{R} \right)^{\frac{5}{2}} \sqrt{1 - \left( \frac{\delta}{R} \right)^{2}}
\]

where \( R \) is the fiber number-weighted average radius, \( \delta \) is the perturbation distance (as shown in Figure 4.1), and \( \Delta \) is the minimum distance between fibers, can be expressed as:

\[
\sqrt{\frac{\pi}{4\alpha}} (R^2 + \delta^2) - R
\]

Permeability for bi-modal filters with hexagonal packing shown in Figure 4.1b, based on Lundstrom and Gebart’s approach (1995) can be written as:

\[
K_{\text{hexagonal}} = \frac{16}{9\sqrt{2\pi}} \left( \frac{\Delta}{R} \right)^{\frac{5}{2}} \sqrt{1 - \left( \frac{\delta}{R} \right)^{2} + \frac{1 - \left( \frac{\delta}{R} \right)}{1 + \frac{\delta}{\Delta}}}
\]

\( \Delta \) is can be expressed as,

\[
\sqrt{\frac{\pi}{6\sqrt{3}\alpha}} (R^2 + \delta^2) + 2(R^2 - \delta^2) - R
\]

It can be seen that the bi-modal permeabilities will change with the packing pattern. Equation 1 and Equation 2 has been proved to be correct for the media with small \( \delta \) and high SVF (Papathanasiou, 2001), which is not always the case of the fibrous filters.
Another interesting work has been done by Brown and Thorpe (2001). For uni-modal filters, the permeability, $K$, is only a function of Solid Volume Fraction, $\alpha$, and fiber radius $R$ (Wang, et. al, 2006, Maze, et. al, 2007):

$$\frac{K}{R^2} = f(\alpha) \quad 4-3$$

Brown and Thorpe (2001) assumed the same relationship between the permeability and solid volume fraction exists for bi-modal media if an equivalent radius can be found and used:

$$\frac{K}{R_{eq}^2} = t(\alpha) \quad 4-4$$

$f(\alpha)$ is the dimensionless permeability, which having different expression based on different theories.

For filtration models with 2D hexagonal packing cylinders, Sangani and Acrivos (1982) obtained an expression by solving series bi-harmonic equations for Stokes Flow:

$$t(\alpha) = -\ln \alpha - 1.49 + 2\alpha - 0.5\alpha^2 \quad \frac{8\alpha}{8} \quad 4-5$$

For idealized geometries with 2D quadratic packing cylinders, Sangani and Acrivos (1982) gave another expression:

$$t(\alpha) = -\ln \alpha - 1.476 + 2\alpha - 1.774\alpha^2 + 4.076\alpha^3 \quad \frac{8\alpha}{8} \quad 4-6$$

Jackson and James (1986) gave an estimated correction of 3-D random webs:

$$f(\alpha) = \frac{3}{20\alpha} [-\ln(\alpha) - 0.931] \quad 4-7$$
Even though attempts are often made to justify the good correlations by theoretical models, yet some of the most successful permeability models are based on pure empiricism (Davies 1973, Brown 1993, Hinds 1999). Davies’s experimental correlation is obtained to calculate the pressure drop of a variety of filter media, which are normally 3D layer geometries, with SVF ranging from 0.6% to 30% (Davies 1973). Dimensionless pressure drop based on Davies’ correlation is:

\[ f(\alpha) = \left[ 6\alpha^{3/2} (1 + 56\alpha^3) \right]^{-1} \]  

Base the 2D quadratic models, Brown and Thorpe (2001) investigated the natural mean fiber radius, such as the number-weighed mean, the surface or the volume weighed mean, could be used as the equivalent radius to describe the behavior of the mixed fiber filters:

\[ R_{eq}^{(\alpha)} = \sum_{i=1}^{2} \frac{n_i R_i^\alpha}{\sum_{i=1}^{2} n_i R_i^{\alpha-1}} \]  

Where \( n_i \) is number of fibers of each diameter in the media. \( \alpha \) can be 1, 2, or 3 corresponding to number-weighted, \( R_{eq}^{(1)} \), area-weighted, \( R_{eq}^{(2)} \), or volume-weighted average diameters, \( R_{eq}^{(3)} \), respectively. Their result shows that the permeability across a bi-modal filter is similar to that of a uni-modal with the same SVF, composed of fibers with the surface area mean diameter of the mixture of fibers, and their experimental results verify the calculation. The similar conclusion has been achieved by Clague and Phillips (1997) by using their three-dimensional disordered fibrous media. They claimed in the case the ratio of coarse to fine fiber radius, \( R_C \) and \( R_F \), is not too large \((R_C / R_F < 3)\), the contribution of the fine fibers and coarse fibers can be calculated as if they were in unimodal media at the same volume fraction.
Our algorithm for generating bi-modal media and numerical scheme used for solving Navier-Stokes equation is simply presented in Section 4.1.2. Our simulation results of 3D-layered fibrous filter media is presented in Section 4.1.3, together with a comparison of the available models followed by the conclusions in Section 4.1.4.

4.1.2- Modeling Idealized Bi-Modal Fibrous Filters

In the current work, the virtual bi-modal filters are generated by using GeoDict, which constructing of the realistic bi-modal media based on stochastic model with structural inputs, followed by the numerical evaluation of the effect of the variation in structures on the media’s permeability (Schladitz, et. al, 2006; Schulz, et. al, 2007). This innovation software treats the geometries as the grids, where the two states empty and solid are marked. In our case, the flow domain is the collection of empty cells and the fibers are defined by the solid cells (GeoDict Manual). One of the advantages of this cubic grid cell approach is avoiding the meshing which normally causes most trouble in traditional Computation Fluid Dynamic procedure.

Most of nonwovens used in filtration industries can be assumed to be 3-D layered structures, as shown in Figure 4.2a. 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. Hence, we assumed that fibers lie horizontally in the plane of web, as shown in Figure 4.2b. The fiber orientation distribution is controlled by density function the \( p(\theta, \varphi) \) in polar coordinate in Geodict, in which \( \theta \) is the through-plane angle and \( \varphi \) is the in-plane angle (Schladitz, et. al, 2006; Schulz, et. al, 2007). For the 3-D layered filters mentioned above, the density function \( p(\theta, \varphi) \) can be expressed in the form of

\[
\frac{4}{\pi} \frac{\beta \sin \theta}{1 + (\beta^2 - 1) \cos \theta^2}
\]

where \( \beta \) is the anisotropy.
parameter and equals to 1 for the isotropic case. This method has been fully detailed and its use is justified in the works of Schladitz, et. al (2006) and Schulz, et. al (2007).

Here, for simplicity, we considered the fibers to be circular cylinders with given diameters. One of the abovementioned 3-D structures of stacked horizontal fibers with nonphysical fiber overlapping is shown in Figure 4.2b. The virtual medium has a solidity of $\alpha = 10\%$ with number fraction of fine and coarse fibers of $F_F = 20\%$ and $F_C = 80\%$, and diameters of fine and coarse fibers of $d_F = 10 \mu m$ and $d_C = 20 \mu m$, respectively.

![Figure 4.2](image1.png)

**Figure 4.2:** (a) Scanning Electron Microscopy (SEM) image shows that bi-modal fiber filters have 3-D layered geometry; (b) 3-D layered fibrous filter having two fiber sizes has been generated by using GeoDict Software.

A steady state laminar incompressible model has been adopted for the flow regime inside our virtual filters. The governing equations: continuity, and Navier-Stokes equation written in vectorial form are as follow:

$$\nabla \cdot u = 0$$  \hspace{1cm} 4-10

$$-\mu \Delta u + \nabla p = f$$  \hspace{1cm} 4-11

In the above equations $u$, $p$, $f$, and $\mu$ represent velocity vector, pressure, density of a body force and viscosity. The periodic boundary has been applied to the flow domain together with the no-
slip condition. The air flow field was solved by finite difference scheme implemented in Geodict code (Ohser and Mucklish, 2000; Schladitz, et. al, 2006; Schulz, et. al, 2007). In realization of the solving the flow field of abovementioned geometric models, the average velocity for a given pressure gradient $\nabla p$ in the stationary state can be calculated by applying Darcy’s law.

We did the benchmarking of Geodict software for single-phase flow, which is air flow here. A series of simulations were run using both finite difference solver Geodict and finite element solver Fluent. As shown in Figure 4.3, simulations had excellent agreement between these two approaches on velocity prediction for a given pressure drop.

![Figure 4.3: Benchmarking shows an excellent agreement in the single phase calculations between Geodict and Fluent.](image)

4.1.3- Results and Discussion

We, firstly, considered one of our bi-modal filtration webs and studied the effect of voxel density on the filters permeability to ensure that the results are voxel-size-independent. To do so, we
increased the number of voxels (by applying smaller size) along the fine fiber diameter from 2 to 14 and computed the permeability of the fabric. As it can be seen in Figure 4.4, increasing the voxel number along the fine fiber diameter beyond 8 has no influence on the permeability of the fabric. Simulation study reported here have more than 8 voxels along the fine fiber diameter.

