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Dual-Scale Modeling of Two-Phase Fluid Transport in Fibrous Porous Media

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DUAL-SCALE MODELING OF TWO-PHASE FLUID TRANSPORT IN FIRBOUS POROUS MEDIA

A Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy at Virginia Commonwealth University.

by

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Abstract

DUAL-SCALE MODELING OF TWO-PHASE FLUID TRANSPORT IN FIBROUS POROUS MEDIA

By Alireza Ashari, MSc

A Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy at Virginia Commonwealth University.

Virginia Commonwealth University, 2010

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The primary objective of this research is to develop a mathematical framework that could be used to model or predict the rate of fluid absorption and release in fibrous sheets made up of solid or porous fibers. In the first step, a two-scale two-phase modeling methodology is developed for studying fluid release from saturated/unsaturated thin fibrous media made up of solid fibers when brought in contact with a moving solid surface. Our macroscale model is based on the Richards’ equation for two-phase fluid transport in porous media. The required constitutive relationships, capillary pressure and relative
permeability as functions of the medium’s saturation, are obtained through microscale modeling. Here, a mass convection boundary condition is considered to model the fluid transport at the boundary in contact with the target surface. The mass convection coefficient plays a significant role in determining the release rate of fluid. Moreover the release rate depends on the properties of the fluid, fibrous sheet, the target surface as well as the speed of the relative motion, and remains to be determined experimentally.

Obtaining functional relationships for relative permeability and capillary pressure is only possible through experimentation or expensive microscale simulations, and needs to be repeated for different media having different fiber diameters, thicknesses, or porosities. In this concern, we conducted series of 3-D microscale simulations in order to investigate the effect of the aforementioned parameters on the relative permeability and capillary pressure of fibrous porous sheets. The results of our parameter study are utilized to develop general expressions for $k_r(S)$ and $P_c(S)$. Furthermore, these general expressions can be easily included in macroscale fluid transport equations to predict the rate of fluid release from partially saturated fibrous sheets in a time and cost-effective manner. Moreover, the ability of the model has been extended to simulate the radial spreading of liquids in thin fibrous sheets. By simulating different fibrous sheets with identical parameters but different in-plane fiber orientations has revealed that the rate of fluid spread increases with increasing the in-plane alignment of the fibers.

Additionally, we have developed a semi-analytical modeling approach that can be used to predict the fluid absorption and release characteristics of multi-layered composite fabric made up of porous (swelling) and soild (non-swelling) fibrous sheets. The sheets
capillary pressure and relative permeability are obtained via a combination of numerical simulations and experiment. In particular, the capillary pressure for swelling media is obtained via height rise experiments. The relative permeability expressions are obtained from the analytical expressions previously developed with the 3-D microscale simulations, which are also in agreement with experimental correlations from the literature.

To extend the ability of the model, we have developed a diffusion-controlled boundary treatment to simulate fluid release from partially-saturated fabrics onto surfaces with different hydrophilicity. Using a custom made test rig, experimental data is obtained for the release of liquid from partially saturated PET and Rayon nonwoven sheets at different speeds, and on two different surfaces. It is demonstrated that the new semi-empirical model redeveloped in this work can predict the rate of fluid release from wet nonwoven sheets as a function of time.
CHAPTER 1 Objectives

The Nonwovens industry is becoming increasingly more sophisticated, and is the fastest growing segment of the fiber and textile complex. Understanding two-phase fluid flow in nonwoven fibrous materials is of great importance in the design and optimization of a variety of products which are extensively used in our daily life. Such products include, but are not limited to, sanitizing wet and dry wipes, incontinence pads, and diapers.

Nonwoven fibrous materials are fibrous webs made up of short or long (filaments) fibers, bonded together to form a textile-like structures. These fibers can be natural, like cotton, or manmade materials like polyester fibers.

Underlying principles in fluid transport in fibrous materials are similar to those of fluid imbibition and drainage in unsaturated granular porous media (e.g., soil). These principles are used to establish cost-effective modeling strategies for simulating performance of fibrous materials in applications involving fluid absorption and release.

The current research is composed of numerical modeling, accompanied with an experimental component both for model validation and completion. The main objective of this project has been to develop a mathematical framework which can be used to model/predict the rate of fluid transport (absorption and release) in fibrous sheets made up of solid (impermeable) and/or porous (fluid-absorbing) fibers. Our model was expected to be capable of predicting the saturation of the wetting fluid inside a fibrous sheet as a
function of time and space. More importantly, it was expected to predict the influence of the sheets microstructural parameters such as porosity, thickness, fiber diameter, fibers’ in-plane and through-plane orientations, and fiber material on the rate of fluid absorption or release. For the case of fluid release simulations (see Figure 1), the model must include the hydrophilicity of the target surface as well as the speed of sheets motion in predicting the rate of fluid release. Our study is aimed at developing valuable guidelines for design and development of new fibrous products.

Figure 1.1: Schematic illustration of a thin fibrous sheet moving on a target surface.

Developing a numerical model that accounts for the influence of all the above microstructural parameters requires excessive computational resources. To circumvent this problem, we have considered a dual-scale modeling approach in which the influence of microstructural parameters is studied via microscale simulations, but the sheet’s saturation profile is obtained using macroscale models (Richards’ partial differential equation, solved via finite element method).

The experimental component of this research is designated to provide empirical coefficients for model adjustment and if validation.
1.1 Novelty of Work

Even though there are a few studies dedicated to modeling fluid absorption in fibrous media, our extensive literature search resulted in no published work on modeling fluid release from fibrous media. The study we are conducting regarding the development of mathematical models for predicting the rate of fluid release as function of the microstructural parameters is the first study of its kind. Moreover, the previous publications failed to discuss the effects of fiber swelling (porous fibers). Also dual-scale modeling has never been implemented for simulating fluid release from fibrous media. In the same manner, our work will also be the first to study the fluid transport in multi-layered and multi-component fibrous structures. In this study, we developed a test method to measure the release performance of the fibrous sheets when moved against a solid surface with different speeds.
CHAPTER 2 Background Information

2.1 Nonwovens

Nonwoven fibrous materials are textile-like structures (webs or mats) made up of fibers (short or long) bonded together mechanically or chemically. Composing fibers can be either natural or synthetic. Drug delivery patches, liquid filtration, air filtration, sanitizing wipes, diapers, and incontinence pads are among many examples of such fibrous products. Figure 2.1 presents examples of nonwovens made of different natural and synthetic fibers.
2.2 Single-Phase Flow in Porous Media

Since fluid flow in a porous medium depends on a number of parameters including fiber diameter, the current study’s main focus is on the outmost significant of those parameters. One of the most important parameters of a porous medium is solid volume fraction (SVF) $\alpha$, defined as the ratio of the total volume of fibers to the bulk volume of the material. Porosity $\varepsilon$ is another way to describe SVF which is defined as $\varepsilon = 1 - \alpha$. Since SVF is defined on an ensemble of fibers, it is considered a global property of a porous medium as opposed to a point property (Bear 1972).

On the same note, another important parameter affecting the flow of a fluid through a fibrous medium is the fiber orientation. Fibrous structures are generally divided into three major categories based on their fiber orientations: random structures (Tomadakis and
Robertson 2005), where fibers’ axes can be randomly arranged in any spatial directions, layered structures (see, for instance, Maze et al. 2007, Zobel et al. 2007), where axes of cylindrical fibers lie randomly in a plane perpendicular to the fluid flow, and unidirectional structures (see, for instance, Chen and Papathanasiou 2006, Chen and Papathanasiou 2008), where axes of the cylindrical fibers are oriented either parallel or perpendicular to the flow direction.

2.2.1 Governing Equations

The majority of fluid flow applications are solved by using the Navier-Stokes equations. These equations are always the governing equations obtained from the principal universal equations in the forms of conservation of mass (continuity) and momentum. For more details regarding derivation of equations, readers are referred to standard fluid dynamic references (see for example, Kundu and Cohen 2008). The Navier-Stokes equations for the incompressible fluid flow through a porous media are simplified to (Kundu and Cohen 2008):

\[ \nabla \cdot v = 0 \]  \hspace{1cm} (2.1)

\[ \rho \left( \frac{\partial v}{\partial t} + v \cdot \nabla v \right) = -\nabla p + \mu \nabla^2 v + \rho F \]  \hspace{1cm} (2.2)

where \( v \) is vector flow velocity having three components in \( x, y \) and \( z \) directions; \( p \) is the fluid pressure, \( \mu \) is the dynamic viscosity, \( \rho \) is the density of fluid, and \( F \) is the external body forces such as centrifugal and gravitational forces. The Reynolds number is defined
as $Re = \frac{\rho U L}{\mu}$ ($U$ and $L$ are characteristic of fluid velocity and length). When $Re$ is small, flow is conditionally linear or laminar (Phillips 1970). In the case of laminar flow, the inertia terms (on the left hand side of the Equation 2.2) become negligibly small compared to the viscous terms (on the right hand side of Equation 2.2), thus resulting in above referenced Stokes equation. By neglecting the external body force, which is usually the case in a single phase flow problem, the Stokes equation can be written as follows (Kundu and Cohen 2008):

$$\nabla^2 v = \frac{1}{\mu} \nabla p$$

(2.3)

which is applicable to fluid flow when $Re<1$.

In 1856 Darcy experimentally demonstrated that volumetric flow rate $Q$ through a porous media is directly proportional to the cross-sectional area $A$, and the pressure drop across the porous media $\Delta p$, and inversely proportional to thickness $T$ of the porous media:

$$Q = -K A \frac{\Delta p}{T}$$

(2.4)

where the proportionality constant $K$ is the medium’s permeability. The negative sign indicates that flow direction goes from the high pressure regime to the low pressure region. Darcy’s law can also be written in terms of superficial velocity $U = \frac{Q}{A}$, fluid viscosity $\mu$, and intrinsic permeability $k$ as (Dullien 1991):
\[ U = -\frac{k \Delta p}{\mu T} \quad (2.5) \]

It is significant to note that unlike the permeability \( K \), the intrinsic permeability \( k \) (having a unit of \( m^2 \)) is only a function of the porous media’s geometry (i.e., independent of the fluid properties). According to the Dupuit-Forchheimer assumption, the relation between superficial velocity \( U \) and local pore velocity \( u \) is defined as \( u = \frac{U}{\varepsilon} \), where \( \varepsilon \) is porosity of the medium. In this work, the term permeability is used to refer to the intrinsic permeability \( k \), unless stated otherwise.

### 2.2.2 Theoretical and Empirical Models to Predict Permeability

Several studies are dedicated solely to the development of theoretical and empirical models for predicting permeability of a fibrous structure. Results of Davies (1973) via dimensionless analysis indicate that permeability \( k \) is only a function of SVF and fiber radius. As mentioned previously, fiber orientation is another important parameter that affects permeability of a fibrous medium. In Figure 2.2 and Figure 2.3, the aforementioned categories are shown with schematic illustrations (see Section 2.2). In the case of a unidirectional structures (UNI) only two unique permeability components of \( k^{UNI}_{TD} = k^{UNI}_{CD} \) and \( k^{UNI}_{MD} \) are necessary to characterize the structure (TD, CD, and MD refer to Thickness Direction, Cross Direction, and Machine Direction, respectively). When flow is perpendicular to the fiber axis (TD and CD), the medium’s pressure drop is higher, \( k^{UNI}_{TD} = k^{UNI}_{CD} \ll k^{UNI}_{MD} \). Likewise, when the structure is layered (LAY), only two permeability...
values are required to characterize the structure as $k_{TD}^{LAY} \ll k_{CD}^{LAY} = k_{MD}^{LAY}$. For the random structures (RAN), $k_{TD}^{RAN} = k_{CD}^{RAN} = k_{MD}^{RAN}$, only one unique permeability exists to characterize the structure (Jaganathan et al. 2008b).

Figure 2.2: Schematic of different fibrous structures based on different fiber orientations a) Unidirectional b) Layered c) Random microstructure (Jaganathan, PhD thesis, NCSU 2009).

Figure 2.3: Schematic of fluid flow in different directions through fibrous porous structure a) unidirectional b) layered c) random, same color represents same permeability (Jaganathan, PhD thesis, NCSU 2009).

Using the Brinkman’s equation, Spielman & Goren (1968) proposed a few analytical expressions for calculating permeability of fibrous structures when the flow is perpendicular ($k_{TD}^{LAY}$) or parallel ($k_{MD}^{LAY} = k_{CD}^{LAY}$) to a layered fibrous medium (see Figure 2.3):
\[
\frac{1}{4\alpha} = \frac{1}{2} + \frac{\sqrt{k_{\text{LAY}}^{\text{TD}}}}{r} \frac{K_1\left(\frac{r}{\sqrt{k_{\text{LAY}}^{\text{TD}}}}\right)}{\sqrt{k_{\text{TD}}}} 
\]

(2.6)

\[
\frac{1}{4\alpha} = \frac{1}{4} + \frac{3}{4} \frac{\sqrt{k_{\text{LAY}}^{\text{CD}}}}{r} \frac{K_1\left(\frac{r}{\sqrt{k_{\text{LAY}}^{\text{CD}}}}\right)}{\sqrt{k_{\text{CD}}}} 
\]

(2.7)

where \( K_1 \) and \( K_0 \) are Bessel functions of second kind, \( r \) is the fiber radius and \( \alpha \) is the solid volume fraction. The following expression is also derived by Spielman and Goren (1968) for flow through isotropic random microstructures, \( k_{\text{CD}}^{\text{RAN}} = k_{\text{MD}}^{\text{RAN}} = k_{\text{TD}}^{\text{RAN}} \) (see Figure 2.3):

\[
\frac{1}{4\alpha} = \frac{1}{3} + \frac{5}{6} \frac{\sqrt{k_{\text{TD}}^{\text{RAN}}}}{r} \frac{K_1\left(\frac{r}{\sqrt{k_{\text{TD}}^{\text{RAN}}}}\right)}{\sqrt{k_{\text{TD}}}} 
\]

(2.8)

For flow parallel to the fibers in unidirectional microstructures, Spielman and Goren (1968) derived the following expression:

\[
\frac{1}{4\alpha} = \frac{1}{2} \frac{\sqrt{k_{\text{MD}}^{\text{UNI}}}}{r} \frac{K_1\left(\frac{r}{\sqrt{k_{\text{MD}}^{\text{UNI}}}}\right)}{\sqrt{k_{\text{MD}}}} 
\]

(2.9)

Davies (1952) proposed another widely used empirical correlation for perpendicular flow through layered fibrous structures as the following:
\[
\frac{k}{r^2} = \left[ 16 \alpha^{1.5} (1 + 56 \alpha^3) \right]^{-1}
\]  

(2.10)

This proves to be in good agreement with the expression of Spielman and Goren (Equation 2.6) for the lower range of SVF (Spielman & Goren 1968).

Using the simple body and face centered cubic representations of three dimensional random fibrous structures and the spectral boundary element method, Higdon and Ford (1996) provided numerical solutions to the permeability of random fibrous structures. Their results are in reasonable agreement with other analytical and experimental studies reported throughout the literature.

### 2.2.3 Virtual Geometries of Fibrous Structures

Three dimensional modeling techniques based on virtual geometries of fibrous structures are the most attractive among researchers. Virtual geometries of fibrous structures have been used by many authors to study the fluid flow in such structures (see for example, Clague and Phillips 1997, Clague et al. 2000, Jeong et al. 2006, Wang et al. 2006, Zobel et al. 2007, Maze et al. 2007). In Figure 2.4, a 3-D model of a nonwoven fibrous structure (virtual geometry) is presented which is used to study the fluid flow and filtration properties (Wang et al. 2006, Zobel et al. 2007). In the virtual structure shown in Figure 2.4, geometries are generated where fibers penetrate into each other or are separated from each other by considering certain inter-fiber spacing. In some cases, fibers may also be allowed to touch each other.
The advantage of virtual geometries relies on their ability to adapt. They can be generated with any required fiber diameter, SVF and fiber orientation. A virtual structure of a filter medium having bimodal fiber diameter distribution is shown in Figure 2.5 (Tafreshi et al. 2009). The structure presented in Figure 2.5 was generated using an algorithm developed originally by ITWM, Germany and implemented in the Geodict code. For instance, virtual geometries generated with unidirectional, layered and random fiber arrangement (Tahir and Tafreshi 2009) are presented in Figure 2.6.

Figure 2.4: Velocity vectors of flow in a virtual 3-D model of nonwoven fibrous media (Wang et al. 2006).
In order to generate more realistic fibrous structures, some authors have introduced crimping and bending of fibers at crossovers in the algorithm of generating the structures (Koponen et al. 1998, Provatas et al. 2000, Faessel et al. 2005, Maze et al. 2007). A growth algorithm developed by Koponen et al. (1998) used to generate a 3-D structure of a paper like material (see Figure 2.7). In the structure shown in Figure 2.7, fibers having a rectangular cross-section were randomly laid in-plane (in x- and y- directions). Furthermore, the fibers were allowed to bend at the point in which they cross over.
Figure 2.6: Virtual geometry of fibrous media with a) unidirectional b) layered c) random fiber arrangements (Tahir and Tafreshi 2009).

Wang et al. (2006) presented a novel technique to generate a 3-D fibrous structure. The $\mu$-randomness method was used appropriately for generating a web of continuous fibers and I-randomness method, resulting in the construction of a web of staple fibers. Zobel et al. (2007) used these techniques to study fluid flow through fibrous structures. Using these techniques, one can implement the actual fiber orientation distribution of a nonwoven structure in generating the virtual geometry.

Obtaining details regarding fiber length, fiber diameter, position, orientation, and curvature of fibers from a real 3-D image of a fibrous structure, Faessel et al. (2005) presents a novel crimped fiber virtual geometry of a fibrous structure. The data was used to generate virtual fibrous structures and generated random, semi-random, and oriented
virtual geometries. Figure 2.8 shows the 3-D virtual geometries generated by Faessel et al. (2005).

Figure 2.7: A 3-D virtual geometry of a fibrous structure (Koponen et al. 1998).

Figure 2.8: 3-D virtual geometries with different fiber orientations a) Random b) semi-random c) oriented fibrous structure (Faessel et al. 2005).

2.2.4 Realistic 3-D Geometries of Fibrous Structures

In this section we explore the several existing techniques to generate the realistic 3-D fibrous structures based on realistic 3-D images. Serial sectioning-imaging is a useful technique to obtain a realistic microstructure of a porous medium imbedded in a polymeric resin. With this technique which is known as the Digital Volumetric Imaging (DVI), 2-D
images are used to virtually reconstruct the original 3-D microstructure (Genabeek and Rothman 1996). Figure 2.9 presents a realistic 3-D fibrous structure generated with the DVI technique (Jaganathan et al. 2008).

Alternatively the X-ray-computed micro-tomography has also been widely used in studying porous materials to generate the realistic 3-D structures; however few works are related to fibrous materials (Maschio and De Arruda 2001, Latz and Wiegmann 2003, Schladitz et al. 2006, Lux et al. 2006). Furthermore, Magnetic Resonance Imaging (MRI) has been used by various authors to obtain a 3-D image of fibrous porous media as another alternative technique (Hoferer et al. 2007). It should be noted that MRI and X-ray tomography are both non-destructive procedures, and have been proved to be quite useful techniques in obtaining pore scale morphology of fibrous structures.

Figure 2.9: An example of 3-D DVI image of a typical hydroentangled nonwoven sample (Jaganathan et al. 2008).
2.3 Two-Phase Flow in Porous Media

There are variety topics which are of great importance to the discussion of nonwoven applications. Fluid flow in the absorption and release of liquid in fibrous media made up of solid and porous fibers and also in composite structures are the focus of the current dissertation. In order to solve these problems, a thorough knowledge of simple two-phase flow problems is very crucial. Understanding the principals of fluid transport (infiltration and/or release) in nonwoven applications such as cosmetic and cleaning wipes, diapers, and medical absorbents are of great interest throughout this dissertation.

Infiltration (absorption) describes the process of moving two or more discrete fluid phases separated by an interface. At the interface, a gradient of density and pressure may be existent between the different phases. There are tangential interfacial forces at the boundaries of the phases at the interface due to existence of the mentioned interface. Interfacial forces are the results of unbalanced cohesion forces between different fluid phases which are presented as the surface tension $\sigma$. The pressure difference across the interface of different phases is balanced with the well known capillary pressure $p_c$ (Dullien 1991). Capillary pressure plays an important role as the driving force on the fluid interface during the infiltration process. Young-Laplace equation is a well known expression which can be used in estimating the magnitude of the capillary pressure as (Dullien 1991):

$$p_c = \sigma \left( \frac{1}{r_1} + \frac{1}{r_2} \right)$$  \hspace{1cm} (2.11)
where \( r_1 \) and \( r_2 \) are the radius of curvatures which exist at the interface of different fluid phases as shown in Figure 2.10.

![Figure 2.10: Schematic of different radius of curvatures and surface tension forces in a fluid-fluid interface (Jaganathan, PhD thesis, NCSU 2009).](image)

However, for the case of circular capillary tube (see Figure 2.11a), Equation 2.11 is reduced to:

\[
p_c = \frac{2\sigma \cos \theta}{r} \tag{2.12}
\]

where \( r \) is the radius of the capillary tube and \( \theta \) is the contact angle of the fluid-solid interface. For the case of fluid flow between two parallel plates (see Figure 2.11b), Equation 2.11 is reduced to (Kundu and Cohen 2008):

\[
p_c = \frac{2\sigma \cos \theta}{b} \tag{2.13}
\]

where \( b \) is the gap between the two plates. Capillary pressure is a parameter which depends on both fluid and geometrical characteristics such as shape, size and distribution of the
pores. Due to the unclear definition of length scale, the fibrous structure in the fluid flow becomes challenging to be defined clearly.

Based on the interactional forces between porous structure and different fluid phases, two-phase problems can be categorized in various ways. In spontaneous infiltration, fluid transport occurs only due to capillary pressure and gravity without any externally applied pressure. In this case, the angle of inclination of the sample ($\alpha$) plays an important role in the direction and magnitude of the gravitational force (see Figure 2.12). Upward infiltration occurs when $\alpha > 0^\circ$ where gravitational forces are against the fluid flow. Downward infiltration occurs when $\alpha < 0^\circ$ where gravity forces are in the same direction of fluid flow. Moreover, horizontal infiltration known as wicking, occurs in the absence of gravitational forces which means that $\alpha = 0^\circ$. 

Figure 2.11: Schematic of capillary fluid flow through a) circular capillary tube b) in-between parallel plates (Jaganathan, PhD thesis, NCSU 2009).
Spontaneous spreading takes place when fluid flow is initiated from a source point. Both spontaneous spreading and spontaneous infiltration occur in the absence of gravitational forces. However, there are some applications in which the fluid is introduced by applying external pressure such as composite molding or as a constant flux.

2.3.1 Governing Equation of One-Dimensional Infiltration into Fibrous Sheet

In a simple experiment, we consider a thin strip of a fibrous sheet which is dipped into an infinite source of liquid at one end as shown in Figure 2.12. In this case the main driving force on the fluid is the capillary force as a result of capillary pressure. The goal is to find the rate of advancing the liquid front or wetted length \( l_e \). For simplicity, it is assumed that the fibrous media is composed of a bundle of circular capillary tubes. In the case of steady-state flow in a circular flow, the well known equation of Hagen-Poiseuille may be considered as the governing equation (Zhmud et al. 2000):

\[
\frac{\rho x x' + x'}{r_c^2} = \frac{2\sigma \cos \theta}{r_c} - \frac{8}{r_c^2} \mu x x' - \rho g x
\]  

(2.14)

where \( r_c \) is the capillary tube radius, \( \rho \) is fluid density, \( \mu \) is fluid viscosity and \( g \) is acceleration due to gravity. By neglecting the gravitational forces and considering a laminar flow, Equation 2.14 is reduced to:

\[
\frac{8}{r_c^2} \mu x x' = \frac{2\sigma \cos \theta}{r_c}
\]  

(2.15)

and after solving the Equation 2.15 results are as follow:
where \( r_e \) is the equivalent capillary radius of the porous medium, and \( l_e \) is the length of the wetted region or advancing front of liquid. Equation 2.16 is Washburn’s widely recognized equation (Mullins et al. 2007), implying that the length of the wetted region \( l_e \) is equal to \( C \sqrt{t} \), where \( C \) is a constant which depends on fluid properties and geometry of the porous medium.

![Figure 2.12: Schematic of a thin inclined fibrous sheet (Jaganathan et al. 2009).](image)

In referring to Washburn’s equation (Equation 2.16), the made assumptions are: unidirectional flow, the region in both sides of interface is fully saturated with different fluid phases, pores are circular capillary tubes and therefore an equivalent capillary radius \( r_e \) is computable (Pan and Zhong 2006, Patnaik et al. 2006, Mullins et al. 2007, Massodi et al. 2007). However, one can see from Equation 2.15 that (Zhmud et al. 2000):
\[
\frac{\sigma \cos \theta r}{4 \mu x} \quad x' \to \infty \quad \text{when} \quad x = 0
\]
(2.17)

which means that the velocity of the fluid at the entrance (x=0) is always infinity. This is known as the irregularity in Washburn’s equation. There has been an abundant amount of research dedicated to modifying Washburn’s equation in order to resolve this irregularity.

Zhmud et al. (2000) modified the Washburn’s equation to:

\[
x(t) = x_\infty \left[ 1 - \exp \left( -\frac{\rho g r}{8 \mu x_\infty} t \right) \right]
\]
(2.18)

where \( x_\infty \) is the steady-state (equilibrium) height which is defined as \( x_\infty = \frac{2 \sigma \cos \theta}{\rho g r} \).

Reed and Wilson (1993) further modified Washburn’s equation by performing the analysis of force balance in an element of fluid in capillary rise:

\[
t = \frac{8 \mu}{g \rho r_c^2} \left[ x_\infty \log_e \left( \frac{x_\infty}{x_\infty - z} \right) - x \right]
\]
(2.19)

Mullins et al. (2007) later used Equation 2.19 to obtain an equivalent capillary radius of the nonwoven fabric in the study of fluid height rise in fibrous samples. Using the energy balance, Massoodi et al. (2007) modified Washburn’s equation even further in predicting the wicking property of polymeric wick as:

\[
l_c = \sqrt{\frac{6 k (1 - \epsilon) \sigma \cos \theta}{\epsilon^2 \mu r}} \sqrt{t}
\]
(2.20)

Even though using Equation 2.20 in predicting the fluid rise in a fibrous sample was not accurate enough, it was found to be in better agreement with the experimental results.
Washburn’s equation is not considered the most appropriate for realistic applications of two-phase flow problems in fibrous media. The base of Washburn’s equation originated from Hagen-Poiseulle’s equation which is derived for the circular capillary tubes. However, extending the application of the equation to a complex fibrous structure is not quite reasonable (Philip 1970). It is essential to know that finding an exact analytical model to obtain equivalent capillary radius of a fibrous structure is almost impossible. As mentioned earlier, Washburn’s equation assumes that the saturation of different fluid phases in the fibrous structure is either zero or one. Therefore, pores are considered to be either fully saturated or fully empty. However, in reality we see that fibrous domain can be partially saturated (saturation can be between zero and one) during absorption and also during the release process. Moreover, Washburn’s equation is only applicable to unidirectional flows and cannot be applied directly to 2-D or 3-D flow regimes.

2.3.2 Richard’s Equation for Partially-Saturated Flow in Porous Media

Darcy’s law can be modified for partially-saturated flows in porous media by considering the permeability $K$ and capillary pressure $p_c$ as function of saturation (Richards 1931, Phillip 1955, Gardner 1958, Dullien 1991, Landeryou et al. 2005). Considering the effects of gravity forces, modified Darcy’s law is written as (Dullien 1991, Landeryou et al. 2005),

$$u = -K(S)\nabla p_c(S) + \rho g \sin \alpha$$

(2.21)
where \( u \) is known as filtration or average velocity and \( S \) is the saturation of wetting phase which is defined as the ratio of the volume of wetting phase to existing pore volume. Also, applying the continuity equation for the transport of wetting phase in porous media we have:

\[
\varepsilon \frac{\partial S}{\partial t} + \nabla \cdot u = 0
\]  
(2.22)

where \( \varepsilon \) is the porosity of the porous media. Combining Equations 2.21 and 2.22, for an inclined fibrous sheet results in (Landeryou et al. 2005):

\[
\varepsilon \frac{\partial S}{\partial t} + \frac{\partial}{\partial x} \left( -K(S) \frac{\partial \rho_c}{\partial x} \right) + \frac{\partial}{\partial y} \left( -K(S) \frac{\partial \rho_c}{\partial y} \right) + \frac{\partial}{\partial x} (-K(S) \rho g \sin \alpha) = 0
\]  
(2.23)

Equation 2.23 can be used for predicting the in-plane fluid infiltration into a thin inclined fibrous sheet. As one can see, Equation 2.23 is highly nonlinear. However, there are some exact analytical solutions and semi-analytical solutions using empirical constants obtained for special cases by Landeryou et al. (2005). In general, solving the Richards’ equation is possible by numerical methods. Nevertheless, diffusive coefficients should be obtained and introduced to the equation. Using chain rules, Equation 2.23 can be expanded to:

\[
\varepsilon \frac{\partial S}{\partial t} = \frac{\partial}{\partial x} \left( K(S) \frac{\partial \rho_c}{\partial S} \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y} \left( K(S) \frac{\partial \rho_c}{\partial S} \frac{\partial S}{\partial y} \right) + \frac{\partial}{\partial x} (K(S) \rho g \sin \alpha)
\]  
(2.24)

where the diffusive coefficient is defined as \( D(S) = K(S) \frac{\partial \rho_c}{\partial S} \). It should be noted that in deriving Equation 2.24, it is assumed that the permeability is the same in x- and y-directions. However, as later in this thesis will be discussed in detail, we expand the application of Richard’s equation to the cases where different permeability exists in
different directions (Ashari et al. 2010). We also expand the application of the Richards’ equation to 3-D problems (Ashari et al. 2011). In order to solve Equation 2.24, expressions of $K(S)$ and $p_c(S)$ are needed.

### 2.3.3 Permeability as a Function of Saturation, $K(S)$

There are different methods used in literature in order to obtain the relation of permeability-saturation. These various methods include Richards’ method, long and short column test, the steady state method, unsteady state method, and air relative permeability measurement (Corey 1994 and Collins 1961). However, these existing empirical correlations were mainly obtained for the application of two-phase flow in soil as the porous media. One of the most famous methods proposed by Brooks and Corey (1964) is to use the well-known power law relation between permeability and saturation as:

$$K(S) = K_s S^n$$

(2.25)

$$n = \frac{2 + 3\lambda}{\lambda}$$

(2.26)

where $\lambda$ is the index of pore-size distribution and $K_s$ is single-phase or absolute permeability of the fibrous sample when $S=1$. For the majority of applications of the two-phase flows in porous structures, Brooks and Corey (1964) propose a value of $n = 4$. For the uniform porous media with a single pore size, $\lambda \rightarrow \infty$ and then $n \rightarrow 3$. The value of $\lambda$ is smaller than the value for porous media with a wide range of pore diameters. van

\[
K(S) = S^{1/2} \left( 1 - \left( 1 - S^m \right)^n \right) \]

(2.27)

where \( m \) is an empirical constant. Proposed empirical permeability-saturation relationships by Brooks and Corey (1964) and also van Genuchten (1980) are originally obtained for the applications of two-phase flow in soil as a porous media. Furthermore in the cases of nonwoven materials, the credibility of these relations should be investigated. By performing an experiment on an inclined nonwoven sample with different range of flow rates, Eames et al. (2003) and Landeryou et al. (2005) obtained the following permeability-saturation relationship as:

\[
K(S) = K_s S^3 \]

(2.28)

where \( K_s \) is single-phase or absolute permeability of the fibrous sample when \( S=1 \). One can see that Equation 2.28 is similar to Equation 2.25 proposed by Brooks and Corey (1964) with the value of \( n=3 \) which implies that the fibrous sample has almost uniform pore size. In addition, Landeryou et al. (2005) found a critical percolation threshold for the permeability-saturation curve at the point of \( S=0.4 \) where permeability goes to zero where \( S \leq 0.4 \) rapidly.
2.3.4 Capillary Pressure as a Function of Saturation, $p_c(S)$

Predicting the capillary pressure-saturation functionality has been performed in different approaches in literature. The height rise test, better known as the *long column test*, is one of the existing methods. In this method the fibrous sample (narrow strips of nonwoven fabric) is mounted vertically and moved above a fluid reservoir (a beaker). In this test, the fluid is allowed to be absorbed against the gravity into the sample from the bottom. The process of fluid absorption will be continued for a certain amount of time until the equilibrium height is reached. At the equilibrium, the advancement of fluid front is stopped and the driving force of capillary pressure is balanced with the gravitational force. Continuing, the sample is cut into equal segments when the fluid reaches the equilibrium height and saturation of each segment is obtained from a weight analysis. Additionally, the value of capillary pressure in each segment is obtained by $\rho g h$ where $h$ is height of segment from the datum line (Collins 1961 and Ghali et al. 1994).