![Figure 4.4: The influence of voxels’ size on the permeability](image)

We then studied the influence of super-position assumption on the permeability of bi-modal filters having different Solid Volume Fraction. To do this, we generated and calculated the pressure drop ($\Delta P$) of a series of 3D virtual bi-modal filters with fine fibers (diameter $d_F = 10 \mu m$ and number fraction $F_F = 20\%$) and coarse fibers (diameter $d_C = 20 \mu m$ and number fraction $F_C = 80\%$), but having different Solid Volume Fraction ($3\% \leq \alpha \leq 25\%$). We recorded the positions of fine and coarse fibers inside the bi-modal filters, and reproduced the same filters only with the fine fibers or only with the coarse fibers (see Figure 4.5).
The super-position pressure drop ($\Delta P_{\text{super}}$) was then calculated by simply adding the pressure drop of the media only having fine fibers ($\Delta P_F$) and the pressure drop of the media only having coarse fibers ($\Delta P_C$). Then super-position permeability ($K_{\text{super}}$) was then calculated through Darcy’s law to compare with the bi-modal filter permeability. Figure 4.6 shows the error percentage caused by super-position for different solid volume fraction. It can be seen that the super-position causes significant error on the permeability of bi-modal filters with high solidity.
Here we report on our numerical simulations aimed at finding a uni-modal equivalent diameter for each bi-modal filter (similar to the work of Brown and Thorpe, 2001). To do this, we generated and calculated the permeability of a series of bi-modal filters with identical fine fiber diameter ($d_F = 10 \, \mu m$), number fraction of fine fibers ($F_F = 50\%$) and solidity ($\alpha = 10\%$), but different coarse fiber diameters, and thus different $\delta/R$ value. We followed an identical procedure to calculate the permeability from the uni-modal filters with fibers based on the number-weighted, area-weighted and volume weighted equivalent diameters (can be calculated from Equation 8) of abovementioned bi-modal filters. Permeability, $K$, of both uni-modal and bi-modal filters is computed and presented in Figure 4.7. The value of $\delta/R$ is changed from 20% to 66.7%, for bi-modal filters having coarse fibers whose radius ranging from 15 \, \mu m to 50 \, \mu m. It can be seen that there is a relatively good agreement between the permeability of bi modal filters and the permeability of uni-modal filters applied area-weighted equivalent diameter, which agreed with the empirical work (Brown and Thorpe, 2001).
Figure 4.7: A relatively good agreement between the permeability of bi-modal filters and the permeability of uni-modal filters applied area-weighted equivalent diameter.

Figure 4.8: A comparison between different theories and a relatively good agreement between the permeability of bi-modal filters and uni-modal filters applied area-weighted equivalent diameter based on Davies empirical equation.
In Figure 4.8, we presented the bi-modal filter pressured drop obtained from simulating the structures in Figure 4.5a (symbol) along with the predictions of previous models. We applied the area-weighted average diameter to different fiber arrangements: 2D quadratic packing based on Sangani and Acrivos’ work (Equation 4-6), 3D random packing based on James and Jackson’s expression (Equation 4-7), 3D layered geometry (Equation 4-8) based on Davis experimental equation. It can be seen that there is a perfect good agreement between our CFD simulations and the Davis’ empirical equation by using area-weighted average diameters. Permeability based the 2-D models resulted in a lower prediction (Brown, 1984) not only because of the ignorance of the uniformity effect existed in fibrous filter structure, but also because of the difference between the geometries in 2 dimensional or 3 dimensional scales. Permeability based on the 3-D random structures results in higher prediction because of the attendance of the flow in the parallel to fiber direction and thus increases the permeability (Jackson and James, 1986, claimed that the permeability of arrays in cross flow direction is almost exactly half that when the arrays are parallel to the flow). The permeability calculated based on Lundstrom and Gebart’s expression of 2D quadratic packing (Equation 4-1) was also presented in Figure 4.8, which seem to over-estimate the permeability. As we mentioned in the literature, the 2D quadratic simulation of Papathanasiou (2001) also showed the similar trends.

Figure 4.9 and Figure 4.10 shows the influence of number fraction of fine fiber ($F_F$) and coarse-to-fine fiber diameter ratio ($R_{CF}$), respectively.

The virtual media shown in Figure 4.9a, have diameter of fine fiber $d_F = 10 \, \mu m$, diameter of coarse fiber $d_C = 20 \, \mu m$, solidity $\alpha = 10\%$ and number fractions of fine fiber, $F_F$, change from 0%, 20%, 40%, 60%, 80% to 100%. It can be seen in Figure 4.9b that increase the number fraction of fine fibers, the permeability of bi-modal filters decreases.
The virtual media shown in Figure 4.10a, have diameter of fine fiber $d_F = 10 \, \mu m$, number fraction of fine fiber $F_F = 50\%$, solidity $\alpha = 10\%$, and coarse-to-fine-fiber diameter ratio, $R_{CF}$, change from 1, 1.5, 2, 3, 4, 5 ($R_C = 10, 15, 20, 30, 40, 50 \, \mu m$). It can be seen in Figure 4.10b that increase the coarse-to-fine fiber diameter ratio, the permeability of bi-modal media increases.
Figure 4.10: a) 3-D virtual filters with different coarse-to-fine fiber diameter ratio. b) The permeability increases with increasing the coarse-to-fine fiber diameter ratio.

The virtual media with different SVF have also been studied here. The bimodal media have diameter of fine fiber $R_F = 10 \, \mu m$, number fraction of fine fiber $F_F = 50\%$, coarse-to-fine-fiber diameter ratio, $R_{CF} = 20 \, \mu m$. SVF changes from 3\% to 20\%. The result (see Figure 4.11) shows the permeability decreases with the solidity of the structure increases, and it also shows that the variation of the permeability of the geometries decreases with the increasing in the solidity.
4.1.4- Conclusions

A conventional approach for predicting permeability of bi-modal filters is to consider them as periodic arrangements of cylinder fibers or applying super-position assumption. In this work, a new set of models which represents bi-modal filters with virtual 3-D layered geometries has been presented, and relationship between permeability and geometrical parameters of bi-modal filters has been studied. Our CFD results show that the super-position assumption is not valid for filters having Solid Volume Fraction higher than 10%. It was also demonstrated that a unimodal surface-weighted equivalent diameter of each bimodal filter can be used in the existing expressions for calculating the permeability for small Coarse-to-Fine-Fiber-Diameter-Ratio, which is in a perfect agreement with the empirical work (Brown and Thorpe, 2001 and see section 4.2).
4.2- Experiment on Filters with Bi-Modal Fiber Distribution

The purpose of this study is to experimentally investigate the role of fiber diameter distribution on the pressure drop of the filter media. For this purpose, bi-modal PET filter media with different coarse-to-fine-fiber-diameter-ratio and mass fractions were produced via carding process. The webs were then cross-laid and bonded by needle punching. The influences of the coarse-to-fine-fiber-diameter-ratio and mass fraction of fine fibers were then investigated with respect to filtration properties, such as permeability. The permeability results indicate that a uni-modal area-weighted equivalent diameter of each bimodal filter can be used in the existing expressions for calculating the permeability, which is in a perfect agreement with our previous simulations.

4.2.1 – Introduction

Many experimental studies have been conducted to calculate the pressure drop of fibrous filters. These work predominantly use filters of one fiber size, and consider fibrous media as uni-modal webs (Davies, 1973). However, fibrous media containing more than one fiber diameter are common, so that the experimental findings of the above-mentioned works no longer applicable. For example, mixture of fibers with two different diameters are popular for producing bi-modal filters to improve the indoor air quality by removing particles from air stream. Bi-modal fibrous filters have better mechanical strength due to the coarse fibers and higher collection efficiency to the fine fibers than uni-modal filter media. However, there are only a few examples in literature of experimental studies of fibrous filters with a fiber diameter distribution (Brown and Thorpe, 2001; Johnson and Deen, 1996). Bi-modal filters are more complicated than the uni-modal filters. For this reason, more systematic research, which takes the fiber diameter distribution in to
account is required. This section will cover our experimental study of needle-punched fibrous media consisting of two fiber size.

4.2.2 – Description of Filters

Carding is a dry laid technology adopted from the traditional textile carding operation. In the carding process, staple fiber webs are produced by using high-speed rolls, as shown in Figure 4.12a. The general objectives of this process includes: 1) opening, blending, and cleaning; 2) short fiber removal; and 3) decrease in the linear density (INDA NW Handbook). The normal carding process produces webs highly oriented in the machine direction.