The centrifuge method is another method used in release process, which a fully wetted sample is centrifuged at different rotational speeds until sample reaches the equilibrium saturation. Capillary pressure is then obtained as a function of rotational speed (Corey 1994).

Another alternative is the pressure cell method which is mainly used in soil. In this method the fibrous sample is mounted on a semi-barrier membrane. In the semi-barrier membrane only the wetting phase of fluid can pass through. Sample and semi-barrier membrane are placed inside a pressurized test chamber. By decreasing the pressure of the
test chamber gradually, the wetting phase can be penetrated into the fibrous sample. Since the volume of absorbed wetting fluid is known, the saturation-capillary pressure relationship can be obtained (Landeryou et al. 2005).

There are many empirical correlations in literature which express the functionality of capillary pressure verses saturation which are mostly obtained for the soil-like pours media. Among all, the correlations of Brooks and Corey (1964), van Genuchten (1980), Landeryou et al. (2005) and Haverkamp et al. (1977) are more popular. Correlation of Brooks and Corey (1964) is given as:

\[
S = \left( \frac{p_d}{p_c} \right)^{\lambda}
\]  

(2.29)

where \( p_d \) is the air-entry pressure (bubble point pressure), and \( \lambda \) is pore diameter index, as explained in Equation 2.26. Also, correlation of van Genuchten (1980) is given as,

\[
S = \left( \frac{1}{1 + (\alpha p_c)^n} \right)^m
\]

(2.30)

where \( \alpha \) is an empirical coefficient, \( m = 1 - \frac{1}{n} \) where \( n \) is an empirical constant which represents the variation of pore diameter distribution. The empirical correlations of Landeryou et al. (2005) and Haverkamp et al. (1977) are given as:

\[
S = \exp\left( \frac{p_c}{p_c} \right)
\]

(2.31)

\[
S = \frac{1}{1 + \left| p_c \right|^b / C}
\]

(2.32)
where $p^*_c$, $b$, and $C$ are empirical coefficients. It is significant to note that Equation 2.31 (Landeryou et al. 2005) was obtained originally for fibrous samples.

2.3.5 Numerical Methods to Solve Richards Equation

In order to solve the saturation form of Richards’ equation (Equation 2.24), it is necessary to substitute the correlations of permeability-saturation and capillary pressure-saturation as discussed in sections 2.3.3 and 2.3.4 into Equation 2.24. One can see that Richards’ equation, even in the simplest form of 1-D, is highly non-linear and must be solved numerically. Among all existing numerical methods, finite element and finite difference methods are the most effective and popular methods in solving Richards’s equation (Narashimhan and Witherspoon 1976, Haverkamp et al. 1979, Huyakorn et al. 1986, Ashari and Tafreshi 2009a, Ashari et al. 2010 and Ashari et al. 2011).

2.4 Microscale Modeling of Transport Properties

As mentioned in section 2.3.5, quantitative analysis of two-phase flow in unsaturated porous media requires functional relationships between the fluid saturation and capillary pressure as well as fluid saturation and relative permeability. These constitutive relations can be obtained both experimentally and numerically, although the experimental methods have been the only viable approach in past decades. The recent advances in full-morphology (FM) modeling (Hazlett 1995, Hilpert and Miller 2001, Vogel et al. 2005, Schladitz et al. 2006, Schulz et al. 2007), have made it possible to obtain such relationships
via microscale modeling. Hilpert and Miller (2001) developed a novel quasi-static microscale (pore-scale) approach for modeling drainage in porous media. They used the concept of pore morphology and local pore-scale physics in their approach which is very similar (with some slight differences) to methods developed by Hazeltt (1995) based on size and connectivity analysis of the digital pore space. They presented a sphere packing procedure in a non-overlapping manner (see Figure 2.13). They found good agreement with experimental observations with their drainage simulations. The Lattice-Boltzmann method has been used in the past as another pore-scaling modeling method in solving drainage. Hilpert and Miller (2001) expressed that the morphology-based model is inexpensive due to less memory and CPU time requirements.

![Figure 2.13: Two-dimensional presentation of release simulation in a two-dimensional pore space for three different stages of capillary pressure of a, b and c. The solid phase is shown in black color while non-wetting phase is shown in red color (Hilpert and Miller 2001).](image)

Vogel et al. (2005) compared three existing models: Lattice-Boltzmann (LB), Full-Morphology (FM) and Pore Network (PN) models in determining capillary pressure-saturation relationship in the porous structure of a macroscopically homogeneous porous
medium (sintered glass). It was concluded that the computational demands of the LB approach are almost five orders of magnitude higher than the other two simpler models as far as calculation time is concerned, and three orders of magnitude higher with respect to required computational memory. They also found that the results of capillary pressure versus saturation curves are consistent among all different methods (see Figure 2.14). However, Vogel et al. (2005) mentioned that the simplified models of FM and PN overestimate the value of saturation in a given capillary pressure due to the required assumption of considering spherical shape in the wetting–nonwetting interface.

![Figure 2.14: Results of capillary pressure–saturation prediction obtained by Vogel et al. (2005) based on different models of Lattice-Boltzmann (thick dashed line), full-morphology (two solid lines) and network model (gray shaded).](image)

Schultz et al. 2007, following the work of Hazlett (1995) and Hilpert and Miller (2001), developed a FM model for studying the two-phase characteristics of the gas diffusion medium in a polymer electrolyte fuel cell. They use the FM method to obtain the
capillary pressure versus saturation curve in drainage process. In their work, based on microstructural properties such as fiber diameter, fiber orientation, and porosity, the microstructure of nonwoven carbon paper is reconstructed based on using a stochastic generation method.

Jaganathan et al. (2008b) used Digital Volumetric Imaging (DVI) to obtain microstructure of a typical hydroentangled nonwoven fabric, and performed a series of numerical simulations to determine the single phase permeability of their media (see Figure 2.15).

![Figure 2.15: An example of flow path-lines through a fibrous medium obtained by Jaganathan et al. (2008b). Flow path-lines are colored by velocity magnitudes.](image)

Using microscale modeling techniques is almost the most accurate way of determining properties of a porous fibrous medium. However, because of its computational requirements, this method has limited utility.
2.5 Macroscale Modeling

In contrast to microscale modeling, macroscale modeling techniques are by far more affordable. Using macroscale modeling gives us the opportunity to model the entire dimensions of a product. However, with this simplicity we have to scarify the precision that can be obtained via microscale modeling techniques. In a macroscale model, the fibrous domain is considered a lumped medium. Macroscale properties of such a lumped model (SVF, permeability, capillary pressure, etc.) are obtained either analytically or empirically and fed to the macroscale governing equations (Richards’ equation, here).

Landeryou et al. (2005) used Richards’ equation to simulate fluid infiltration in a nonwoven PET fabric at macroscales. However, they obtained capillary pressure and permeability expressions via experimental (see Figure 2.16). In addition, they performed a series of experiments to compare their modeling with experimental results. Mao and Russel (2003) predicted an unsteady rate of fluid flow in homogenous anisotropic nonwoven structures, as well as heterogeneous patterned nonwoven fabrics having dual-scale porosities. They used Richards’ equation in different areas of the nonwoven structure having different permeabilities and different porosities. However, Mao and Russel (2003) used existing experimental and analytical relationships for capillary pressure and permeability expressions.
Figure 2.16: Experimental results obtained by Landeryou et al. (2005) for functionality of
a) capillary pressure and b) permeability verses saturation.

The work of Nabipour et al. (2008) on macroscale modeling of two phase flows in
soils should also be noted within this discussion. Nabipour et al. (2008) also used existing
experimental relationships for permeability and capillary pressure of their media. Nasseri
et al. (2008) refined the existing analytical methods to solve the 1-D unsteady Richards’
equation. However, similar to the above-mentioned studies, they also used existing
experimental relationships for capillary pressure and permeability of their media.

2.6 Dual-Scale Modeling

As we mentioned in section 2.5, macroscale modeling is simple, computationally
affordable, and gives us the chance to consider the full scale of the real sample in our
study. However, because the microscale movement of fluid around the fibers can not be
predicted in macroscale, precision is lower than microscale modeling results. Furthermore,
constitutive equations of capillary pressure-saturation and permeability-saturation should
be introduced to the model. As mentioned in section 2.3.4, there are many empirical
correlations of capillary pressure-saturation and permeability-saturation which have been obtained mainly for application of two-phase flow in soil-like porous media. Nevertheless, there is almost no significant relation for the application in nonwoven and fibrous samples. Those empirical equations that exist in the literature for fibrous samples were developed mainly for specific samples with known structural properties (such as SVF and fiber diameter) which cannot be directly applied for the fibrous structures with different structural properties. In this regard, to increase the precision of necessary constitutive equations (capillary pressure-saturation and permeability-saturation) for the relevant SVF and fiber diameter of structure, we obtained these relations using the micro-scale modeling techniques described in section 2.4. Once we obtained the necessary constitutive equations in the microscale, we implement them in the macroscale framework and governing equations of two-phase flow, such as Richards’ equation, to predict the saturation profile.

The only example of a dual-scale two phase flow modeling in fibrous nonwoven media is the work of Jaganathan et al. (2009) in which 1-D Richards’ was used to predict fluid infiltration rate in thin inclined fibrous sheets. In Figure 2.17 we present results of their microscale permeability simulations. The capillary pressure expression in the work of Jaganathan et al. (2009) was obtained experimentally (see Figure 2.18). These authors compared their results with own experiments or those available in the literature (see Figure 2.19).
Figure 2.17: Permeability-saturation result obtained via micro-scale modeling. Results are shown in a dimensionless form, $K/K_s$ (Jaganathan et al. 2009).

In the current project, we use dual-scale modeling for both absorption and drainage simulations in composite media, for the first time. Our literature search shows no previous work conducted for studying fluid release from fibrous media. Similarly, no work has been reported on modeling fluid absorption in multi-layered fibrous sheets with three-dimensionally anisotropic microstructure. Figure 2.20 shows a schematic presentation of dual-scale modeling technique that we use in our release model.
Figure 2.18: Experimental results of capillary pressure-saturation of wetting phase obtained by Jaganathan et al. (2009). Empirical correlations of van Genuchten (1980) and Landeryou et al. (2005) are fitted to the results.
Figure 2.19: Results obtained from numerical solution of Richards’ equation compared with experimental result based on a) wetted length verses time for inclination angle of 90° and b) saturation profile verses distance from the datum line at t=1000 s for various inclination angles (Jaganathan et al. 2009).
Figure 2.20: Schematic showing the concept of dual-scale modeling.
CHAPTER 3 A Two-Scale Modeling of Motion-Induced Fluid Release from Thin Fibrous Porous Media

Content of chapter is published in Chemical Engineering Science, 64, pp 2067-2075 (2009) in an article entitled “A Two Scale Modeling of Motion-Induced Fluid Release from Thin Fibrous Porous Media”, by Ashari, A. and Tafreshi, H.V.

3.1 Introduction

Fluid delivery via fibrous materials has become widely popular in recent years. Drug delivery patches, sanitizing wipes, facial scrubs, and very many other hygiene and industrial products take advantage of the unique properties of the fibrous materials in storing a fluid and releasing it when brought in contact with moving or absorbing solid surfaces. Underlying principles in fluid absorption and/or release in/from fibrous materials is similar to those of fluid imbibition and drainage in unsaturated granular porous media. These principles will be used here for establishing modeling strategies to include microscale properties of fibrous media in developing predictive numerical models for cost-effective product design and development.

Two-phase flow in porous media has been studied in various fields via numerical simulations and experiments. These include, but are not limited to, underground oil and gas fields (Ciegi et al. 2006), water absorption in concretes (Lockington and Parlange 2003), and rocks (Li 2008) among many others. Literature of fluid modeling in unsaturated fibrous media, on the other hand, is somewhat scarce. Most of the published works on
fibrous media are only concerned with fluid absorption with no attention to the fluid release. The majority of these works are experimental (see, for instance, Hsieh and Yu 1992, Miller and Schwartz 2000) although there are some numerical simulations available as well (see, for instance, Thompson 2002, Mao and Russell 2003, and Lucas et al. 2004). For a complete review of the previous works on fibrous media readers are referred to the recent book of Pan and Gibson (2006).

In this work, for the first time, we present a two-scale two-phase 3-D modeling work aimed at simulating the release of delivery fluid from thin fibrous sheets when rubbed against a targeting surface. Our work is based on developing 3-D microscale models resembling internal geometry of fibrous sheets. The virtual geometries will then be used in establishing relationships for the relative permeability and capillary pressure in terms of medium’s saturation. These relationships are hence implemented in a macroscale model, based on the Richards’ equation (Richards 1931) for fluid propagation in unsaturated porous media.

Section 3.2 describes our macroscale model for release rate prediction. The required constitutive equations are obtained via microscale modeling and are described in detail in section 3.3. In this section, we first explain our 3-D fibrous microstructures and then describe how these microscale geometries are used to calculate absolute permeability, relative permeability, and capillary pressure needed for the macroscale model. Here, we also review relevant empirical correlations and discuss them in the context of our simulations. Numerical simulation of Richards’ equation and the deployed boundary conditions are discussed in section 3.4. Finally, our fluid release results are presented in
section 3.5 together with a discussion on the influence of the mass convections coefficient, kf, on the release rate.

### 3.2 Macroscale Modeling via Richards’ Equation

In this section we present our macroscale model based on the Richards’ equations. Starting with the conservation of mass in a 1-D domain for the wetting phase, we obtain (Scheidegger 1974):

\[
\varepsilon \frac{\partial S}{\partial t} + \frac{\partial v_z}{\partial z} = 0
\]

where \( \varepsilon \) is the porosity of the media and \( S \) is the fluid saturation, i.e., the ratio of liquid volume to that of the pores and \( v_z \) is the fluid velocity in the z-directions (thickness direction). Assuming a creeping flow, we utilize the Darcy’s law (Dullien 1991):

\[
v_z = \frac{-K(S) \frac{\partial p_c}{\partial z}}{\mu}
\]

where \( K(S) \) is permeability of the medium (a function of saturation) and \( p_c \) is the capillary pressure. \( \mu \) is the fluid viscosity. Here we assume the gas pressure to be equal to the atmospheric pressure. Combining conservation of mass (Equation 3.1) and Darcy’s law for the liquid phase (Equation 3.2) results in a single diffusive equation (Landeryou et al. 2005) for saturation (\( S \)):

\[
\varepsilon \frac{\partial S}{\partial t} + \frac{\partial}{\partial z} \left( \frac{-K(S) \frac{\partial p_c}{\partial z}}{\mu} \right) = 0
\]

Since the capillary pressure \( p_c \) is a function of saturation (\( S \)), we obtain:
\[
\varepsilon \frac{\partial S}{\partial t} = \frac{\partial}{\partial z} \left( \frac{K(S) \partial p}{\mu} \frac{\partial S}{\partial z} \right)
\]  

(3.4)

Equation 3.4 is a nonlinear scalar 1-D partial differential equation which needs to be solved numerically. In this paper, we solve this equation to simulate fluid release from fibrous media. Note that as the material is assumed to be hydrophilic and so the fluid will not drain spontaneously. This means that an external mechanism is required to extract the fluid from the medium.

Fluid transport out of the medium depends on the surface energy of the target surface (contact angle between the fluid and the target surface) as well as the speed of the relative motion between the sheet and surface. In this work, we model this with a mass convection boundary condition. The convection coefficient used in the formulation, incorporates the effect of the speed and the properties of the surface and needs to be obtained empirically.

It is worth mentioning that the model considered in this work is not exactly what one may expect to use for modeling a drying process. Drying of a wet sheet is due to the gradient of species (water vapor) concentration in an air-vapor bicomponent mixture (see Vahedi Tafreshi et al. 2006 for more details). Our formulations here are written for the liquid phase (e.g., water). The ambient air outside the porous medium is not included in the model and evaporation is ignored due to the dynamics of the system.
3.3 Constitutive Equations from Microscale Modeling

Quantitative analysis of two-phase flow in unsaturated porous media requires functional relationships between the fluid saturation and capillary pressure as well as fluid saturation and relative permeability. These constitutive relations can be obtained both experimentally and numerically, although the experimental methods have been the only viable approach in the past decades. The recent advances in Full-Morphology (FM) modeling (Hazlett 1995, Hilpert and Miller 2001, Vogel et al. 2005, Schladitz et al. 2006, and Schulz et al. 2007), has made it possible for us to obtain such relationships via microscale modeling. In the following section, we present our microscale modeling aimed at obtaining relevant correlations for the capillary pressure and relative permeability as functions of medium’s saturation.

3.3.1 Generating Fibrous Microstructures

Microstructure of a fibrous media can either be obtained by 3-D imaging (see for instance, Jaganathan et al. 2008a,b,c and Jaganathan et al. 2009) or by constructing a digital microstructure based on stochastic models (see for instance, Wang et al. 2006, Maze al. 2007). The latter has been considered in the current work. Most of the nonwoven fibrous materials can be assumed to be 3-D “layered” structures. Our media is assumed to be composed of polyester fibers with an average fiber diameter of 15µm and a Solid Volume Fraction (SVF) of 10%. Fibers are randomly oriented in the xy-plane (in-plane) and are horizontally stacked on top of one another to form a “layered” 3-D structure. In addition, the fibrous system is assumed to be macroscopically homogeneous in the in-plane...
direction. We used the GeoDict code from Fraunhofer-IWTM Germany in generating our 3-D microstructures. GeoDict is a voxel-based code in which each voxel is either “empty” or “filled” (or solid). In our case, fluid domain and solid fibers are represented by empty and filled voxels. The fiber orientation distribution is controlled by a density function \( p(\phi, \varphi) \) in polar coordinates, in which \( \phi \) is the through-plane angle and \( \varphi \) is the in-plane angle (Schladitz et al. 2006). For the above-mentioned 3-D layered media, \( p(\phi, \varphi) \) can be expressed as:

\[
p(\phi, \varphi) = \frac{1}{4\pi} \frac{\beta \sin \phi}{(1 + (\beta^2 - 1)\cos^2 \phi)^{3/2}}
\]

where \( \beta \) is the anisotropy parameter. It should be noted that due to assumed isotropy in the xy-plane, \( p(\phi, \varphi) \) is independent of polar coordinate, \( \varphi \). The case of \( \beta = 1 \) describes a three-dimensionally isotropic system. By increasing \( \beta \), fibers tend to become parallel to the xy-plane and form a layered structure. In other words, the fiber orientation of the stochastic microstructure generation is reflected by the anisotropy factor \( \beta \), and it has to be set to a large value to suppress fibers from orienting in the z-direction. This algorithm has been fully described by Schladitz et al. (2006) and is implemented in GeoDict code. Note that it is assumed here that fibers are continuous and their curvature (crimp) is negligible. In the current study, a simulation domain with a size of 450×450×300 voxels with a resolution of 2µm/voxel has been used as shown in Figure 3.1.
Figure 3.1: Two different views of the virtual fibrous microstructure considered in this work. The domain size is 450×450×300 voxels with each voxel being 2µm.

3.3.2 Capillary Pressure as a Function of Saturation

Leverett in 1939 was the first who obtained an empirical relationship between the capillary pressure and saturation, the Leveret function, for granular porous media. Since the seminal work of Leverett (1939), there have been many studies in the past decades, dedicated to establishing a relationship between capillary pressure and saturation. Almost all of these works, however, were conducted for underground and/or soil applications (see
Haverkamp et al. 1977, van Genuchten 1980, Udell 1983, Udell 1985, Wang and Beckerman 1993, Eames et al. 2003, and Ishakoglu and Baytas 2005). To the knowledge of the authors, the only correlation originally developed for fibrous materials is that of Landeryou et al. (2005) who used an auto-porosimeter to study liquid rise in nonwoven needle-felt fabrics. Note that the correlation of Landeryou et al. (2005) was obtained for in-plane (as opposed to through-plane) fluid flow in fibrous media. The empirical correlation of Landeryou et al. (2005) is shown in Table 3.1 along with those of Haverkamp et al. (1977), van Genuchten (1980), and Leverett (1939) and their corresponding empirical coefficients. These empirical coefficients depend on the microstructure of the porous media and need to somehow be obtained for a given material. In the present study, we perform a series of microscale simulations to obtain our own capillary pressure-saturation data and use them to find the above-mentioned required empirical coefficients.

Unlike previous studies, here we use a morphological method to obtain a relation between the capillary pressure and media’s saturation. Here, Young-Laplace equation is used to identify the capillary radius, \( r_c \), corresponding to a given capillary pressure:

\[
p_c = \frac{2\sigma \cos \theta}{r_c}
\]

(3.6)

where \( \sigma \) is the surface tension between wetting and non-wetting phase and \( \theta \) is the contact angle between wetting and solid phases. Here we used a contact angle of 80 degree based on the work of Zhu et al. (2005). In this technique, morphological openings are used to determine parts of pore space where spherical structuring elements could be fitted.
Table 3.1 Different empirical correlations proposed for capillary pressure-saturation relationship

<table>
<thead>
<tr>
<th>Model</th>
<th>Correlations</th>
<th>Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Leverett (1939)</td>
<td>( p_c = a S + b S^2 + c S^3 + d )</td>
<td>( a= 2650.58 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( b=-13504.58 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( c=27472.38 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( d=-16376.12 )</td>
</tr>
<tr>
<td>Haverkamp et al. (1977)</td>
<td>( S_e = \frac{S - S_i}{1 - S_i} ) for ( p_c &lt; 0 )</td>
<td>( S_i=0 )</td>
</tr>
<tr>
<td></td>
<td>( S_e = \frac{1}{1 +</td>
<td>p_c</td>
</tr>
<tr>
<td></td>
<td>( S_e = 1 ) for ( p_c \geq 0 )</td>
<td>( b=3.93 )</td>
</tr>
<tr>
<td>Van Genuchten (1980)</td>
<td>( S = \left(1 + \left(\frac{p_c}{p_c^*}\right)^{\gamma \alpha m}\right)^n )</td>
<td>( p_c^* = 768.76 )</td>
</tr>
<tr>
<td></td>
<td>( m = 1 - \frac{1}{n} )</td>
<td>( n=4.43 )</td>
</tr>
<tr>
<td>Landeryou et al. (2005)</td>
<td>( S = \exp\left(\frac{p_c}{p_c^*}\right) )</td>
<td>( p_c^* = -500.27 )</td>
</tr>
</tbody>
</table>

without intruding the fiber boundaries. This process corresponds to the concept of granulometry discussed by Soille (1999). Liquid intrusion and extrusion porosimetry can be simulated using this approach. In the current paper, we use a modified full-morphology
algorithm developed based on the works of Hazlett (1995) and Hilpert and Miller (2001) and implemented in the Geodict Code (a detailed description of the implementation can be found in Schultz et al. 2007 and Becker et al. 2008). Steps involved in simulating this quasi-static fluid intrusion are as briefly described below.

This algorithm assumes that the pore space of the medium is initially filled with the wetting phase and the medium is connected from one side to a large reservoir of nonwetting fluid. The nonwetting fluid, then, intrudes into the fibrous structure as the reservoir’s pressure is increased. Based on the Young-Laplace equation (Equation 3.6), it is assumed that only a certain pore diameters can be intruded for each pressure increment. In order to simulate fluid intrusion, we first consider a spherical structuring element ($B_r$) of radius of $r$ which is then used in a morphological operation “erosion” of pore space defined as:

$$\varepsilon_{B_r}(X) = \{ x : B_{x,r} \subseteq X \}$$  \hspace{1cm} (3.7)

where $X$ is the pore space and $B_{x,r}$ is the structuring element centered at point $x$ (Schulz et al. 2007). The radius $r_c$ of these structuring elements is obtained using the Young-Laplace equation (Equation 3.6) for particular given capillary pressure. This erosion operation results in the center points, where a given sphere can fit without intruding the fiber boundaries. Note here that erosion operation gives all possible center points in a domain where a given sphere could be fitted, but we only need those eroded regions which are directly or indirectly connected to nonwetting fluid reservoir which is kept at one end of domain. So we remove all those eroded space which are not connected to the reservoir,
this process is called connectivity analysis. Mathematically, this connectivity analysis of pore space to reservoir \( C_R X \) (where \( R \) is subspace of \( X \) to be connected to reservoir) is defined as: \( C_R X = \{ x \in X : \exists x_0 \in R : \exists \) path in \( X \) connecting \( x \) to \( x_0 \} \) (Becker et al. 2008).

Although the above steps give center points where a given sphere could be fitted, it does not actually provide actual pore volume intruded for a particular pressure. The eroded space (center points) is then dilated using the same structuring element defined as:

\[
D_{x,r} [e_{B_{x,r}} (X)] = \{ x : B_{x,r} \cap e_{B_{x,r}} (X) \neq \emptyset \} \tag{3.8}
\]

Once this dilation step is completed, pressure is incremented in predetermined steps to find the next smaller structuring element, using the Young-Laplace equation, and the above procedure is repeated. Note that the nonwetting fluid reservoir can be placed at any side of the simulation domain. Here all other boundaries are assumed to be impermeable to the fluid. Also note here that since the full-morphology model treats the nonwetting fluid intrusion problem as a purely geometric problem, it is not sensitive to the fluid’s contact angle or surface tension (Schulz et al. 2007).

An important step in the above procedure is connectivity of the intruding fluid to the reservoir. Ignoring this step, one obtains what is called the Geometric Pore Size Distribution (GPSD) of the material (Jaganathan et al. 2008c). In the case of GPSD, the erosion process is directly followed by the dilation without checking for the connectivity. This procedure is called “opening” the pore space by structuring element \( B_r \),

\[
O_r (X) = \bigcup \{ B | B \subseteq X \} \tag{3.9}
\]
A detailed comparison of full morphology method with other image analysis technique could be found in Vogel et al. (2005).

Simulation domain and the drainage process are shown in Figure 3.2. The domain is connected to imaginary reservoirs of wetting and non-wetting phases from bottom and top boundaries, respectively. It can be seen that by increasing the capillary pressure, air progressively enters the domain and replaces the wetting phase (water). In this Figure, red represents the non-wetting phase. Figure 3.3 is obtained by plotting the capillary pressure versus the corresponding wetting phase saturation during the drainage process.

In order to find a relevant correlation for the capillary pressure-saturation relation, our FM results (Figure 3.3) are fitted with the proposed empirical correlations of Leverett (1939), van Genuchten (1980), Haverkamp et al. (1977), and Landeryou et al. (2005) and the necessary coefficients are obtained from the curve fitting (see Figure 3.4). It can be seen that both van Genuchten (1980) and Haverkamp et al. (1977) correlations show relatively good agreement with our morphology data. The Leverett function, on the contrary, shows somehow different trends. Except for the saturations close to 1, the logarithmic correlation of Landeryou et al. (2005) also presents an acceptable prediction. Our curve fitting resulted in \( a = 2650.58, b = -13504.58, c = 27472.38 \) and \( d = -16376.12 \) for the correlation of Leverett (1939), and \( p_{c}^* = 768.76 \) and \( n = 4.43 \), for that of van Genuchten (1980). In addition, we obtained \( C_i = 877.98, b = 3.93 \) and \( S_i = 0 \) for the correlation of Haverkamp et al. (1977), and \( p_{c}^* = -500.27 \) for that of Landeryou et al. (2005).
Figure 3.2: Morphological simulation of wetting phase drainage from a fibrous medium. Corresponding capillary pressures are a) 385 Pa, b) 646 Pa, c) 748 Pa, d) 888 Pa, e) 1233 Pa, and f) 3500 Pa. The non-wetting phase is shown in red.

As mentioned earlier, we have implemented the Richards’ equation in a macroscale model for simulating the fluid release from a fibrous sheet. We used the correlations of
Haverkamp et al. (1977) and Landeryou et al. (2005) in our macroscale simulations (see the next sections) and compared their results.

Figure 3.3: Capillary pressure versus saturation obtained from our morphological analysis.

Figure 3.4: Different correlations are fitted to our morphological data to obtain the required empirical coefficients for each correlation.
3.3.3 Relative Permeability-Saturation Relationship

Absolute permeability can be defined as the proportionality constant between the average fluid velocity and the applied pressure gradient which is calculated when the entire pore space is filled with a single-phase fluid. To compute the absolute permeability of our media, we solve the Stokes equations with periodic boundary conditions using the finite difference method of the GeoDict code. The Stokes equations for conservation of mass and momentum are as follow:

\[
\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0
\]  
(3.10)

\[
\frac{\partial p_x}{\partial x} = \mu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right)
\]  
(3.11.1)

\[
\frac{\partial p_y}{\partial y} = \mu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right)
\]  
(3.11.2)

\[
\frac{\partial p_z}{\partial z} = \mu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right)
\]  
(3.11.3)

where \( v_x, v_y, \) and \( v_z \) are velocity in the x, y, and z directions, respectively. GeoDict treats each voxel as a computational cell and circumvent the mesh generation process in the complex 3-D geometry of a fibrous medium. Based on the Darcy’s law the relation between mean velocity and pressure drop in each direction are as follow:

\[
v_x = \frac{1}{\mu} \left( k_{xx} \frac{\partial p_x}{\partial x} + k_{xy} \frac{\partial p_y}{\partial y} + k_{xz} \frac{\partial p_z}{\partial z} \right)
\]  
(3.12.1)
\[ v_y = \frac{1}{\mu} \left( k_{yx} \frac{\partial p_c}{\partial x} + k_{yy} \frac{\partial p_c}{\partial y} + k_{yz} \frac{\partial p_c}{\partial z} \right) \]  
(3.12.2)

\[ v_z = \frac{1}{\mu} \left( k_{zx} \frac{\partial p_c}{\partial x} + k_{zy} \frac{\partial p_c}{\partial y} + k_{zz} \frac{\partial p_c}{\partial z} \right) \]  
(3.12.3)

where \( k_{ij} (i, j = x, y, z) \) is the permeability tensor. Specifying an arbitrary small pressure drop in the z-direction, e.g., 20 Pa across the thickness, we obtain, \( k_{xz} = 3.22E-13 \), \( k_{yz} = 7.82E-13 \), and \( k_{zz} = 1.44E-10 \), respectively. Note that \( k_{xz} \) and \( k_{yz} \) are almost 3 orders of magnitude smaller than \( k_{zz} \). We, therefore, neglect any fluid flow in the x and y directions (in-plane flow) in formulating our macroscale model. In addition we obtain the diagonal component of permeability in x and y direction, \( k_{xx} = 2.536E-10 \) and \( k_{yy} = 2.604E-10 \), respectively. As it can be observed, obtained values for diagonal x and y permeabilities are quite same and almost 2 times greater than obtained permeability value in z (thickness) direction which is due to layered feature of the structure. It should be noted that since there is not any external pressure gradient in x and y direction on the structure, we do not have such a fluid flow in defined drainage problem.