In order to achieve a randomized fiber orientation distribution and obtain uniform webs, the cross-lapping process needs to be used. Cross-lapping is the stacking of highly oriented fibrous filter layer onto one another, as shown in Figure 4.12b. Since the angle of lapping can be controlled, we can improve the uniformity and fiber orientation distribution of the webs and obtain uniform media. Figure 4.12c shows that the feed belts feed the fibrous webs (after cross-lapping) into the needling zone, where the webs are punched between the plates, and then be pulled through a pair of take-up rollers.

![Figure 4.12a: A schematic drawing of the needle-punching process used in this work: Roller top carding process (TT 504 note).](image-url)
The bi-modal PET fibrous media were made in the Nonwovens Cooperative Research Center’s staple lab, and the influence of coarse-to-fine-fiber-diameter-ratio and mass fraction of fine fibers was studied.

The specifications for the four fibrous filters used in the coarse-to-fine-fiber-diameter-ratio study are listed in Table 4.1. The fine fibers used in this series of media are 1.5 denier, and the coarse fibers were 4, 6 or 15 denier. The fiber diameters were determined by image analysis to be 12.40 ± 0.42 µm, 20.71 ± 1.34 µm, 22.15 ± 0.85 µm, 39.23 ± 1.16 µm for the 1.5, 4, 6, and 15 denier fibers, respectively. The mass- fraction-of-fine-fiber \( M_F = \frac{\text{Mass of Fine Fiber}}{\text{Mass of Coarse Fiber}} \) used in this study is 50%, as shown in Table 4.1. The coarse-to-fine-fiber-diameter-ratio is defined as the \( R_{CF} = \frac{d_C}{d_F} \), and the bi-modal nonwoven media having different \( R_{CF} \) are shown in Figure 4.13.
Table 4.1: Staple fiber media having different coarse-to-fine-fiber-diameter-ratio used in this study

<table>
<thead>
<tr>
<th>( R_{CF} )</th>
<th>( d_F )</th>
<th>( M_F )</th>
<th>( d_C )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.40 ( \mu m )</td>
<td>100%</td>
<td>N/A</td>
</tr>
<tr>
<td>1.67</td>
<td>12.40 ( \mu m )</td>
<td>50%</td>
<td>20.71 ( \mu m )</td>
</tr>
<tr>
<td>1.92</td>
<td>12.40 ( \mu m )</td>
<td>50%</td>
<td>23.83 ( \mu m )</td>
</tr>
<tr>
<td>3.16</td>
<td>12.40 ( \mu m )</td>
<td>50%</td>
<td>39.23 ( \mu m )</td>
</tr>
</tbody>
</table>

Figure 4.13: Staple fiber media having different coarse-to-fine-fiber-diameter-ratio: a) \( R_{CF} = 1.92 \) and b) \( R_{CF} = 3.16 \).

We controlled the fine fiber diameter, \( d_F \), coarse fiber diameter, \( d_C \), and solidity of the media, \( \alpha \), to study the influence of the mass-fraction-of-fine-fiber on the permeability of bi-modal media. Two series of nonwoven media with \( R_{CF} = 1.92 \) and \( R_{CF} = 3.16 \) were made (see Table 4.2.1 and Table 4.2.2). The finer fiber mass fraction, \( M_F \), was increased from 0%, 25%, 50%, 75% to 100% for each series. The bi-modal nonwoven media having different mass fractions are shown in Figure 4.14.
Table 4.2.1: Staple fiber media having different mass fraction of fiber fine with $R_{CF} = 1.92$

<table>
<thead>
<tr>
<th>$R_{CF}$</th>
<th>$d_F$</th>
<th>$M_F$</th>
<th>$d_C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.92</td>
<td>12.40 µm</td>
<td>100%</td>
<td>23.83 µm</td>
</tr>
<tr>
<td>1.92</td>
<td>12.40 µm</td>
<td>75%</td>
<td>23.83 µm</td>
</tr>
<tr>
<td>1.92</td>
<td>12.40 µm</td>
<td>50%</td>
<td>23.83 µm</td>
</tr>
<tr>
<td>1.92</td>
<td>12.40 µm</td>
<td>25%</td>
<td>23.83 µm</td>
</tr>
<tr>
<td>1.92</td>
<td>12.40 µm</td>
<td>0%</td>
<td>23.83 µm</td>
</tr>
</tbody>
</table>

Table 4.2.2: Staple fiber media having different mass fraction of fine fiber with $R_{CF} = 3.16$

<table>
<thead>
<tr>
<th>$R_{CF}$</th>
<th>$d_F$</th>
<th>$M_F$</th>
<th>$d_C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.16</td>
<td>12.40 µm</td>
<td>100%</td>
<td>39.23 µm</td>
</tr>
<tr>
<td>3.16</td>
<td>12.40 µm</td>
<td>75%</td>
<td>39.23 µm</td>
</tr>
<tr>
<td>3.16</td>
<td>12.40 µm</td>
<td>50%</td>
<td>39.23 µm</td>
</tr>
<tr>
<td>3.16</td>
<td>12.40 µm</td>
<td>25%</td>
<td>39.23 µm</td>
</tr>
<tr>
<td>3.16</td>
<td>12.40 µm</td>
<td>0%</td>
<td>39.23 µm</td>
</tr>
</tbody>
</table>

Figure 4.14: Staple fiber media having different mass fraction of fibers: a) $M_F = 75\%$ and b) $M_F = 50\%$
4.2.3 – Results and Discussion

The permeability of the media was measured using the TSI 3160 (see Chapter 1). The air velocity used here was 0.53 m/s, which is the industrial standard for air filtration tests. For each web, five samples (cut along the MD and the CD), were used. The average pressure drop was obtained from the samples and the permeability was calculated from the pressure drop by Darcy’s law.

Figure 4.15a shows the comparison of the permeabilities obtained from the TSI tests and Davies empirical correlations (see Equation 4-8) for the uni-modal fiber filters. It shows that with increasing fiber diameter, the permeability of the fabric increases. Note that for uni-modal filters with different fiber diameter, the solid volume fractions of the media varied slightly in the experiment. Figure 4.14a also shows the discrepancy exists between the experiment value and Davies’ empirical data, which is explained by term of Error Percentage in Figure 4.15b (Error Percentage was simply defined as, $\frac{K_{\text{experiment}} - K_{\text{davies}}}{K_{\text{experiment}}} \times 100$ , here).

Figure 4.15b shows that the Error Percentage of the permeability decreases with increasing fiber diameter. This is because the extent of non-uniformity, which caused by the needle-punching, decreases due to the compatible sizes of the needles used for needle-punching and the average filter pore diameter when coarse fibers are used for filter media.

Equation 4-12 shows that the relationship between the error percentage and fiber diameter fits with a 2nd order polynomial regression with $R^2 = 0.99$:

$$Error \ Percentage = -0.007d_f^2 - 0.0146d_f + 19.007$$

4-12
Note that in Figure 4.14b, the solid line is the regression value was calculated from Equation 4-12.

**Figure 4.15:**

a) The permeability of uni-modal staple fiber media increases with increasing the fiber size;
b) The permeability Error Percentage decreases with increasing fiber size in the uni-modal filter
Figure 4.16 compares the permeability obtained from the bi-modal media tested with the TSI filter test machine and the permeability calculated from the Davies empirical equation of uni-modal fibrous filters based on number-weighted, $R^1_{eq}$, area-weighted, $R^2_{eq}$, or volume-weighted average diameters, $R^3_{eq}$. The equivalent diameters can be calculated from Equation 4-9. The comparison reveals a constant discrepancy between bi-modal experimental data and the Davies equation with the area-weighted average diameter.

![Figure 4.16: Permeability for Bi-modal filter has constant discrepancy with the permeability calculated from uni-modal filters with the area-weighted average diameter.](image)

The discrepancy between the permeability obtained from the bi-modal filter experiment (red dot) and the permeability calculation data from uni-modal filter with the area-weighted average diameter (solid green line) was caused by holes produced in the needle-punching process. In order to eliminate this discrepancy, we used Equation 4-11 to modify the permeability of bi-modal media. Thus creating agreement between the experimental data and the Davies equation with area weighted equivalent diameter, as shown in Figure 4.17. Figure 4.17 also shows that the permeability increases with increasing coarse-to-fine fiber diameter ratio of bi-modal media.
Figure 4.17: The modified permeability of bi-modal filter media has good agreement with uni-modal filter media with area weighted equivalent diameter.

Figure 4.18a: Permeability of bi-modal filters decreases by increasing the mass fraction of fine fiber with $R_{CF} = 1.92$. 
The similar agreement between bi-modal filters and uni-modal filters with the area-weighted average diameter was found in the study of the mass fraction of the fine fiber, as shown in Figure 4.18a and Figure 4.18b for $R_{CF} = 1.92$ and $R_{CF} = 3.16$ respectively.