It is important to ensure that the size of simulation domain is sufficiently large so that the permeability values are not dependent on the domain size. Here we used the Brinkman screening length criterion which is given by \( \sqrt{k_{zz}} \). According to (Clague et al. 2000), a box size of about 14 times larger than the Brinkman’s length is sufficient to smooth out the local heterogeneities. Here we used the expression of Jackson and James
(1986), \( \frac{k_{zz}}{r^2} = \frac{3}{20(1 - \phi)} [-\ln(1 - \phi) - 0.931] \), to obtain an estimate of the relevant domain size, prior to the simulations. Moreover, we have also examined our results for size-dependency and concluded that the domain size considered for our simulations is adequately large to represent of the whole media. For more information on the effect of domain size on permeability calculations see (Clague et al. 2000; Jaganathan et al. 2008a,b,c).

To ensure that GeoDict’s calculations are accurate, we compared its results with those of the well-established CFD code from Fluent Inc. In this respect, a fibrous medium was generated in GeoDict and exported to Fluent with exactly identical boundary conditions. Each voxel of the domain was used as a quadrilateral computational cell in Fluent. The medium had an SVF of \( \alpha = 10\% \) and a fiber diameter of \( d_f = 10 \mu m \). The simulation domain was consisting of 200 voxels in x, y and z directions with each voxel size being 1 micrometer. Through-plane permeability constant of this medium was calculated by using GeoDict and Fluent and were found to be 1.66e-10 m2 and 1.70e-10 m2, respectively. Obviously, the discrepancy (2.5% error) is negligible. Note that the sole purpose of the above comparison was to check GeoDict’s absolute permeability calculations with Fluent by conducting the computations on identical geometries. Therefore, the domain size did not need to be too large to ensure size-independency and also there were no repetition (Vahedi Tafreshi et al. 2009).

Total permeability can be defined as:

\[
K(S) = K_r(S) \tag{3.13}
\]
where $K_s$ is the single-phase (absolute or intrinsic) permeability of the material. The relative permeability, $K_r$, is not determined by the pore structure alone; it also depends on the media’s saturation. Calculation of the total permeability, being a function of saturation, is difficult and requires solving the Navier-Stokes equations. Following the work of Schultz et al. (2007), we assume that the relative permeability of each phase can be decoupled from one another. This assumption is valid in our morphological analysis in which the stream of one phase does not affect the configuration of phases. In this technique, the two-phase problem is decomposed into flows of single independent phases. Therefore, Stokes flow equations are solved at each saturation level during the drainage simulation.

The relative permeability calculation is carried out by combining the FM method with a numerical solution of the Stokes equation. Using the FM method, we incrementally intrude the non-wetting fluid into the medium. The wetting phase saturation (and the overall porosity of the medium) therefore, changes depending on the volume of the pores that are now occupied by the non-wetting phase (being a function of the applied capillary pressure). By assuming that the wetting and non-wetting phases are decoupled from each other at each intrusion increment (the non-wetting phase considered to be in a stationary state like a solid phase), the permeability of this porous medium to the flow of the wetting phase can be obtained by solving the Stokes equations throughout the domain. It should be noted that the void space in a disordered fibrous medium is actually shared between all the
pores, i.e., pores are all interconnected. Therefore, there are no individual open or closed pores.

As expected, relative permeability calculation is computationally expensive. Our relative permeability calculations (in a domain of 450×450×300 voxels) took more than 3 days on a workstation with 32 GB of RAM and a 3 GHz CPU. Figure 3.5 shows our relative permeability results versus wetting phase saturation.

Figure 3.5: The equation of Brooks and Corey is fitted to our relative permeability data to obtain the required empirical coefficients $n=6.01$ and $\lambda=0.66$.

Similar to the case of capillary pressure, there are many available studies dedicated to establishing a relationship between the relative permeability and saturation in soils and granular porous media. There are, however, not many published works on developing such relationships for fibrous materials.
Brooks and Corey (1964) proposed the following general form for the wetting phase relative permeability in porous media:

\[ K_r = S^n \] \hspace{1cm} (3.14)

with

\[ n = (2 + 3\lambda) / \lambda \] \hspace{1cm} (3.15)

where \( \lambda \) is the pore size distribution index. Fitting Equation 3.14 into our relative permeability simulation data, results in \( n = 6.01 \) and \( \lambda = 0.66 \).

### 3.4 Numerical Simulation

We use the FlexPDE program to solve the Richards’ equation along with the aforementioned constitutive equations. FlexPDE is a general purpose mathematical program developed by PDE Solutions Inc. for solving partial differential equations by finite element method. Equation 3.4 along with Equation 3.11 and of Haverkamp et al. (1977), Landeryou et al. (2005), and Leverett (1939) are coded in FlexPDE to be solved in a 1-D domain. Our nonwoven sheet is assumed to be 1 mm thick with a SVF of 10% and a fiber diameter of 15µm. In order to model the transport of wetting phase from the sheet, we implemented a mass convection boundary condition at the bottom boundary. This boundary condition is placed to mimic the fluid release from the media as the material is moved against a stationary surface (see section 3.5).

Richards’ equation is a scalar equation developed for calculating saturation throughout the material’s thickness as a function of time. To simulate the release of fluid
from the sheet onto the target surface, one needs to set appropriate boundary conditions at the bottom boundary. Since the sheet is considered to be thin, for the sake of simplicity, we assume that the fluid release from the bottom boundary is solely due to the relative motion between the sheet and the target surface. In other words, we assume that the thin sheet is not significantly compressed while delivering the fluid to the target surface (see Figure 3.6).

Figure 3.6 A schematic illustration of the fluid convection from the lower boundary.

Here neither of Dirichlet (fixed saturation value) nor Neumann (fixed saturation flux) boundary conditions are appropriate for our simulations. We, instead, simulated the fluid release via a mass convection boundary condition.

Based on the governing Richards partial differential equation (Equation 3.4), the outward flux is 

$$- \frac{K(S) \partial p_c}{\mu} \frac{\partial S}{\partial z}.$$  

Here, we consider a mass convection boundary condition as:

$$- \frac{K(S) \partial p_c}{\mu} \frac{\partial S}{\partial z} = k_f \gamma (S_{in} - S_{out}) \quad (3.16)$$
where $\gamma$ is the fluid’s specific gravity, $S_{in}$ is the saturation value at the bottom boundary, $S_{out}$ is the saturation outside the domain (if any). The coefficient $k_f$ plays an most important role in this boundary condition. It has the dimension of $m^2/\text{Pa.s}$ and should be found empirically in order to emulate the effect of fluid delivery on to the solid surface. As we have no prior knowledge of any appropriate numeric value for $k_f$, we started our simulations with $k_f = 1$ and incrementally reduced it to study its effect on fluid delivery. Here we also set the external saturation, $S_{out}$, equal to zero to simulate the case of dry target surface. Note that by assigning a non-zero value to $S_{out}$ one can simulate delivery of a fluid to a wet surface.

### 3.5 Results and Discussion

As mentioned in section earlier, correlations of Haverkamp et al. (1977), van Genuchten (1980), and Landeryou et al. (2005) for the relationship between the capillary pressure and saturation were all relatively close to our simulation data. For comparison purposes, we used correlations of Landeryou et al. (2005), Haverkamp et al. (1977), and Leverett (1939) in three separate simulations and plotted their corresponding medium’s average saturation as a function of time in Figure 3.7. The above average saturation is calculated by integrating the individual saturation values throughout the domain. As it can be seen, there is perfect agreement between the predictions of Landeryou et al. (2005) and Haverkamp et al. (1977) while the correlation of Leverett (1939) shows small degrees of
deviation at lower saturations which is negligible. Such a difference is expected from the
different behavior of Leverett (1939) capillary pressure-saturation relation compare to
those of Haverkamp et al. (1977) and Landeryou et al. (2005) presented in Figure 3.3.
Since the derivative of capillary pressure-saturation directly implemented in nonlinear
diffusive coefficient in Richards’ equation \( \frac{\partial p_c}{\partial S} \) term in nonlinear coefficient

\[- \frac{K(S) \partial p_c}{\mu} \frac{\partial S}{\partial z} \]  

in Equation 3.4) such a differences is expectable. It should be noted that
the permeability term \( K(S) \) (which is small value), is directly multiplied to the capillary
pressure term and the observed behavior in Figure 3.7 is the net product of these two main
terms divided by viscosity of the fluid, \( \mu \).

Figure 3.7: Medium’s average saturation versus time is calculated using the correlations of
Haverkamp et al. (1977) and Landeryou et al. (2005).
Figure 3.8 shows the medium’s saturation profiles at different times for the case of $k_f = 10^{-8}$. It can be seen that the saturation decreases almost uniformly across the thickness. Only when the saturation goes below a value of about 0.3, a gradient can be observed across the thickness. This indicates that for the fibrous medium simulated in this work, the fluid release is controlled by the boundary condition imposed at the surface in contact with the wall, as opposed to the permeability or capillary pressure caused by the fibrous medium.
As discussed earlier, we have considered a mass convection boundary condition to simulate the mass convection from the bottom of the solution domain due to the relative motion between the medium and the solid surface. As it can be observed from Equation 3.14, the flux of fluid from the bottom boundary is proportional to $f_k$ which needs to be determined experimentally. In this section, we study the effect of this coefficient on the rate of fluid release and so the performance of the fluid delivery process using a fibrous thin sheet.

In order to study the effect of $k_f$ on the rate of fluid release, the medium’s average saturation is plotted as a function of time for different $k_f$ values. As it can be seen in Figure 3.9, the rate of fluid release remains unchanged for $k_f > 10^{-4}$ (only $k_f \leq 1$ are shown in the Figure) while decreasing $k_f$ delayed the fluid delivery as the rate of fluid release decreases. At $k_f \equiv 10^{-6}$, for instance, almost 30% of the initial fluid is released from the sheet in less than one second which is probably not very realistic. The release rate tends to become more realistic at smaller values of $k_f$ (e.g., $k_f = 10^{-9}$) and remains to be determined experimentally in future studies. It is interesting to note that, regardless of $k_f$, all the saturation profiles converge together at very low saturations.
Figure 3.9: Effect of mass convection coefficient, $k_f$ on the medium’s average saturation and consequently, fluid release.
CHAPTER 4 General Capillary Pressure and Relative Permeability Expressions for Through-Plane Fluid Transport in Thin Fibrous Sheets


4.1 Introduction

Fibrous materials have been used for fluid absorption and release for many years. However, only in recent years has optimizing their microstructure become important. This is, in part, due to the inception of many new applications demanding controlled fluid absorption, storage, and release. Drug delivery patches, sanitizing wipes, wound dressings, and very many other hygiene and industrial products are among the applications taking advantage of the unique properties of fibrous materials in absorbing, storing, and releasing a fluid. For a complete review of the previous works on fibrous media readers are referred to the recent book of Pan and Gibson (2006).

Quantitative relations for capillary pressure, $p_c$, and relative permeability in terms of the media’s saturation, $S$, are required for predicting the rate of fluid transport in porous materials. Such relationships have been empirically obtained for granular porous media over the last few decades for applications in the oil and gas industries or soil sciences. Unfortunately, there are no such relationships available for fibrous materials except for the work of Landeryou et al. (2005), who used an auto-porosimeter to study liquid rise in
needle felt fabrics. The correlation of Landeryou et al. (2005) was obtained for in-plane (as opposed to through-plane) fluid infiltration in fibrous media. The only available study reporting on a capillary pressure–saturation, $p_c(S)$, and relative permeability–saturation, $k_r(S)$, relationship for through-plane fluid transport in a fibrous medium is that of our group (Ashari and Tafreshi 2009a). In that work, we simulated fluid release from a partially saturated fibrous sheet using a combined micro- and macro-scale modeling approach. Results of our previous work, however, were obtained for a specific fibrous material. Our objective in this work, on the other hand, is to develop, for the first time, general $p_c(S)$ and $k_r(S)$ expressions valid for a whole family of fibrous sheets with a practical range of fiber diameter, thickness, and porosity. These expressions are required, for instance, in solving the Richards’ equation (Richards 1931), among many others. The Richards’ equation is a partial differential equation relating the fluid’s continuity equation to Darcy’s law, and is often used in literature to predict the percentage of fluid saturation in a porous medium as a function time and space, $S(x,y,z,t)$ (e.g., see Landeryou et al. 2005, Jaganathan et al. 2009 and Ashari and Tafreshi 2009a).

It is worth mentioning that $p_c(S)$ and $k_r(S)$ expressions can only be obtained via experimentation (Landeryou et al. 2005) or computationally expensive microscale simulations (Ashari and Tafreshi 2009a and Jaganathan et al. 2009), and they are only valid for the material used in the experiment or simulation. Developing generalized $p_c(S)$ and $k_r(S)$ expressions is very important as they enable us to circumvent the need for conducting expensive microscale simulations (or laborious experiments), and help in
performing fast and affordable macroscale calculations for fluid transport in partially saturated porous media.

In this work, we generate a large series of 3-D microstructures resembling the internal geometry of fibrous sheets. These virtual geometries will be then used to study capillary pressure and relative permeability in terms of a medium’s saturation. We consider the effect of different parameters such as the medium’s thickness, fiber diameter, solid volume fraction (SVF), fluid’s surface tension, and contact angle on \( p_c(S) \) and \( k_r(S) \) relations.

The next section describes our microscale modeling conducted for obtaining a relation between capillary pressure and medium’s saturation. In this section, we also present our generalized \( p_c(S) \) expressions and examine their accuracy. In Section 4.3, we report on our relative permeability study and present our general expression for \( k_r(S) \). This section is followed by our conclusions in Section 4.4.

### 4.2 Capillary Pressure as a Function of Saturation

Leverett was the first to obtain an empirical \( p_c(S) \) expression for granular porous media in 1939. Since then, there have been many other studies focused on developing such relationships for underground or soil applications (e.g., Haverkamp et al. 1977, Udel 1985, Wang and Beckerman 1993, Eames et al. 2003, Ishakoglu and Baytas 2005 and van Genuchten 1980). The empirical coefficients used in these correlations depend on the
microstructure of the porous media used in a given experiment and need to be obtained for each and every given material.

In the present study, we perform a series of microscale simulations to build a general  \( p_c(S) \) expression valid for the whole family of fibrous sheets when the fluid transport takes place in the through plane direction.

### 4.2.1 Fibrous Microstructures and Saturation Simulation

The microstructure of a fibrous medium can either be obtained by 3-D imaging (e.g., Jaganathan et al. 2008a and Jaganathan et al. 2008b) or by constructing digital microstructures based on stochastic models (Vahedi Tafreshi et al. 2009). The latter has been considered in the current work. Most thin sheet non-woven materials can be considered as 3-D “layered” fibrous structures. In these media, fibers are randomly oriented in the x–y plane (in-plane) and are horizontally stacked on top of one another to form a layered structure. In the current work, we use a program called Geodict from Fraunhofer-IWTM Germany to generate our 3-D fibrous microstructures (www.geodict.com). GeoDict is a voxel-based code in which each voxel is either “empty” or “filled” (or solid). In our case, fluid domain and solid fibers are represented by empty and filled voxels. The fiber orientation distribution is controlled by a density function  \( p(\phi, \varphi) \) in polar coordinates, in which \( \phi \) and \( \varphi \) are the through-plane and in-plane angles,
respectively (Schladitz et al. 2006). For the abovementioned 3-D layered media, $p(\phi, \varphi)$ can be expressed as:

$$p(\phi, \varphi) = \frac{1}{4\pi} \frac{\beta \sin \phi}{(1 + (\beta^2 - 1)\cos^2 \phi)^{3/2}}$$  \hspace{1cm} (4.1)$$

where $\beta$ is the anisotropy parameter. A large $\beta$ value results in a layered fibrous structure (see Schladitz et al. 2006 for more details). Note that it is assumed that fibers are continuous with no curvature. A layered fibrous structure with a size of 750×750×500 voxels, a SVF of 10%, and a fiber diameter of 15µm is shown in Figure 4.1. Note that the voxel size used in the simulations presented in this work is consistently 2µm.