4.2.4 – Conclusions

The aim of this work is to check if our simulation findings for bi-modal filter permeability (a uni-modal area-weighted equivalent diameter of each bimodal filter can be used in the existing expressions for calculating the permeability) are correct. We made bi-modal fiber media with changing parameters, such as the coarse-to-fine fiber diameter ratio ($R_{CF}$) and the mass fraction of fine fiber ($M_F$). The testing results show that the same relationship exists between the uni-modal filters and the bi-modal filters, which mean our experimental findings, support our previous simulation conclusions.
References:


Geodict Manual.


CHAPTER 5

PERMEABILITY OF MONO-FILAMENT & MULTI-FILAMENT WOVEN FILTER

This chapter is taken from following manuscripts:


5.1- On the Pressure Drop of Monofilament-Woven Fabric

Pressure drop of monofilament woven fabrics is often calculated via the so-called orifice model in which a discharge coefficient is assigned to the weave’s unit cell. In all previous models of woven fabrics, the filaments were assumed to have circular cross-sections – an assumption which is not entirely accurate especially when there is a considerable tension in the warps and wefts. Following the methodology developed by Lu and Tung (1996), a new set of expressions are derived for calculating the most constricted open area, and so the discharge coefficient, of plain-woven monofilament fabrics having filaments with elliptical cross-sections. Conducting numerical simulations for computing the pressure drop of such fabrics, we observed a logarithmic relationship between the discharge coefficient and the Reynolds number. It was also shown that the discharge coefficient decreases by increasing the aspect ratio of the filaments’ cross section.

5.1.1- Introduction

Permeability of monofilament woven fabrics is of great importance in many applications and has been vastly studied in the past. In 1971, Rushton and Griffiths reviewed various theories of fluid flow through woven monofilament fabrics developed by then and concluded that the so-called orifice analogy is the most appropriate modeling approach for calculating permeability of a monofilament fabric. In the orifice model, the open area between the filaments is treated as a submerged orifice and, depending on the geometry of the opening, a discharge coefficient is determined for the pore (Pedersen 1969). Inspired by the work of Pedersen (1969), Lu and Tung (1996) developed an orifice model for calculating the permeability of monofilament fabrics. In their model, the discharge coefficient is presented by equation (1) as follows.

\[ C_d = \sqrt{\frac{\rho u^2 (1 - \alpha_c^2)}{2\Delta P \alpha_c^2}} \] 5-1
where, $\rho$, $V$, $\alpha_c$ and $\Delta P$ are flow density, superficial velocity, Effective Fractional Open Area (EFOA) and pressure drop, respectively. EFOA is given by $\alpha_c = A_c / l_f^2$, where $A_c$ is the most constricted area and $l_f$ is the filaments’ center-to-center distance.

Since the infancy of the orifice model, discharge coefficient has been related to the flow Reynolds number in the following form (Pedersen 1969, Gooijier et al. 2003, Wakeman and Tarleton 2005):

$$C_d = k_c \cdot \text{Re}^m_c$$

5-2

where $k_c$ and $m_c$ are constants for fabrics having filaments with circular cross-sections. Note that Reynolds number is defined differently in different studies. Following the work of Pedersen (1969), Lu and Tung (1996) defined their Reynolds number based on the wetted perimeter of the orifice, $W_c$, where the flow is most constricted:

$$\text{Re} = \frac{4 \rho V l_f^2}{W_c \mu}$$

5-3

here $\mu$ is the flow viscosity. Lu and Tung (1996) presented the following equations for $\alpha_c$ and $W_c$, respectively.

$$\alpha_c = \frac{\sqrt{\Phi_f^2 + 1}}{2\Phi_f} + \Phi_f \cdot \frac{1}{2} \ln \left( \frac{1 + \sqrt{\Phi_f^2 + 1}}{\Phi_f} \right) - \frac{1}{\Phi_f} \cdot \sqrt{\Phi_f^2 + 1} \left( 1 - \frac{1}{\Phi_f} \right)$$

5-4

$$W_c = 2d_f \left[ \sqrt{\Phi_f^2 + 1} \left( 1 - \frac{1}{\Phi_f} \right) E \left( k, \frac{\pi}{2} \right) + \sqrt{\Phi_f^2 + 1} \right]$$

5-5

Here $d_f$ is the filament diameter and $E(k, \pi/2)$ is the Elliptical integral of the second kind, where

$$\Phi_f = \frac{l_f}{d_f} \quad \text{and} \quad k = 1 - \frac{\Phi_f^2}{(1 + \Phi_f^2)(\Phi_f - 1)^2}.$$
In this paper we only consider cases where warps and wefts are made of exactly identical filaments and are under identical tensile forces. The work of Lu and Tung (1996) as well as all other previous models (Armour and Cannon 1968, Pedersen 1969, Rushton and Griffiths 1971, Gooijier et al. 2003, Wakeman and Tarleton 2005) consider the filaments to have circular cross-sections. This assumption may simplify the modeling effort but is not entirely accurate. This is because the existing tension in the warps and wefts causes the filaments to be push against each other in a direction normal to the plane of the fabric. The filaments’ circular cross-section therefore, tends to become elliptical (Hu 2004). This is especially true in the case of multifilament yarns where the filaments can move around and allow the cross-section to deform. As will be discussed later in this note, the shape of the filaments’ cross-section can greatly influence the air flow pattern, and consequently the pressure drop of the fabrics. The study reported in this note, is aimed at establishing a relationship between $C_d$ and $Re$ in monofilament fabrics with filaments having elliptical cross-sections. Note that the modeling methodology presented here can be used together with the available lump permeability models of Gebart (1990) and/or Moholkar and Warmoeskerken (2004) to simulate the air permeability of fabrics having multifilament yarns with elliptical cross-sections (Wang et al. 2006).

In section 5.2.2, we follow the work of Lu and Tung (1996) to develop a new set of expressions for calculating $\alpha_e$ and $W_e$ for the case of filaments with elliptical cross-sections. This will be followed by a series of Computational Fluid Dynamics (CFD) simulations aimed at calculating the fabrics’ discharge coefficient as a function of Reynolds number.

5.1.2- Woven Fabric with Elliptical Cross-section

Here we follow the methodology developed by Lu and Tung (1996) to derive analytical expressions for calculating $\alpha_e$ and $W_e$ for the case of monofilament fabrics with filaments having
elliptical cross-sections. These new expressions will be used in equations (1) and (3) to obtain a relationship between $C_d$ and $Re$.

To describe a monofilament woven fabric made of identical filaments of circular cross-sections one would only need two parameters: filament diameter, $d_f$, and filaments’ center-to-center distance, $l_f$. When the filaments have elliptical cross-sections, however, three parameters are needed. These are the filaments major and minor diameters and the filaments’ center-to-center distance, $l_f$ (see Figure 5.1). In this paper, filaments major and minor diameters and their ratio, aspect ratio, are referred to as $d_x$, $d_y$, and $a_r = d_x / d_y$, respectively. According to Hu (2004), filaments in typical monofilament woven fabrics have cross-sectional aspect ratios in the range of $1 < a_r < 3$.

![Diagram of monofilament fabrics with filaments having circular and elliptical cross-sections.](image)

**Figure 5.1**: Monofilament fabrics with filaments having circular (a) and elliptical (b) cross-sections.
Following Lu and Tung (1996) we obtained equations 5-6 and 5-7 as follow.

$$\alpha_e = \frac{\sqrt{\Phi_y^2 + 1}}{2\Phi_y} + \frac{\Phi_y}{2} \ln \left( 1 + \frac{\sqrt{\Phi_y^2 + 1}}{\Phi_y} \right) - \pi \frac{\sqrt{\Phi_y^2 + 1}}{4} \frac{1 - \frac{1}{\Phi_y}}{\Phi_y} - \Omega$$

where

$$\Omega = \int_0^l \sqrt{\frac{l_f^2 + d_y^2}{\Phi_x^2 + \left(1 - \frac{2x}{l_f}\right)^2}} \, dx$$

$$W_e = 2d_y \left[ \sqrt{\Phi_y^2 + 1} \left( 1 - \frac{1}{\Phi_y} \right) E\left(k', \frac{\pi}{2}\right) + \sqrt{\Phi_y^2 + 1} \right]$$

where $\Phi_x = l_f / d_x$, $\Phi_y = l_f / d_y$, and $k' = 1 - \frac{\Phi_y^4}{(1 + \Phi_y^2)(\Phi_y^2 - 1)^2\Phi_x^2}$.

In the special case of $d_x = d_y$, equations 5-6 and 5-7 reduce to 5-4 and 5-5 with the exception of a factor of $\pi / 4$ in the forth term of equation 5-4. Based on the work of Lu and Tung (1996), the most constricted area of a plain-woven fabric is a 3-D surface with a convoluted shape. The difference between our expression and that of Lu and Tung (1996) lies in the simplifications considered in both derivations. Nevertheless, we found insignificant differences between the pressure drop predictions of our expressions and those of equations 5-4 and 5-5 when compared against the results of numerical simulations of plain-woven fabrics.

### 5.1.3-Modeling Flow through Monofilament Woven Fabrics

The well-known finite volume method developed by Patankar (1980) and implemented in Fluent code is used here to solve the continuity and the conservation of momentum in a steady state mode (equations are not shown for the sake of brevity). Laminar incompressible flow is assumed to prevail inside our solution domain (see Figure 5.2) for the face velocities considered here (Re < 15). Due to the periodicity of the woven geometry, only the unit cell of the plain
weave pattern is considered for the simulations. The mathematical equations describing the shape of a filament’s centerline for woven fabrics is well-documented through the pioneering works of Peirce (1937) and recent review of Hu (2004) and will not be repeated in this short note. Briefly, the filament’s geometry is imported to Gambit, a preprocessor for Fluent code, via a journal file. The journal file describes all the operations needed to reconstruct the geometry of the filament. Depending on their geometries, these structures are meshed using 200,000 to 400,000 tetrahedral elements, refined close to the filament surfaces. Air is assumed to enter the simulation domain through a velocity-inlet and leave it from a pressure-outlet boundary condition. The inlet and outlet boundary conditions are placed far from any strong gradients as we used uniform our boundary conditions. Symmetry boundary condition is considered for the sides of the computational box. For the air flow on the fiber surfaces, we assumed a no-slip boundary condition as the flow is in the continuum regime.

![Figure 5.2](image)

**Figure 5.2**: Simulation domain together with the boundary conditions.
To ensure the accuracy of our CFD results, we conducted a mesh-independence study in which the number of cells considered for a simulation was varied in a wide range and the fabric’s pressure drop was monitored. As shown in Figure 5.3, we increased the interval size between the grid points on the perimeter of the filaments from 2.5 µm up to 5 µm (40 to 20 per \( d_x \) where \( d_x \) is 100 µm) and computed the pressure drop of the fabric. As it can be seen results are mesh-independent for as long as the interval size is smaller than about 3.3 µm. The grids interval size in the simulations reported in this note were always smaller than 3 µm.

![Figure 5.3: Effect of mesh size on the pressure drop calculations.](image)

### 5.1.4-Results and Discussion

Here we report on our numerical simulations aimed at establishing a relationship between \( C_d \) and \( Re \) when the filaments have elliptical cross-sections. To isolate the effect of filaments’ aspect ratio from other parameters influencing a fabric’s pressure drop, we considered different monofilament fabrics with \( d_y \) being the only difference between them. In these simulations
was changed in such a way that filament cross-sectional aspect ratio, \( a_r \) was varied from 1 to 3. The case of filaments with circular cross-section has also been studied for comparison with the work of Lu and Tung (1996) as mentioned before.

Conducting a series of simulation for the case of \( a_r = 1 \), we obtained the following expression for the discharge coefficient of the plain-woven fabrics for \( \text{Re} < 15 \):

\[
C_d = k_c \cdot \text{Re}^{m_c} \quad \text{5-8}
\]

where \( k_c = 0.11 \) and \( m_c = 0.45 \) based on equation 5-6 and 5-7 while \( k_c = 0.15 \) and \( m_c = 0.46 \) based on equation 5-4 and 5-5. Equation 5-8 is similar to the one obtained by Lu and Tung (1996), however, their constants are slightly different from ours (\( k_c = 0.18 \) and \( m_c = 0.49 \)). This is due to the fact that their expression is the result of fitting a curve into a combined set of experimental data obtained for four different types of pore geometries (from plain, twill, and sateen weaves). Note that as pointed out by Brasquet and Le Cloirec (2000), different weave patterns lead to different relationships between the pressure drop and face velocity. Using equations 5-4 – 5-5 and 5-6 – 5-7 for predicting the results of numerical simulation of plain-woven fabrics, we observed a good general agreement between the models, as mentioned before. It is also worth mentioning that our \( k_c \) and \( m_c \) values are close to those of Gooijier et. al (2003).

Using our CFD simulations, we calculated the fabric discharge coefficients versus Reynolds number. It can be seen that discharge coefficient decreases by increasing the cross-section’s aspect ratio. This indicates that the pressure drop of a fabric increases by increasing the aspect ratio of its filaments’ cross-sections. More interestingly, we observed a change in the relationship between \( C_d \) and \( \text{Re} \) once the cross-sectional aspect ratio is increased beyond a value of about \( a_r = 1.2 \). This was found by considering different aspect ratios starting from 1 to 1.5 and
was observed that a transition from the power-law dependence to logarithmic relationship occurs at the above aspect ratio.

From the results presented in Figure 5.4 one can obtain a general equation for $C_d$ versus $Re$ which is valid for a wide range of practical aspect ratios and $Re < 15$:

$$C_d = c_e a_r^{0.44} \ln Re + m_e a_r^{0.18}$$

where $c_e = 0.10$ and $m_e = 0.11$.

![Figure 5.4: Discharge coefficient versus Re for fabrics having filaments with different cross-sectional aspect ratios.](image)

To check whether this equation can reliably predict the discharge coefficient of monofilament fabrics with elliptical cross-sections, three different cases of $a_r = 1.25, 2.25$ and $2.75$, (which were not included in the above regression procedure) at different Reynolds numbers were simulated. Pressure drop predictions obtained from equation 5-9 shows a good agreement with those of CFD simulations indicating the validity of our general expression (see Table 5.1).
Table 5.1: A comparison between the predictions of equation 5-9 and numerical simulations

<table>
<thead>
<tr>
<th>$a_r$</th>
<th>Re</th>
<th>$C_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
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</tr>
<tr>
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</tr>
<tr>
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<td>5.69</td>
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</tr>
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</tr>
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</tr>
</tbody>
</table>

5.1.5 -Conclusion

A conventional approach for calculating pressure drop of monofilament fabrics is to consider them as a series of parallel orifices where the discharge coefficient of these orifices, $C_d$, is a function of flow Reynolds number, $Re$. Previous theoretical models are based on the assumption that filaments have circular cross-sections. In almost all woven fabrics, warps and wefts are under some degrees of tension. This causes the warps and wefts to be pushed against each other at the crossovers and results in the deformation of the filaments’ cross-sections. In this work, a new set of expressions are derived for predicting the pressure drop of monofilament woven fabrics with filaments having elliptical cross-sections. A new relationship is established between the fabric’s discharge coefficient, $C_d$, and $Re$ which incorporates the cross-sectional aspect ratio of the filaments. It was demonstrated that discharge coefficient decreases by increasing filaments’ cross-sectional aspect ratio. Our CFD results also indicate that the discharge coefficient of such fabrics has a logarithmic relationship with the Reynolds number.
5.2 - A Note on Permeability Simulation of Multifilament Woven Fabrics

A conventional approach for modeling permeability of multifilament fabrics is to consider their warps and wefts to be individual thick filament made of homogeneous porous media and solve the flow equations for such monofilament fabrics. In this work, for the first time, the full 3-D geometry of an idealized multifilament woven fabric, wherein the filaments are packed in Hexagonal arrangements, is generated to compute its permeability and compare with the homogeneous anisotropic lumped model of Gebart (1992). While a relatively good agreement is obtained, our results indicate that Gebart’s model slightly underestimate the permeability of multifilament fabrics even at high yarn’s solid volume fractions.

5.2.1 - Introduction

Because of their strength, flexibility, and high permeability, woven materials have found enormous applications in our daily life and industry. Permeability of multifilament woven fabrics has been vastly studied in the past. Most of these works, however, are experimental and many of them are designed for specific applications (Sadiq et al., 1995; Brasquet and Le Cloirec, 2000; Wassink et al., 2003; Bijeljic et al., 2004; Moholkar and Warmoeskerken, 2004; Benesse et al., 2006). This, in part, is due to the complexity of the geometries of such fabrics. As will be discussed later in this note, conducting a computational study on multifilament woven fabrics requires considerable computing power even for idealized geometries. For this reason, all previously published simulations of the multifilament fabrics are based on monofilament geometries made of porous materials (Bruschke and Advani, 1993; Papathanasiou, 1996; Papathanasiou, 1997; Phelan and Wise, 1996; Ngo and Tamma, 2001; Nedanov and Advani, 2002; Song et al., 2003; Wong et al., 2006). In such studies, the flow field is divided into two zones of intra-yarn and inter-yarn and solved separately. The intra-yarn zone is obtained via 2-D
simulations whereas the inter-yarn zone is often calculated in 3-D space. Assuming the yarn to be a porous filament greatly reduces the computational requirements, but instead, requires accurate information regarding the yarn’s permeability. Gebart in 1992 conducted 2-D simulations for the flow of Newtonian fluid perpendicular to and parallel with the unidirectional filaments in a yarn. Gebart obtained the following permeabilities for a yarn made up of hexagonally packed continuous filaments. Permeability along the filaments:

\[ K_\parallel = \frac{2d_f^2}{53} \frac{(1-\alpha_y)^3}{\alpha_y^2} \]  

5-10

and perpendicular to the filaments:

\[ K_\perp = \frac{4}{9\pi \sqrt{6}} \left( \frac{\pi}{2\sqrt{3}\alpha_y} - 1 \right)^5 d_f^2 \]  

5-11

Here \( \alpha_y \) and \( d_f \) are the yarn Solid Volume Fraction (SVF) and the filament diameter, respectively. It can be seen that the yarns permeabilities are different in different direction. Except for the work of Tung et. al (2002), who studied the permeability of multifilament woven cloths for different weave patterns, almost all other published simulations have recognized the anisotropy of the yarn’s permeability.