Figure 4.1: 3-D view of a virtual fibrous microstructure. The domain size is 750×750×500 voxels with each voxel being 2µm.
4.2.2 Full Morphology Technique

We use a morphological method to develop a relationship between capillary pressure and saturation. This method was originally developed by Hazlett (1995) and Hilpert and Miller (2001), and has also been used by Vogel et al. (2005) and Schulz et al. (2007) for different applications. In this model, a quasi-static distribution of water and air for an arbitrary capillary pressure of $p_c$ is simulated in a 3-D domain and repeated for the whole range of saturation ($0 < S < 1$). The simulation starts from a water-saturated medium, and continues until almost all the wetting phase is pushed out of the domain. The underlying principle of the full morphology (FM) method is that at a given capillary pressure, $p_c$, the pore space accessible to air (the non-wetting phase) is determined by the pore size via the Young–Laplace Equation 4.2. In this regard, the domain is decomposed into different pore sizes with pore radii being the ordering parameter. By increasing the capillary pressure, corresponding pores are incrementally filled with the non-wetting phase while the rest of the pores remain water-filled. Detailed explanation of the FM method can be found in the works of Soille (1999), Hilpert and Miller (2001), Schulz et al. (2007) and Becker et al. (2008).

The FM method is basically a method for finding the relative permeability of a porous medium. It is based on a critical assumption that the non-wetting phase will stay immobile (like a solid object) during the flow of the wetting phase. The FM method will obviously fail to be accurate if such an assumption proves to be invalid. It should also be noted that the FM technique is known for slightly overestimating the wetting phase.
saturation at a given capillary pressure as it assumes spherical local interfaces between the wetting and non-wetting phases (Vogel et al. 2005). Nevertheless, the FM method, even with its current limitations, is still the only method that allows affordable computation of relative permeability in 3-D.

The Young–Laplace equation has been used to assign a radius, \( r_c \), to the given capillary pressures here, i.e.,

\[
p_c = \frac{2\sigma \cos \theta}{r_c}
\]

where \( \sigma \) is the surface tension between the wetting and nonwetting phases and \( \theta \) is the contact angle between the wetting phase and the solid surface. Here, we used a contact angle of \( \theta_w = 80^\circ \) for the water–air–polyester fibers (Zhu et al. 2005) in all the simulations. The effect of contact angle is included in our general expressions as will be discussed later in section 4.2.

An example of our FM simulations performed for a fibrous structure (750×750×500 voxels) with a fiber diameter of 20\( \mu \)m and a SVF of 5% is shown in Figure 4.2 at different capillary pressures. The fibrous medium is connected to imaginary reservoirs of wetting and non-wetting fluids from bottom and top boundaries, respectively. It can be seen that by increasing the capillary pressure, the non-wetting phase progressively enters the domain and replaces the wetting phase. The wetting phase is shown with red color in this Figure.
4.2.3 Curve Fitting with Empirical Correlations

In a previous study (Ashari and Tafreshi 2009a), we compared our simulation results with the empirical $p_r(S)$ correlations of Leverett (1939), van Genuchten (1980), Haverkamp et al. (1977), and Landeryou et al. (2005) to demonstrate that both van Genuchten (1980) and Haverkamp et al. (1977) correlations have relatively good agreement with the results of our FM simulations, especially at saturations less than 0.4. We therefore use the correlation of van Genuchten (1980) and Haverkamp et al. (1977) in the current work. The empirical $p_r(S)$ correlations of Haverkamp et al. (1977) and van Genuchten (1980) are shown in Table 4.1.

Figure 4.2: Some intermediate stages of the FM method are shown for illustration. The non-wetting phase (air) is shown in red. The wetting phase (water) is invisible. The medium is initially filled with the wetting phase and the non-wetting phase is intruded with pressure; (a) 250 Pa, (b) 361 Pa, (c) 424 Pa and (d) 883 Pa. It can be seen that wetting phase is drained from the domain as the capillary pressure increases.
4.2.4 Parameter Study

In this section, we study the influence of sheet’s thickness, fiber diameter, SVF, fluid’s surface tension and contact angle on $P_c(S)$. Before we start our parameter study, it is important to ensure that the simulation results are independent of the choice of the box’s x–y dimensions. An appropriate size is one in which the population of fibers is high enough for virtual microstructures to represent the entire sheet. It should be noted that for a specific domain size and SVF, the finer the fiber diameter, the higher the population of the fibers in the simulation domain. Increasing the population of the fibers improves the statistical variation of the results. In this regard, we performed a series of FM simulations with identical overall properties (thickness of 1mm i.e., 500µm, fiber diameter of 25µm, SVF of 10%, contact angle of 80, and surface tension of 0.073 N/m) but different in-plane domain sizes of 50×50, 100×100, 250×250, 500×500, 750×750 and 900×900 voxels. Note that a fiber diameter of 25µm is the largest, and therefore the most critical, fiber diameter considered in this study. Our capillary pressure–saturation results are shown in Figure 4.3. It can be seen that our data are independent of the size of the simulation domain as long as the in-plane dimensions are greater than 250×250 voxels. We continued the rest of simulations presented in this section with fixed in-plane dimensions of 750×750 voxels.
### Table 4.1 Different empirical correlations proposed for capillary pressure-saturation relationship

<table>
<thead>
<tr>
<th>Model</th>
<th>Correlations</th>
<th>Constants</th>
</tr>
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| Leverett (1939)           | \[ p_c = a S + b S^2 + c S^3 + d \]                                         | \( a = 2650.58 \)
|                           |                                                                              | \( b = -13504.58 \)       |
|                           |                                                                              | \( c = 27472.38 \)        |
|                           |                                                                              | \( d = -16376.12 \)       |
| Haverkamp et al. (1977)   | \[ S_e = \frac{S - S_i}{1 - S_i} \]                                        | \( S_i = 0 \)             |
|                           | \[ S_e = \frac{1}{1 + |p_c|^p / C_i} \]                                    | \( C_i = 877.98 \)        |
|                           | \( S_e = 1 \)                                                              | \( b = 3.93 \)            |
|                           | for \( p_c < 0 \)                                                          |                            |
|                           | \( S_e = 1 \)                                                              |                            |
|                           | for \( p_c \geq 0 \)                                                       |                            |
| Van Genuchten (1980)      | \[ S = \left( 1 + \left( \frac{p_c}{P_c} \right)^n \right)^{-m} \]        | \( p_c^* = 768.76 \)      |
|                           | \( m = 1 - \frac{1}{n} \)                                                  | \( n = 4.43 \)            |
| Landeryou et al. (2005)   | \[ S = \exp \left( \frac{p_c}{P_c} \right) \]                             | \( p_c^* = -500.27 \)     |
Figure 4.3: Results of FM analysis for six cases with different in-plane domain size of 50×50, 100×100, 250×250, 500×500, 750×750 and 900×900 voxels but identical thickness of 500 voxels (each voxel is 2µm).

4.2.4.1 Effects of Sheet Thickness

To study the dependency of $p_c(S)$ on a material’s thickness, eight different media with identical dimensions of 750×750 voxels, but different thickness of 125, 250, 500, 1000, 1500, 2000, 3000, and 3800 voxels were considered. The SVF and fiber diameter were kept at 10% and 15µm, respectively. Figure 4.4a shows the capillary pressure versus the wetting phase saturation for media with different thicknesses. Simulations for each thickness were repeated five times in order to obtain statistically meaningful average values. For the sake of clarity, we have only plotted the average values in Figure 4.4a.
demonstrate the influence of the above repetition on the capillary pressure estimation, we have shown the error bars for the results obtained with the thinnest (most susceptible to statistical error) sample in Figure 4.4b.

As it can be seen in Figure 4.4a, results of different thickness values perfectly match with one another for a saturation of up to about 60%. Beyond this, the results of different thickness start to slightly depart from each other. Figure 4.4a indicates that \( p_c(S) \) is independent of the media’s thickness as long as the thickness is not too small. Our experience with non-woven sheets used for fluid release (wet wipes) suggests that saturation normally stays below a value of about 50%. For this reason, in developing our general expressions, we considered a saturation range of \( 0 < S < 0.6 \). As it can be seen in Figure 4.4a, for the range of \( S < 0.6 \), \( p_c(S) \) is independent of thickness. In this regard, we chose a thickness of 500 voxels (1mm) for the rest of the simulations presented in this section.
Figure 4.4: (a) Capillary pressure–saturation curves of drainage process for media with different thicknesses. The in-plane dimensions of the samples are equal to 750×750 voxels. (b) Capillary pressure versus saturation for media with a size of 750×750×125 voxels. The results are averaged over five repetitions.
4.2.4.2 Effect of Fiber Diameter

To study the dependency of \( p_c(S) \) on fiber diameter, four different samples with identical dimensions of 750×750×500 voxels with different fiber diameters of 10, 15, 20, and 25µm were considered (see Figure 4.5a). Here SVF, surface tension, and contact angle are considered to be 10%, 0.072 N/m, and 80°, respectively. Figure 4.5a reveals that \( p_c(S) \) curves move down as fiber diameter increases. This implies that the average pore size of a medium decreases by decreasing the fiber diameter and, therefore, higher pressures are required for intruding a non-wetting fluid into the wetted medium (i.e., harder to release the fluid). Figure 4.5a clearly shows that \( p_c(S) \) is dependent on fiber diameter.

As mentioned earlier, we are searching for generalized \( p_c(S) \) expressions that cover a range of saturations less than 60%. We fitted the empirical correlations of Haverkamp et al. (1977) and van Genuchten (1980) to our FM results for \( S < 0.6 \) to obtain their corresponding empirical coefficients \( C_i \) and \( b_i \). For the sake of clarity, we only plotted the correlation of Haverkamp et al. (1977) in Figure 4.5b.

4.2.4.3 Effects of Solid Volume Fraction (SVF)

In this section, the effect of SVF on \( p_c(S) \) is studied. Similar to the approach presented in the previous subsections, here we considered four samples with identical dimensions of 750×750×500 voxels and a fiber diameter of 15µm, but different SVFs of 5%, 7.5%, 10% and 12.5% (see Figure 4.6a). It can be seen that the \( p_c(S) \) curves move up as SVF increases. Similar to the case of fiber diameter increase, this implies that the
average pore size of a medium decreases by increasing the SVF and, therefore, higher pressures are required for intruding a non-wetting phase into the wetted medium (i.e., harder to release the fluid). We fitted the empirical correlations of Haverkamp et al. (1977) and van Genuchten (1988) to our FM results for \( S < 0.6 \) to obtain their corresponding empirical coefficients \( C_i \) and \( b_i \). Again, for the sake of clarity, we only plotted the correlation of Haverkamp et al. (1977) in Figure 4.6b.

### 4.2.4.4 Effect of Contact Angle and Surface Tension

In this section, we study the effect of contact angle and surface tension. In order to demonstrate the above dependency, we present the effect of contact angle and surface tension on \( p_c(S) \) results for a fibrous medium with a size of 750×750×500 voxels, a fiber diameter of 15\( \mu \)m, and a SVF of 10\%. Figure 4.7a shows the case where a fixed contact angle of 80° was used while Figure 4.7b shows similar results when the surface tension was kept constant at 0.073 N/m. It can be seen that the difference between the data points is equal to \( \sigma/\sigma_w \) and \( \cos \theta/\cos \theta_w \) for the results shown in Figure 4.7a and b, respectively. These ratios are therefore included in our general expressions (see next subsection).
Figure 4.5: (a) Capillary pressure–saturation curves of the drainage process for media with different fiber diameters but identical SVF of 10%. The domain dimensions are 750×750×500 voxels. (b) Curve fitting using the correlation of Haverkamp et al. (1977).
Figure 4.6: (a) Capillary pressure–saturation curves of the drainage process for media with different SVFs but same fiber diameter of 15 μm. The domain dimensions are 750×750×500 voxels. (b) Curve fitting using the correlation of Haverkamp et al. (1977).
Figure 4.7: (a) Results of FM analysis for media with identical domain size, fiber diameter, SVF, and contact angle but different surface tensions of 0.0276 and 0.07275 N/m. (b) Results of FM analysis for media with identical domain size, fiber diameter, SVF, and surface tension but different contact angles of 60° and 80°.
4.2.5 General Capillary Pressure Expressions

In this section, we present our general \( p_c(S) \) expressions developed based on the empirical correlations of Haverkamp et al. (1977) and van Genuchten (1980). Considering Equation 4.2, it can be seen that capillary pressure is directly proportional to \( \sigma \) and \( \cos \theta \). We, therefore, construct our generalized expressions as:

\[
p_c^{\text{Hav}} = C_1 \frac{\sigma \cos \theta}{\sigma_w \cos \theta_w} (S^{-1} - 1)^{1/b_1} \tag{4.3}
\]

\[
p_c^{\text{Gen}} = C_2 \frac{\sigma \cos \theta}{\sigma_w \cos \theta_w} (S^{b_2 / (1-b_2)} - 1)^{1/b_2} \tag{4.4}
\]

where Equation 4.3 and 4.4 are developed based on the work of Haverkamp et al. (1977) and van Genuchten (1980), respectively. The \( C_i \) and \( b_i \) constants (\( i = 1 \) or \( 2 \)) are obtained from the curve fitting exercise described in the previous subsection, and are plotted in Figure 4.8a and b. Note that our generalized expressions are obtained to study through-plane fluid transport in fibrous sheets. The expressions are valid for a fiber diameter range of 10–25µm, a SVF range of 5–12.5%, and different surface tensions and contact angles.

In order to test the accuracy of the proposed expressions, we generated a series of simulation data with a set of parameters that have not been used in the curve fitting exercise (fiber diameter of 17.5µm, SVF of 8.5%, contact angle of 50°, and surface tension of 0.05 N/m). The predictions of our new expressions are presented in Figure 4.9 and show reasonable agreement with the results of FM simulation. Our general expressions, however, slightly underestimate the capillary pressure at saturations beyond 0.4. This discrepancy in our general expressions is actually inherited from the original
correlations of Haverkamp et al. (1977) and van Genuchten (1980) (Ashari and Tafreshi 2009a). Nevertheless, we believe that the slight mismatch at high saturations does not significantly affect the value of our general equations.

4.3 Relative Permeability as a Function of Saturation

Using modeled or imaged geometries, many authors have studied the single-phase permeability of fibrous materials (e.g., Jaganathan et al. 2008a, Jaganathan et al. 2008b, Jackson and James 1986, Spielman and Goren 1968, Higdon and Ford 1996, Tomadakis and Robertson 2005, Zobel et al. 2007). There are many simple expressions in the abovedicted publications and their references that one can conveniently use to predict the single-phase permeability of a homogeneous fibrous medium. There are however, not many expressions for predicting the two-phase (relative) permeability of a fibrous material. This is partly because the relative permeability depends on the saturation in addition to the SVF and fiber diameter. In the current work, we numerically solve the Stokes flow in the interstitial space between the fibers, and the exiting non-wetting phase at each saturation state obtained via the aforementioned FM method, to obtain the relative permeability of the wetting fluid. We run series of simulations to study the effect of SVF and fiber radius on permeability as a function of saturation in order to develop a general \( k_r(S) \) correlation valid for the most practical range of fiber diameters (10–20µm) and SVFs (5–12.5%) used in making thin fibrous sheets.
Figure 4.8: Dependency of coefficients, $C_1$ and $C_2$ (a) and $b_1$ and $b_2$ (b) on fiber diameter and SVF.
Figure 4.9: A comparison between the predictions of our general $p_c(S)$ expression and the results of FM analysis conducted on a medium that was not used in the expression development. The medium has a fiber diameter of 17.5µm, SVF of 8.75% and is wetted with a fluid with a contact angle of 50° and a surface tension of 0.05 N/m. Reported values are averaged over five repetitions.