The Gebart’s expressions have been widely used in the literature and have given reasonable predictions of the experimental data. Gebart’s expressions, however, have never been accurately validated by experiment. This is simply because these expressions are derived for an idealized arrangement of the filaments in the yarns which is impossible to duplicate in an experiment. Recent developments in the available computational resources have made it possible for us to simulate a series of idealized 3-D multifilament geometries with accuracies better than any previous calculations for comparison with Gebart’s expressions. Note that because of the existing
tension in the warps and wefts, the yarn’s cross-section tends to become elliptical especially at the crossovers (Hu, 2004). However, as our focus here is evaluating the Gebart’s expressions, an idealized model is considered for the yarn’s cross-section and the filaments’ arrangement. The study reported in this note, is aimed at solving the flow field inside the multifilament fabrics in one step using a continuous flow field, i.e., without breaking the simulation domain into inter-yarn and intra-yarn zones. Such calculations result in an accurate flow field prediction. Figure 5.5a shows the unit cell of a monofilament woven fabric followed by a similar cell made of idealized multifilament yarns shown in Figure 5.5b. The yarns are made of 139 filaments packed in a hexagonal arrangement with no crossovers.

Figure 5.5: a) Unit cell of a monofilament woven fabric from top and side views. b) Unit cell of a multifilament woven fabric with 139 filaments packed in a hexagonal arrangement within yarns having the same diameter as the monofilament fabric.
It is worth mentioning that woven fibrous filters have been used in air filtration since decades ago. For such applications, particle collection efficiency and permeability are equally important. Calculating trajectory of airborne or waterborne particles through multifilament fabrics for simulating the collection efficiency of woven filters, for instance, is only possible via the approach presented in this work. Here, we solve the flow field inside a series of multifilament woven fabrics using the CFD code from Fluent Inc. Our modeling scheme is presented in the next section followed by the results and conclusions in section 5.1.3.

5.2.2 – Modeling Idealized Multifilament Woven Fabrics

A steady state laminar incompressible flow is assumed to prevail inside our woven fabrics when exposed to an air flow with a velocity of 0.1 m/s. The finite volume method (Patankar, 1980) implemented in Fluent code is exploited to solve the continuity and the conservation of momentum around the filaments and yarns (equations are eliminated for the sake of brevity). Due to the periodicity of the woven geometry, only the unit cell of the weave pattern is considered for the simulations. The mathematical equations describing the shape of a yarn’s centerline for woven fabrics is well-documented through the pioneering works of Peirce (1937) and recent review of Hu (2004) and will not be repeated in this short note. The yarn’s geometry is imported to Gambit, a preprocessor for Fluent code, via a journal file. The journal file describes all the operations needed to reconstruct the geometry of the yarn. Depending upon the SVF of the yarns, the multifilament fabrics (see Figure 5.5b) are meshed using 8,000,000 to 10,000,000 tetrahedral elements, refined close to the filament surfaces. Boundary conditions considered for the simulations are shown in Figure 5.6a. Air is assumed to flow into the simulation domain through a velocity-inlet and leaves it from a pressure-outlet boundary condition. The inlet and outlet boundary conditions are placed at a distance, $L$, upstream and
downstream of the fabric far from any strong gradients. Symmetry boundary condition is considered for the sides of the computational box. For the air flow on the fiber surfaces, we assumed a no-slip boundary condition as the flow is in the continuum regime, i.e., $Kn_f = 2\lambda / d_f << 1$, where $Kn_f$ is the fiber Knudsen number, $\lambda$ is the mean free path of the air molecules (about 64 nm).

The porous media model of Fluent is employed in this study. This model incorporates a flow resistance in a specified region which, in our case, is the space occupied by the yarns. A porous medium in Fluent is modeled by the addition of a momentum sink term to the standard fluid flow equations. This momentum sink contributes to the pressure gradient in the porous cells, creating a pressure drop that is proportional to the fluid velocity in the cells. Based on Darcy’s law, the pressure drop within the porous region is:

$$\Delta p_i = \sum_{j=1}^{3} \frac{\mu}{K_{ij}} v_j \Delta n_i$$

where $K_{ij}$ is the diagonal permeability tensor and $\Delta n_i$ is the thicknesses of the medium in the $i$-direction. If the yarns were exactly parallel with the $x$ and $y$ coordinates we then would have $K_{xx} = K_{\perp}$ and $K_{yy} = K_{\parallel}$. However, because of the yarns’ curvature, one needs to specify three direction vectors for the yarns. The first vector specifies direction of the yarn’s axis, $s_{||}$, while the two others represent directions perpendicular to this axis, $s_{\perp}$ and $s'_{\perp}$. Here for simplicity we considered two different approximate methods for specifying the above direction vectors (shown in Figure 5.6b). Trial simulations, however, showed no differences in the fabric’s permeability upon considering such changes and so the first method was chosen for all the simulations.
5.2.3-Results and Conclusions

We, firstly, considered one of our multifilament fabrics and studied the effect of mesh density on the fabrics permeability to ensure that the results are mesh-independent. To do so, we increased the number of mesh points on the perimeter of the filaments inside the yarns from 7 up to 15 and computed the permeability of the fabric. Note that we also increased the number of mesh points

Figure 5.6: a) Simulation box together with the boundary conditions. b) Two different set of direction vectors considered for assigning $K_{\perp}$ and $K_{||}$ inside the porous yarns.
on the edges of the simulation box with almost the same proportion to control the skewness of the cells. As it can be seen in Figure 5.7, increasing the grid points at the filament’s perimeter beyond 12 have no influence on the permeability of the fabric. Simulations reported here have more than 12 grid point at the filament perimeters.

![Graph showing the effect of number of mesh at the perimeter of a filament in the fabric's pressure drop](image)

**Figure 5.7:** Effect of number of mesh at the perimeter of a filament in the fabric’s pressure drop

Dimensionless permeability, $K/r_y^2$, of the multifilament fabrics with $L_y=0.4$ mm and $d_y=2r_y=0.2$ mm are computed and presented in Figure 5.8. The intra-yarn SVF, $\alpha_y$, is changed from 33% to 67.6%, for yarns having filament diameters ranging from $d_y=9.75$ to 13.95 micrometer. Similar simulations are performed for fabrics made of monofilament porous yarn with the same $d_y$ and $L_y$, and $K_1$ and $K_\perp$ are taken from Eq. 1 and 2. It can be seen that there is a relatively good agreement between the predictions of Gebart’s expression and our full 3-D simulations as expected. Gebart’s expression however, seem to underestimate the fabrics’ permeability by 10% to 15% even at high SVFs (SVF > 0.6) where it was claimed to be accurate Gebart (1992).
Figure 5.8: Comparison between the fabric’s permeability obtained via the Gebart’s expressions for the permeability of yarns and our full 3-D simulations.

5.3 – Simulating Permeability of 3-DMultifilament Woven Fabrics Under Tension

Pressure drop (permeability) is a critical property of the woven fabrics. In this work an accurate prediction of the airflow field inside multifilament woven fabrics is reported. Unlike all previously reported numerical simulations, a full 3-D model of the multifilament fabrics, in which filaments are assumed to have identical diameters and packed in hexagonal configurations, is developed for the purpose of conducting one-step flow field simulations in continuous domains. This new approach allows us to obtain detailed information regarding the flow field in the intra-yarn and inter-yarn regions. Permeability of multifilament fabrics has been computed for yarns having different filament occupation ratio (thus different yarn intra Solid Volume Fractions), spacing, and cross-sectional aspect ratio. Our results indicate that fabric’ pressure drop increases
by increasing the filament occupation ratio and increases by decreasing the yarn-to-yarn distance. Keeping the filament occupation ratio constant, we also increased its cross-sectional aspect ratio and noticed that fabric’s pressure drop increases.