4.3.1 Relative Permeability Calculation

As mentioned before, the FM method is based on the assumption that the relative permeability of wetting and non-wetting phases can be considered decoupled from each other, which is often valid when capillary pressures are large in comparison with the viscous forces (Becker et al. 2008). The FM method calculates the relative permeability of a medium by solving the Stokes equations for the wetting phase at each saturation level. This has been done here using the finite difference FFF–Stokes solver of GeoDict.
(Wiegmann 2007). The Stokes equations for the conservation of mass and momentum are as follows:

\[
\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \tag{4.5}
\]

\[
\frac{\partial p_x}{\partial x} = \mu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right) \tag{4.6.1}
\]

\[
\frac{\partial p_y}{\partial y} = \mu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right) \tag{4.6.2}
\]

\[
\frac{\partial p_z}{\partial z} = \mu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right) \tag{4.6.3}
\]

where \(v_x, v_y, \) and \(v_z\) are velocity in the x, y, and z directions, respectively. GeoDict treats each voxel as a computational cell and circumvent the mesh generation process in the complex 3-D geometry of a fibrous medium. Based on the Darcy’s law the relation between mean velocity and pressure drop in each direction are as follow:

\[
v_x = \frac{1}{\mu} \left( k_{xx} \frac{\partial p_c}{\partial x} + k_{xy} \frac{\partial p_c}{\partial y} + k_{xz} \frac{\partial p_c}{\partial z} \right) \tag{4.7.1}
\]

\[
v_y = \frac{1}{\mu} \left( k_{yx} \frac{\partial p_c}{\partial x} + k_{yy} \frac{\partial p_c}{\partial y} + k_{yz} \frac{\partial p_c}{\partial z} \right) \tag{4.7.2}
\]

\[
v_z = \frac{1}{\mu} \left( k_{zx} \frac{\partial p_c}{\partial x} + k_{zy} \frac{\partial p_c}{\partial y} + k_{zz} \frac{\partial p_c}{\partial z} \right) \tag{4.7.3}
\]

where \(k_{ij} (i,j = x,y,z)\) is the permeability tensor. Our simulation results indicate that off-diagonal elements of the permeability tensor, \(k_{xz}\) and \(k_{yz}\), are almost 3 orders of magnitude
smaller than the diagonal element, \( k_{zz} \). We, therefore, assume that the lateral fluid flow (i.e., in the x or y direction) caused by the pressure gradient in the through-plane direction, will be insignificant.

In the permeability calculation, it is important to ensure that the size of simulation domain is sufficiently large, so that the permeability values are not dependent on the domain size. Here, we used the Brinkman screening length criterion, which is given by \( \sqrt{k_{zz}} \). According to Clague et al. (2000). A box size of about 14 times larger than the Brinkman’s length is sufficient to smooth out the local heterogeneities. Here we used the expression of Jackson and James [24],

\[
\frac{k_{zz}}{r^2} = \frac{3}{20(1 - \phi)}\left[-\ln(1 - \phi) - 0.931\right],
\]

To obtain an estimate of the relevant domain size, prior to the simulations. Moreover, we have also examined our results for size-dependency and concluded that the domain size considered for our simulations is adequately large to represent of the whole medium. For more information on the effect of domain size on permeability calculations (see refs. Jaganathan et al. 2008a,b,c).

To ensure that GeoDict’s calculations are accurate, we compared its results with those of the well-established CFD code from Fluent Inc. In this respect, a fibrous medium was generated in GeoDict and exported to Fluent with exactly identical boundary conditions.

Each voxel of the domain was used as a quadrilateral computational cell in Fluent. The medium had an SVF of \( \alpha = 10\% \) and a fiber diameter of \( d_f = 10\mu\text{m} \). The simulation
domain consisted of 200 voxels in x, y and z directions with each voxel size being 1µm. The through-plane permeability constant of this medium was calculated by using GeoDict and Fluent, and was found to be 1.66e−10m² and 1.70e−10m², respectively. Obviously, the discrepancy (2.5% error) is negligible. Note that the sole purpose of the above comparison was to check GeoDict’s absolute permeability calculations with Fluent by conducting the computations on identical geometries. Therefore, the domain size did not need to be too large to ensure size-independency and also there were no repetition (Vahedi Tafreshi et al. 2009).

The total permeability can be defined as:

\[ k(S) = k_w k_r(S) \] (4.8)

Following the work of Schulz et al. (2007), we assume that the relative permeabilities of each phase can be decoupled from one another. This means that the flow of the wetting phase does not affect the distribution of the non-wetting phase. The abovementioned Stokes equations are then solved at each saturation level during the drainage simulation. Note that the wetting phase saturation is obtained using the FM method.

As expected, the relative permeability calculation is computationally expensive. Calculating the relative permeability at 7 saturation levels in a simulation domain of 400×400×300 voxels, for instance, takes more than 3 days on a workstation with 32 GB of RAM and a 3GHz CPU. The simulation results for a series of structures with different fiber diameters of 10, 12.5, 15, and 20µm with a domain size of 450×450×350 voxels and a SVF of 10% are presented in Figure 4.10. It should be noted that each simulation was repeated at least three times.
To examine whether or not one can use the existing single-phase permeability correlations for relative permeability prediction, we considered the work of Higdon and Ford (1996) obtained for Simple Cubic fiber networks. The reason for choosing this permeability model among others is that it is valid for a wider range of porosities and its predictions are closer to our simulation data than many others alternative models. The underlying hypothesis for using a single-phase permeability model (i.e., work of Higdon and Ford 1996) to predict the relative permeability is that the pore space occupied by the nonwetting fluid can be treated as an additional solid phase added uniformly to the fibers in the form of a diameter increase. With this assumption, porosity of the media will be a function of instantaneous saturation, $\varepsilon(S)$, and can be defined as follows:
\[ \varepsilon(S) = \frac{V_m - V_{nw}(S) - V_f}{V_m} \]  

where \( V_m \), \( V_{nw}(S) \), and \( V_f \) are the medium’s total volume, volume of the non-wetting phase, and volume of the fibers, respectively. Manipulating Equation 4.9, porosity can be obtained as:

\[ \varepsilon(S) = \varepsilon(1) S \]  

where \( \varepsilon(1) \) is the porosity of the medium when fully saturated with the wetting phase (no solid phase other than the fibers). As can be seen in Figure 4.10, predictions of the Simple Cubic fiber network of Higdon and Ford (1996) under-predict the relative permeability of the medium by more than an order of magnitude at low saturations. The prediction, however, improves as saturation increases. The results presented in Figure 4.10 imply that while the above hypothesis may lead to somewhat acceptable predictions at high saturations, its accuracy significantly deteriorates with decreasing the saturation percentage. Here we conclude that single-phase permeability models can be used to study how the relative permeability of a fibrous medium varies with saturation. However, these correlations are not quantitatively accurate enough.

### 4.3.2 Parameter Study

It is known that single-phase permeability is independent of the material’s thickness. Naturally, the relative permeability should also be independent of thickness because, as discussed in section 4.2, saturation is independent of thickness (see Figure 4.4). To examine this, we computed the relative permeability of two statistically identical media
with an in-plane domain size of 400×400, but different thicknesses of 300 and 450 voxels. The SVF and fiber diameter were fixed at 10% and 10µm, respectively, and saturation level was kept at about 30%. The discrepancy between the results of these simulations (not shown for the sake of brevity) was found to be within the margin of statistical error. This indicates that relative permeability of a fibrous sheet can be considered independent of its thickness.

In order to study the effect of a medium’s original porosity, \( \varepsilon(1) \), on the dimensionless permeability results, we simulated a series of media with a domain size of 400×400×300 voxels and a fiber diameter of 15µm having different SVFs of 5%, 7.5%, 10% and 12.5%. We plotted these data along with the results of Higdon and Ford (1996) in Figure 4.11. These results indicate that relative permeability is not strongly influenced by the material’s SVF. Similar conclusions can also be made from the predictions of Higdon and Ford (1996). This means that for most fibrous sheets, relative permeability is independent of the SVF.

### 4.3.3 General Relative Permeability Expression

In this section, we propose a general expression for calculating the relative permeability of fibrous sheets. Our expression is based on the empirical correlation of Brooks and Corey (1964), obtained for granular porous media:

\[
    k_r(S) = S^n
\]  

(4.11)

with
where $\lambda$ is the pore size distribution index. Combining Equation 4.8 and 4.11, we propose our general relative permeability expression as follows:

$$\frac{k(S)}{r_f^2} = a S^n$$  \hspace{1cm} (4.13)

where the single-phase permeability $k_z = a r_f^2$. The coefficient $a$ and exponent $n$ are obtained via curve fitting using our data shown in Figure 4.11 ($a = 2.23$ and $n = 3.18$). Interestingly, our exponent, $n=3.18$, is in agreement with the empirical $n = 3.0$ of Landeryou et al. (2005) obtained for in-plane fluid absorption.

Figure 4.11: Effect of SVF on dimensionless permeability. FM–Stokes simulation results are plotted for different SVFs of 5, 7.5, 10 and 12.5 for structures with fiber diameter of 15µm.
CHAPTER 5 Modeling Fluid Spread in Thin Fibrous Sheets: Effects of Fiber Orientation


5.1 Introduction

Literature regarding fluid flow modeling in partially-saturated fibrous media is very scarce. Most of the published studies to date are empirical in nature, and were conducted for specific purposes/applications (Pan and Gibson 2006). Because of this, the results of one study are often of no use to the other. There are a few theoretical studies conducted for predicting fluid spread in fibrous media. The well-known work of Lucas (1918) and Washburn (1921) was the first mathematical model developed to predict fluid infiltration in a porous medium made up of series of capillary tubes. This approach of modeling the complex pore space of a fibrous medium with a series of capillary tubes has been often criticized (Eames et al. 2003 and Mullins et al. 2007). This is mainly because there is no direct method of finding the Lucas-Washburn’s required equivalent capillary diameter, and it is hard to establish a fundamental relationship between the predictions of Lucas-Washburn model and the microstructural parameters of the media (e.g., porosity, fiber diameter...). Another over-simplification in the Lucas-Washburn model is the assumption that the medium is either fully-saturated or fully dry, ignoring the partially-saturated region.
between the two. Mao and Russell (2003 and 2008) proposed capillary pressure and relative permeability expressions for anisotropic homogenous fibrous media. The work of Mao and Russell (2003 and 2008) is based on series of assumptions similar to those of Lucas-Washburn’s model, and therefore is inaccurate when the partially-saturated region in the medium is not negligible, as the capillary pressure and relative permeability expressions derived by Mao and Russell exhibit no dependence on saturation. Hyvaluoma et al. (2006) developed a Lattice-Boltzmann simulation scheme to study liquid penetration inside paper sheets and reported excellent agreement between their work and the expression developed by Marmur (1988). The work of Hyvaluoma et al. (2006) also ignores the partially saturation part of the domain.

It is worth mentioning that Adams et al. (1988) also simulated the radial penetration of liquids in planar anisotropic porous media. Their work, however, was mostly formulated for pressure-driven fluid spread (such as the case of resin impregnation in fiber-reinforced composite manufacturing), and so the dependency of capillary pressure on saturation was ignored.

There are also a few statistical/semi-statistical simulations developed for studying fluid spread in fibrous media (e.g., Tompson 2002, Lucas et al. 1997, Lucas et al. 2004, Zhong et al. 2006). The major difficulty with such simulations is that it is often hard to directly relate measurable microstructural parameters of a real fibrous material (e.g., fiber diameter, fiber orientation distribution …) to the irregularity and randomness parameters used in statistical models. For a more complete review of the previous theoretical and experimental studies, readers are referred to the book of Pan and Gibson (2006).
In a recent work, Landeryou et al. (2005) presented a comprehensive study on the problem of fluid imbibition in isotropic partially-saturated fibrous sheets under different inclinations, both experimentally and theoretically. Simulations of Landeryou et al. (2005) were based on the work of Richards (1931) who developed a diffusive absorption model for two-phase flow in partially-saturated granular porous media. Our work in this paper follows the work of Landeryou et al. (2005) in using Richards’ equation for predicting the rate of fluid spread in fibrous sheets. Our emphasis, however, is on the effect of fiber in-plane orientation on fluid imbibition and spread. Moreover, we use a dual-scale simulation method, where the constitutive equations of capillary pressure and relative permeability are obtained via microscale 3-D simulations and utilized in a 2-D macroscale model based on the Richards’ equation derived here for anisotropic media.

In the next Section, we develop Richards’ equation for 2-D anisotropic media and also present our microscale simulations conducted to obtain the required capillary pressure and relative permeability constitutive equations. Section 5.3 describes our macroscale numerical simulation designed to solve Richards’ equation. In section 5.4, we present the results of these simulations and discuss them in comparison with the work of Marmur (1988). The conclusions drawn from our study are given in section 5.5.

5.2 Problem Formulation and Implementation

5.2.1 Richards’ Model of Fluid Infiltration in Porous Media

Starting with the conservation of mass for a wetting phase, we have:
where $\varepsilon$ is porosity and $S$ is moisture saturation, i.e., ratio of the liquid volume to that of the pores. $v_x$ and $v_y$ are the fluid velocities in the x and y directions. Assuming a creeping flow and using Darcy’s law, it can be shown that (Dullien 1991):

$$v_x = -\frac{1}{\mu} \left( K_{xx}(S) \frac{\partial p_c}{\partial x} + K_{xy}(S) \frac{\partial p_c}{\partial y} \right)$$  \hspace{1cm} (5.2)$$

$$v_y = -\frac{1}{\mu} \left( K_{yy}(S) \frac{\partial p_c}{\partial y} + K_{yx}(S) \frac{\partial p_c}{\partial x} \right)$$  \hspace{1cm} (5.3)$$

where $K_{ij}(S)$ is the permeability tensor, and is a function of saturation. In the above equations, $p_c$ and $\mu$ are capillary pressure and fluid viscosity, respectively. As will be discussed later in the next section, $K_{xy}(S)$ and $K_{yx}(S)$ are often negligibly small and can be dropped from further consideration. Combining conservation of mass and Darcy’s law for the moisture results in a single diffusive equation for saturation, we have:

$$\varepsilon \frac{\partial S}{\partial t} - \frac{1}{\mu} \left( \frac{\partial}{\partial x} \left( K_{xx}(S) \frac{\partial p_c}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy}(S) \frac{\partial p_c}{\partial y} \right) \right) = 0$$  \hspace{1cm} (5.4)$$

Since the capillary pressure $p_c$ is a function of saturation, using the chain rule we obtain:

$$\varepsilon \frac{\partial S}{\partial t} - \frac{1}{\mu} \left( \frac{\partial}{\partial x} \left( K_{xx}(S) \frac{\partial p_c}{\partial S} \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy}(S) \frac{\partial p_c}{\partial S} \frac{\partial S}{\partial y} \right) \right) = 0$$  \hspace{1cm} (5.5)$$

Equation 5.5 is a general scalar nonlinear equation which needs to be numerically solved for saturation as a function of time and space.
5.2.2 Constitutive Equations

As can be seen from Equation 5.5, mathematical expressions for capillary pressure, \( p_c(S) \), and relative permeability, \( K_y(S) \), are needed for solving Richards’ equation. Such relationships are often obtained experimentally for specific applications, and therefore limited in their usefulness elsewhere. To circumvent this limitation, we utilized a series of 3-D microscale simulations to obtain mathematical relationships for \( p_c(S) \) and \( K_y(S) \). The former was made possible by a so-called Full Morphology (FM) computational method and the latter was carried out via a combined FM-Stokes approach (Hazlett 1995, Hilpert and Miller 2001, Vogel et al. 2005, Schulz et al. 2007, Ashari and Tafreshi 2009a, Ashari and Tafreshi 2009b, Jaganathan et al. 2008c and Jaganathan et al. 2009). The FM and FM-Stokes algorithms are implemented using the GeoDict code from Fraunhofer-IWTM Germany.