5.3.1-Introduction

Because of their strength, flexibility, and high permeability, woven materials have found enormous applications in our daily life as well as modern industry. Permeability of multifilament woven fabrics has been vastly studied in the past. Most of these works, however, are experimental and many of them are designed for specific applications (Sadiq et al., 1995; Brasquet and Le Cloirec, 2000; Wassink et al., 2003; Bijeljic et al., 2004; Moholkar and Warmoeskerken, 2004; Benesse et al., 2006). This, in part, is due to the complexity of the geometries of such fabrics. As will be discussed later in this paper, conducting a computational study on multifilament woven fabrics requires considerable computing power even for idealized geometries. For this reason, all previously published simulations of the multifilament fabrics are based on monofilament geometries made of porous materials (Bruschke and Advani, 1993; Papathanasiou, 1996; Papathanasiou, 1997; Phelan and Wise, 1996; Ngo and Tamma, 2001; Nedanov and Advani, 2002; Song et al., 2003; Wong et al., 2006). In such studies, the flow field is divided into two zones of intra-yarn and inter-yarn and solved separately. The intra-yarn zone is obtained via 2-D simulations whereas the inter-yarn zone is often calculated in a 3-D space. Assuming the yarn to be a porous filament greatly reduces the computational requirements, but instead, requires accurate information regarding the yarn’s permeability at each point along the length of the crimped yarns. Our approach, on the other hand, is to model the full 3-D geometry of the multifilament fabrics without splitting the solution domain into inter-yarn and intra-yarn. This allows for the prediction of the fabrics’ permeability as well as the flow pattern among the
filaments and tracking airborne particles through the fabric if needed. In a previous study, we performed a series of porous monofilament simulations based on the permeabilities derived by Gebart (1992) to compare with our full 3-D simulations. It was shown that the lump model underestimates the fabrics permeability by about 15% (Wang et al. 2006).

Consider, for instance, $n$ number of fibers with a length of $l_f$ and a diameter of $d_f$ randomly stacked on top of each other to form a nonwoven fibrous structure. The permeability of this nonwoven medium can easily be calculated via the well known Davis equation upon calculating its SVF. This is because the permeability of such nonwoven structures is only a function of their SVF. Now consider the above fibers divided into four groups of equal count and placed them next to each other to form a woven structure. The SVF of this structure is no longer the only parameter needed for determining its permeability. Our objective in this paper is to study parameters that can affect the permeability of a multifilament fabric.

### 5.3.2-Modeling Structure of Multifilament Fabrics under Tension

Multifilament fabrics consist of warps and wefts, made of randomly (or semi-randomly) packed filaments, woven together in a periodic manner. Systematic study of woven fabrics began in 1937 by Pierce who derived an expression for the geometry of monofilament woven fabrics made of circular yarns. The recent work of Hu 2004 review most relevant literature regarding the geometries of multifilament woven fabrics. Considering some general assumptions, we construct 3-D models of the multifilament woven fabrics. To construct a multifilament woven geometry, we start with its equivalent monofilament replicate having identical center-to-center distance, $L_f$, and yarn diameters. Note that the yarn’s cross-section is normally noncircular because of inter-yarn pressures which lead to yarns in-plane flattening (Hearle 1978, Hu 2004). Our monofilament yarns are assumed to have elliptical cross-sections. Assuming the cross-sections of
the warps being elliptical with their centers located at \(O\left(\frac{L_f}{2}, \frac{d_y}{2}\right)\) and \(O'\left(-\frac{L_f}{2}, -\frac{d_y}{2}\right)\), as shown in Figure 5.9a (ellipses \(e_1\) and \(e_1'\)), we have:

\[
\frac{
\left(x - \frac{L_f}{2}\right)^2
}{\left(\frac{d_x}{2}\right)^2} + \frac{
\left(y - \frac{d_y}{2}\right)^2
}{\left(\frac{d_y}{2}\right)^2} = 1
\]

5-13

and

\[
\frac{
\left(x + \frac{L_f}{2}\right)^2
}{\left(\frac{d_x}{2}\right)^2} + \frac{
\left(y + \frac{d_y}{2}\right)^2
}{\left(\frac{d_y}{2}\right)^2} = 1
\]

5-14

Figure 5.9a also shows another two other settings needed to describe the centerline of the weft yarn. Consider the ellipses with diameters \(d_1 + d_2\), in the x-direction, and \(2d_2\), in the y-direction, to have the same centers as the warp. The large ellipses, also sharing the centers \(O\) and \(O'\), have diameters \(d_1 + 2d_2\), in the x-direction, and \(3d_2\), in the y-direction.

The ellipses \(e_2\) and \(e_2'\) are defined as follows:

\[
\frac{
\left(x - \frac{L_f}{2}\right)^2
}{\left(\frac{d_x + d_y}{2}\right)^2} + \frac{
\left(y - \frac{d_y}{2}\right)^2
}{\left(\frac{d_y}{2}\right)^2} = 1
\]

5-15

and

\[
\frac{
\left(x + \frac{L_f}{2}\right)^2
}{\left(\frac{d_x + d_y}{2}\right)^2} + \frac{
\left(y + \frac{d_y}{2}\right)^2
}{\left(\frac{d_y}{2}\right)^2} = 1
\]

5-16

Similarly, ellipses \(e_3\) and \(e_3'\) are
\[
\frac{(x - \frac{L_f}{2})^2}{(d_x + 2d_f)^2} + \frac{(y - \frac{d_y}{2})^2}{\left(\frac{3}{2}d_y^2\right)} = 1
\]

and

\[
\frac{(x + \frac{L_f}{2})^2}{(d_x + 2d_f)^2} + \frac{(y + \frac{d_y}{2})^2}{\left(\frac{3}{2}d_y^2\right)} = 1
\]

We assume the centerline of the weft yarn in this plane consists of three parts: two arcs, AC and BD, and a connecting straight line, AB. The line AB is tangent to ellipses \(e_2\) and \(e_2'\) and is defined as:

\[
y = -\sqrt{\frac{l_f^2d_y^2}{4} - 3d_y^2\left[\left(\frac{d_x + d_y}{2}\right)^2 - \frac{l_f^2}{4}\right] - \frac{l_f^2d_y}{2}} - \frac{\frac{d_x + d_y}{2}^2 - \frac{l_f^2}{4}}{2}
\]

Substituting (4) into (2.1) and (2.2), we obtain the coordinates of points A and B. Two other lines, \(A'B'\) and \(A''B''\), parallel with the line AB but \(d_y/2\) apart, are intercepted by ellipses \(e_f\), \(e_f'\), \(e_i\), and \(e_i'\) to obtain the coordinates of points \(B', A', B'\), and \(A''\), respectively.

To generate multifilament fabrics, filaments are assumed to be pack in hexagonal arrangement and stay parallel with the yarn’s centerline, i.e., filaments do not cross each other. To change the SVF of a yarn with fixed diameters, the filaments diameters are varied while their count and positions are kept constant. Figure 5.9b shows the unit cell of an elliptical multifilament woven fabric with \(d_x = 0.3\text{mm}, d_y = 0.1\text{mm} \) and \(L_f = 0.35\text{mm}\). Here the yarn’s SVF and filaments diameter are 0.484 and 12\(\mu\text{m}\), respectively.
Figure 5.9: (a) shows the elliptical woven fabric generation algorithm and (b) shows a unit cell of multifilament woven fabric with $d_1 = 0.3\text{mm}$, $d_2 = 0.1\text{mm}$, $L_f = 0.35\text{mm}$ and filament diameter $12\mu\text{m}$.

5.3.3-Modeling Permeability of Woven Fabrics under Tension

A steady state laminar incompressible flow is assumed to prevail inside woven fabrics when exposed to an air flow with a velocity of $0.05 \text{ m/s}$. The finite volume method (Patankar, 1980) implemented in Fluent code is exploited to solve the continuity and the conservation of momentum around the filaments and yarns. The governing equations: continuity, conservation of linear momentum, and energy written in vectorial form are as follow:

\[
\frac{D\rho}{Dt} + \rho \nabla \cdot V = 0
\]

\[
\rho \frac{DV}{Dt} = -\nabla p - \mu \nabla \times (\nabla \times V) + 4/3 \mu \nabla (\nabla \cdot V)
\]
In the above equations $\rho$ and $\mu$ represent air density and viscosity, respectively. Due to the periodicity of the woven geometry, only the unit cell of the weave pattern is considered for the simulations. The yarn’s geometry is imported to Gambit, a preprocessor for Fluent code, via a journal file. The journal file describes all the operations needed to reconstruct the geometry of the yarn. Boundary conditions considered for the simulations are shown in Figure 5.10. Air is assumed to flow into the simulation domain through a velocity-inlet and leaves it from a pressure-outlet boundary condition. The inlet and outlet boundary conditions are placed at a distance, $L$, upstream and downstream of the fabric far from any strong gradients. Symmetry boundary condition is considered for the sides of the computational box. For the air flow on the fiber surfaces, we assumed a no-slip boundary condition as the flow is in the continuum regime. This is because for the air thermal condition and the fiber diameter considered in this paper, the continuum flow prevails. Depending upon the SVF of the yarns, the multifilament fabrics are meshed using 5,000,000 to 10,000,000 tetrahedral elements, refined close to the filament surfaces. Figure 5.11 shows a typical mesh on one of the symmetry planes and Figure 5.12 shows velocity vectors colored by the velocity magnitude inside abovementioned structure.

![Simulation box with boundary conditions](image)

**Figure 5.10:** Simulation box together with boundary conditions
Figure 5.11: An example of the generated mesh on one of the symmetry boundaries is shown.

Figure 5.12: Velocity field shown with velocity vectors inside a 3-D virtual multi-filament woven filter.

Velocity contours in x-y plane and y-z planes in multifilament fabrics have been shown in Figure 5.13 and Figure 5.14, respectively. Successive slices of the multi-filament woven fabric ($d_x = 0.2\text{mm}$, $d_y = 0.2\text{mm}$, $L_f = 0.4\text{mm}$) were taken at levels of 0.05 mm and 0.04 mm along z-direction and x-direction.
Figure 5.13: Top-sectional velocity contours of successive sections taken an increasing depth of 0.05 mm for multifilament woven fabrics.

Figure 5.14: Velocity contours of successive sections in y-z plane taken an increasing depth of 0.04 mm for multifilament woven fabrics.
5.3.4-Results and Conclusions

As mentioned before, in order to simulate the fluid flow through a woven fabric, the solution domain should be meshed. To ensure that our results are mesh-independent, we considered one of our multifilament fabrics and studied the effect of mesh density on its permeability. We increased the number of mesh points around the perimeter of the filaments starting from 7 up to 19. The results of mesh density analysis are presented in Figure 5.15. As it can be seen, increasing the mesh density results in an initial increase in the fabric’s permeability. Further increase in the mesh count beyond 12 points, however, did not show any significant change in the fabrics permeability. All the fabrics simulated in this study have been meshed using tetrahedral elements and with at least 15 grid points around their filaments.

![Figure 5.15: The influence of the mesh density on the filter pressure drop (Permeability)]](image)

In the next subsections we present our simulation results obtained for multifilament fabrics having different structural properties, including yarn’s intra SVF, yarn’s aspect ratio and yarn’s center-to-center distance.
5.3.4.1-Effect of Yarn SVF

To investigate the influence of the yarn solidity on the fabric’s pressure drop, different fabrics with different yarn SVF but identical number of filaments packed in hexagonal arrangement were simulated. This was achieved by changing the diameter of the filament while their positions within the yarn were fixed, as shown in Figure 5.16a.

Figure 5.16a: Multifilament woven fabrics have different occupation ratio, thus different intra yarn SVF.

Figure 5.16b: The influence of filaments’ occupation ratio on the intra yarn SVF.
Figure 5.16c: An increase from 75% to 95% in the filaments’ occupation ratio leads to a 25% increase in pressure drop.

The yarns center-to-center distance was assumed to be 350 µm and the yarns were considered to have an aspect ratio of 3 and a major diameter of 300 µm. It can be seen that the fabric’s yarn intra-SVF increases by increasing the occupation ratio (Figure 5.16b), which can be defined as the ratio of filament diameter to the maximum filament diameter, thus influences the pressure drop (Figure 5.16c). This effect, however, is almost negligible when compared to the influence that the yarns center-to-center (see next section) has on the fabric’s pressure drop. A 20% increase in the yarn SVF, for instance, causes an almost 25% increase in the pressure drop.

5.3.4.2-Effect of Yarn Aspect Ratio

To learn the influence of yarns aspect ratio of the fabric’s pressure drop, we considered two series of multifilament fabrics having identical yarn cross-section area 0.03 mm². These yarns are made up of continuous filaments with a diameter of 12.75 µm (occupation ratio 85%) and 13.88 µm (occupation ratio 92.5) packed together with intra-yarns’ SVFs of 55% and 65%, respectively.
The yarns cross-section is elliptical with an aspect ratio ranging from 1 to 3 (see Figure 5.17a). Figure 5.17b shows the fabric’s pressure drop as a function of yarns aspect ratio. It can be seen that increasing the yarn aspect ratio, fabric’s pressure drop increases. Figure 5.17b also shows the aspect ratio influences on the monofilament woven fabrics which having the yarn’s cross-section of 0.03 mm$^2$ and aspect ratio from 1 to 3. Compared with the pressure drop of multi-filament woven fabric, we noticed a big increase in the pressure drop of monofilament woven fabrics.

Figure 5.17: a) Multifilament woven fabrics have different occupation ratio, thus different intra yarn SVF; b) The influence of filaments’ occupation ratio on the pressure drop of multi-filament woven fabric.
5.3.4.3-Effect of Yarns Center-to-Center Distance

To study the influence of yarns center-to-center distance of the fabric’s pressure drop, we considered a series of multifilament fabrics having identical wefts and warps. These yarns are made up of continuous filaments with a diameter of 12 µm packed together with a SVF of 48%. The yarns cross-section is elliptical with an aspect ratio of 3 and a major diameter of 300µm (see Figure 5.18a).

![Multifilament woven fabrics](image)

**Figure 5.18:** a) Multifilament woven fabrics have different yarn center-to-center distance; b) The influence of yarns’ center-to-center distance on the pressure drop of multi-filament woven fabric.
Figure 5.17b shows the fabric’s pressure drop as a function of yarns center-to-center distance. It can be seen that increasing the distance between the yarns decreases the fabric’s pressure drop. Note that a 10% increase in the yarns center-to-center distance has caused a more than 200% decrease in the pressure drop of the fabric. This indicates that most of the flow goes through the open area between the yarns.
References:


CHAPTER 6

OVERALL CONCLUSIONS & RECOMMENDATIONS FOR FUTURE WORK
6-1 Overall Conclusions

In this thesis a new approach was proposed for simulating the pressure drop and nanoparticle collection efficiency of nonwoven fibrous filters. Our new approach is based on developing computational model geometries that can resemble the internal microstructure of a given fibrous filter. Fluid flow governing equations are numerically solved in these geometries to obtain the velocity and pressure field. This information are then used to calculate the medium’s pressure drop, at a given face velocity, or track trajectories of airborne nanoparticles through the filter. Our results are compared with those obtained from the lumped models developed over that last decades and superior accuracy was observed when compared with empirical data.

From the methodologies developed and demonstrated in this thesis one can conclude that, thanks to the recent progress in the available computing power, it is now possible to model the filtration efficiency (pressure drop and collection efficiency) of a typical air filter and optimize its properties before attempting to set up a manufacturing trail. This new design strategy can significantly reduce the cost of developing new products.

The only constraint that can somewhat limit the extent of our virtual design/testing to reach out to all sects of filtration industry at this date, is perhaps the availability of computational resources. With the fast pace of progress in developing high-performance computers, however, it is expected that such a design optimization procedure will be extensively used in industry in the very near future.
The following specific conclusions are drawn from the research conducted here.

- Modeling Spun-bonded filters, our pressure drop calculation and collection efficiency prediction, unlike the previous models, showed a perfect agreement with the empirical data.

- Modeling filters made of short fibers, we observed that the fiber length has no significant influence on the materials’ though-plane permeability as long as the SVF remains constant.

- Modeling bimodal filter media our results indicate that there exists an area-weighted equivalent average diameter for each bimodal filter that can be used in the existing expressions for calculating the permeability of unimodal filters.

- Conducting numerical simulations for computing the pressure drop of monofilament fabrics with elliptical cross-sections, a logarithmic relationship between the discharge coefficient and the Reynolds number was observed for plain-woven monofilament fabrics having filaments with elliptical cross-sections.

- Our CFD simulations based on the 3-D geometries of idealized multifilament woven fabrics indicate that homogeneous anisotropic lumped model of Gebart (1992) underestimate the permeability of multifilament fabrics at high yarn’s solid volume fractions.
6-2 Recommendations for Future Work

- Non-uniformity of the fibrous structure is crucially important to filtration properties of a filter. To the knowledge of author, there is no comprehensive model capable of predicting the influence of the non-uniformity in collection efficiency and pressure drop of a given filter. Such a model can help to overcome the deficiencies caused by the manufacturing process.

- Most of the cross-sections of the fibers/filaments discussed in this research are circular. One can study the influence of the fibers’ cross-sectional shape on the performance of the media.

- The modeling framework considered in this thesis was constrained by the assumption of no-slip boundary condition at the fiber surface which is only valid for fibers with relatively large diameters (i.e., Knudsen numbers $<< 1$). Future generations of fibrous filters have more nanofiber contents and modeling such media requires a somewhat different wall-boundary treatment.

- Majority of aerosol filter media are electrostatically charged. A similar modeling strategy can be considered for modeling charged filters.

- To the knowledge of the author, no mathematical model exists that can predict the pressure drops of multifilament woven fabrics as a function of the yarn’s tension. Developing such a relationship is of great importance for developing responsive woven fabrics.