5.2.2.1 Capillary Pressure

The most popular mathematical relationships for capillary pressure, \( p_c(S) \), are the empirical correlations of Haverkamp et al. (1977) and van Genuchten (1980) which were originally developed for granular porous materials. Landeryou et al. (2005) have recently used an auto-porosimeter to obtain a \( p_c(S) \) relationship in fibrous materials (nonwoven needle-felt polyester fabrics). We have previously shown that the above empirical correlations are in more or less good agreement with each other as well as our FM simulations (Ashari and Tafreshi 2009a and b).
The FM technique was originally developed by Hazlett (1995) and Hilpert and Miller (2001) and has been used by Vogel et al. (2005) and Schulz et al. (2007) for different porous media. In the FM method, the quasi-static distribution of liquid and gas for different capillary pressures are simulated in 3-D domains. The FM technique is used here to simulate water (wetting phase) imbibition in 3-D fibrous microstructures. The simulations start with an initially air-filled (nonwetting phase) medium. By incrementally decreasing the capillary pressure, volume of the pores with their narrowest local diameter smaller or equal to that of an inscribing sphere, whose size is determined via the Young-Laplace equation, are added together to obtain the volume of the pores that will be filled with water at the given capillary pressure (see Figure 5.1). By repeating this procedure over a range of capillary pressures, one can obtain a relation between capillary pressure and the percentage of void space that is filled with water (i.e., saturation). As mentioned earlier, the Young-Laplace equation is used in the FM method to find a relevant pore radius for each capillary pressure.

\[ p_c = \frac{2\sigma \cos \theta}{r_c} \]  

(5.6)

where \( \sigma \) is the surface tension between wetting and nonwetting phase and \( \theta \) is the contact angle between the wetting phase, nonwetting phase and the solid walls (65 degrees in this work).
Figure 5.1: Different stages of the imbibition of wetting phase obtained through morphology analysis. Here fibers, nonwetting phase (air), and wetting phase (water) are shown with blue, red, and background colors, respectively. It can be seen that by decreasing the capillary pressure, the nonwetting phase is being replaced by the wetting phase increasing the wetting phase saturation of the medium. a) $p_c = 4092$ Pa, b) $p_c = 2025.7$ Pa, c) $p_c = 1346$ Pa, and d) $p_c = 1100$ Pa (almost fully-saturated).

Here, we considered layered media with fiber angles obtained from normal-variate random distributions with a zero mean angle (along the x-direction) and standard deviations of 40, 22.5, and 0 degrees. Fibrous structures with standard deviations of 40, 22.5, and 0 degrees in our simulations represent Near-Isotropic, Machine Direction-
oriented (machine direction is the x-direction), and Unidirectional media, as shown in Figure 5.2a, b and c, respectively. From a practical point of view, our Near-Isotropic media represent typical spun-bonded and melt-blown nonwoven sheets where the fibers’ orientation slightly favors the machine direction. Our MD-oriented media represent nonwoven sheets made from carded fiberwebs, where fibers are mostly aligned in the machine direction (Jaganathan et al. 2008b). Our Unidirectional media represent an extreme situation where can only be seen in filament tows or fiber bundles.

We consider fibrous sheets with a Solid Volume Fraction (SVF) of 10% and a fiber diameter of 15µm. The 3-D simulation domains considered for capillary pressure and relative permeability simulations (next subsection) were 750×750×250 and 400×400×250 voxels, respectively, with each voxel being 2µm. Each simulation reported here is conducted, with the results averaged, over an ensemble of at least five statistically identical microstructures, to verify consistency in results. We considered an expression similar to that of Landeryou et al. (2005) for curve fitting to our FM results:

\[ p_e = p^*_e \ln S + C \]  

(5.7)
Figure 5.2: Top view of some of the 3-D microstructures used in this study; a) an example of a medium with random fibrous structure, b) an example of a medium with MD- oriented (somewhat oriented) fibers, and c) an example of a medium with unidirectional fibers.
The coefficients \( p_c^* = 1261.4, \ C = -714.96 \), \( p_c^* = 1415.99, \ C = -775.36 \) and
\( p_c^* = 1453.87, \ C = -745.17 \) are obtained by fitting Equation 5.7 to our FM results (see Figure 5.3) for the Near-Isotropic, MD-oriented, and Unidirectional media, respectively.

Even though the capillary pressure curves are quite close to each other, it still can be noted that saturation percentage is slightly less in the sheets with random fiber orientations at each capillary pressure. In other words, it is slightly easier for water (wetting phase) to penetrate into a medium with unidirectional or somewhat unidirectional (MD-oriented) medium.

Figure 5.3: Capillary pressure vs. wetting phase saturation obtained via the FM technique for Near-isotropic, MD-oriented, and Unidirectional structures.
5.2.2.2 Relative Permeability Expression

We have previously shown that single-phase (or absolute) permeability of a fibrous medium is a diagonal tensor (Ashari and Tafeshi 2009b, Jaganathan et al. 2008b and Tahir and Vahedi Tafreshi 2009). The off-diagonal elements of the permeability tensor are often 2-3 orders of magnitude smaller than the diagonal elements. The total permeability of a partially-saturated medium can be considered as the product of single-phase and relative permeability tensors (Dullien 1991):

\[
K_{xx}(S) = K_{xx}^s K_{xx}^r(S) \tag{5.8}
\]

\[
K_{yy}(S) = K_{yy}^s K_{yy}^r(S) \tag{5.9}
\]

where superscripts s and r stand for single-phase and relative permeability, respectively. Note that single-phase permeability constants, \( K_{xx}^s \) and \( K_{yy}^s \), are the medium’s permeability at \( S=1 \). The relative permeability constants, \( K_{xx}^r(S) \) and \( K_{yy}^r(S) \), on the other hand, depend on the medium’s saturation. Calculation of total permeability requires solving the Stokes equation at different states of saturation \( 0<S<1 \).

We use the FM-Stokes method here to obtain the relative permeability of our fibrous sheets. The FM-Stokes method assumes that the total and relative permeability of the phases can be decoupled, i.e., the flow of one phase does not entrain the other phase. With this assumption, the two-phase problem is actually decomposed to a series of single-phase flow problems with each flowing in slightly different media (same fibrous medium but at different saturation levels). The Stokes flow equations are solved for the wetting
phase using the finite difference FFF-Stokes solver of the Geodict program (Wiegmann 2007). More details on FM-Stokes method can be found in (Schulz et al. 2007).

Figure 5.4 shows the results of our relative permeability calculations for three families of Near-Isotropic (near-random), MD-oriented, and Unidirectional fibrous structures. As mentioned earlier, each simulation was conducted for an ensemble of five statistically identical fibrous structures. Note that the relative permeability values are always smaller than unity, as the permeability values are normalized by the fully-saturated permeability values, $K^s_{ij}$. For the near-isotropic, MD-oriented, and unidirectional structures, we obtained the following respective values:

\[
\begin{pmatrix}
K^s_{xx} = 2.00 \times 10^{-10} & K^s_{xy} = 1.77 \times 10^{-12} \\
K^s_{yx} = 2.02 \times 10^{-12} & K^s_{yy} = 1.39 \times 10^{-10}
\end{pmatrix},
\begin{pmatrix}
K^s_{xx} = 2.57 \times 10^{-10} & K^s_{xy} = 3.39 \times 10^{-12} \\
K^s_{yx} = 5.22 \times 10^{-12} & K^s_{yy} = 1.25 \times 10^{-10}
\end{pmatrix}, \text{ and}
\begin{pmatrix}
K^s_{xx} = 3.77 \times 10^{-10} & K^s_{xy} = 1.46 \times 10^{-14} \\
K^s_{yx} = 2.94 \times 10^{-14} & K^s_{yy} = 1.35 \times 10^{-10}
\end{pmatrix}.
\]

As the numbers show, the off-diagonal values for permeability are quite negligible compared to the diagonal elements.

Previous experimental studies have revealed that relative permeability is proportional to the third power of saturation (Landeryou et al. 2005 and Wang and Beckerman 1993). Brooks and Corey (1964) proposed the following equations for relative permeability of the wetting phase:

\[
K^r_j(S) = S^n
\]  

(5.10)

By fitting this equation to our relative permeability data (Figure 5.4), different values of exponent $n$ are obtained for different microstructures.
Figure 5.4: Relative permeability constants, $K_{xx}'(S)$ and $K_{yy}'(S)$, vs. saturation of wetting phase obtained via the FM-Stokes simulations for a) Near-isotropic, b) MD-oriented and c) Unidirectional structures.
5.3 Macroscale Numerical Simulation

In this paper, we used the FlexPDE program to solve the Richards’ equation (Richards 1931) in our fibrous sheets. FlexPDE is a mathematical program developed by PDESolutions Inc., designed for solving partial differential equations via the finite element method. Equation 5.5 is coded in FlexPDE to be solved in a 2-D domain as shown in Figure 5.5. The material is assumed to be a thin 5cm × 5cm sheet with a SVF of 10% and a fiber diameter of 15µm. Taking advantage of the existing symmetry, only one quarter of the sheet surface has been considered for the calculations. A fully-saturated (S=1) source of infinite moisture is considered in the lower left-hand corner of the domain. For the top and right boundaries, a Neumann (zero flux) boundary condition is considered. The two remaining boundaries were treated as symmetric boundaries.

Figure 5.5: Solution domain and the boundary conditions.
5.4 Results and Discussion

Solving the Richards’ equation, we obtain the media’s saturation as a function of time and space. Figure 5.6 shows the contour plots of saturation in the isotropic, MD-oriented, and unidirectional media at two different moments of \( t = 0.41 \) and 4.2 seconds. It can be seen that water spreads almost isotropically in the sheet with random fiber orientation, but penetrates much faster in the direction of the fibers in the media with oriented microstructures leading to elliptical spread patterns. The reason for this is that, as a wetting fluid enters a fibrous structure, it flows along the length of the fibers much more than past them, as it is the path of less resistance. If the majority of a material’s fibers are in the x-direction, then fluid flow through the medium will be more prevalent in the x-direction. The difference in the values of single phase permeability in the x and y directions (\( K_{xx}^s \) and \( K_{yy}^s \)) for a given microstructure, reflects this behavior. \( K_{xx}^s \) and \( K_{yy}^s \) values for sheets with nearly random orientation are close together, while \( K_{xx}^s \) for the MD-oriented and Unidirectional media is greater than \( K_{yy}^s \) by a factor of 2, and a factor of 3, respectively.

To obtain more quantitative comparisons between fluid penetration in the above sheets, saturation values are plotted along the \( x = 0 \) and \( y = 0 \) lines (i.e., vertical and horizontal boundaries) for isotropic, MD-oriented, and Unidirectional media at four different moments of time. Figure 5.7 illustrates these plots, with a target overlaid on each plot for the corresponding dimensionless \( x \) or \( y \) value of 0.65, and the corresponding time of 1.54 seconds into penetration. As can be seen, at \( t = 1.54 \text{ sec} \), saturation is \( S=0.60 \),...
$S=0.68$, and $S=0.84$ at a dimensionless distance of 0.65 in the x-direction, and $S=0.45$, $S=0.40$, and $S=0.20$ at the same distance in the y-direction, for our isotropic, MD-oriented, and Unidirectional media, respectively.

Figure 5.6: Contour plots of saturation at $t = 0.41$ and 4.2 seconds for a) Near-isotropic, b) MD-oriented and c) Unidirectional structures. Different colors from red to blue represent
different saturation values from one to zero, respectively. Coordinates are normalized by the sheet’s dimensions.

Figure 5.7: Saturation values along y = 0 and along x = 0 at different times of t = 9e-6, 0.11, 1.54, and 10 seconds) for a) Near-isotropic, b) MD-oriented, c) Unidirectional structures. Coordinates are normalized by the sheet’s dimensions. Target corresponds to dimensionless distance of 6.5 in corresponding x or y, and time at 1.54 seconds.
Finally, a comparison between the total amounts of water absorbed by the above media over time is presented in Figure 5.8. It can be seen that increasing the directionality of the fibers in a medium can help increase the rate of moisture uptake, as the rate is highest in the unidirectional and lowest in the isotropic media.

![Figure 5.8: Plot of liquid volume versus time for Near-isotropic, MD-oriented, and unidirectional media. Note that the reported values are for the domain size shown in Figure 6 (one quarter of the sheet).](image)

Some of the simulations conducted using FlexPDE were also performed using the finite volume CFD code from Fluent Inc enhanced with two User Defined Functions (UDFs) to ensure the accuracy of our results. Specifically, we programmed the Richards equation for the Fluent code via a UDF to be solved by the Fluent finite volume PDE solver. The first UDF calculates the saturation profile and the other the total liquid volume inside the media per unit thickness in L/mm. Solving Equation 5.5 using both finite
element and finite volume methods allows us to better validate our results against possible numerical errors (e.g., mesh dependency, convergence …). Figure 5.9a and b present the volume of water absorbed in an MD-oriented sheet over a period of ten seconds, and the saturation profile along the x-axis (y=0) of a sheet at $t=0.5$ seconds, respectively. In these Figures we compare the results of FlexPDE program with those of the Fluent-UDF with two (Figure 5.9a) and three (Figure 5.9b) different mesh counts. It can be seen that good agreements exist between the results of these two different numerical techniques, upon using a properly refined mesh for the finite volume calculations. It is also worth mentioning that the finite element computations conducted with FlexPDE were considerably faster and more accurate than the finite volume calculations of Fluent-UDF for a given mesh count.

Following the work of Hyvaluoma et al. (2006), we also compare our results with the analytical model of Marmur (1988). The simple relationship obtained by Marmur (1988) has also been used by Borhan and Rungta (1993) and Danino and Marmur (1994) for studying in-plane radial motion of fluids in paper sheets and good agreements were observed. Note that Marmur’s model is developed for isotropic media. The assumptions employed in the work of Marmur (1988) are somewhat similar to those used by Lucas-Washburn, and so do not consider the partially-saturated region of the media. Marmur’s equation for the radial penetration of fluids in thin porous media is given as:

$$\left(\frac{R}{R_0}\right)^2 \left(\ln\left(\frac{R}{R_0} - \frac{1}{2}\right) + \frac{1}{2}\right) + \frac{\sigma r_u \cos \theta}{6\mu R_0^2} = t$$

(5.11)
Figure 5.9: Volume of absorbed water versus time (a) and saturation values along the line $y=0$, at time $t=0.5$ seconds (b) obtained using FlexPDE and Fluent codes with different mesh densities.
where $R$ is the radius of the wetted area (assumed to be fully-saturated), $R_0$ is the radius of the liquid source, $r_a$ is the average pore radius inside the fibrous media and $t$ is the time. Note that $r_a$ is a parameter that cannot be directly measured or estimated. Here, using the information presented in Figure 5.8, we calculate a radius for an imaginary fully-saturated circular region in the media as a function of time (note that the values reported in Figure 5.8 are for one fourth of the sheet). The Marmur’s equation (Equation 5.11) was then fitted to our results and a value for the average pore radius, $r_a$, was obtained to be about 20 µm (see Figure 5.10).

![Graph](image)

**Figure 5.10:** Radius of an imaginary fully-saturated circular region is calculated from the results of Figure 5.6. The equation derived by Marmur (1988) is fitted to our results.
CHAPTER 6 A Semi-Analytical Model for Simulating Fluid Transport in Multi-Layered Fibrous Sheets Made up of Solid and Porous Fibers


6.1 Introduction

Products designed for fluid absorption or release, such as wound dressings, absorbent dry wipes, sanitary wet wipes, among many others, are ubiquitous and of crucial importance in industry and everyday life. Engineered composite nonwoven fabrics (often multi-layered) continue to rise in sophistication day by day, and thoughtful and methodical approaches to their design and development require in-depth understanding of two-phase diffusive fluid transport in fibrous media.

The majority of published studies discussing fluid transport in fibrous media are purely empirical, and consequently, their applications are limited to the products or conditions for which the experiments were conducted (see Pan and Gibson 2006 for a review). While there have been a few analytical, statistical, or numerical modeling studies in which fluid absorption in dry fibrous media has been investigated (see for instance, Marmur 1988, Lucas et al. 1977, Tompson 2002, Lucas et al. 2004, Hyvaluoma et al. 2006 and Mao and Russell 2008), no modeling works were reported to account for a given
medium’s anisotropy and partial saturation at the same time. Inspired by the seminal work of (Landeryou et al. 2005), we recently developed a dual-scale (microscale-macroscale) modeling methodology suitable for simulating fluid transport in partially-saturated anisotropic fibrous media (Jaganathan et al. 2009 and Ashari et al. 2010). Unlike the work of (Landeryou et al. 2005), the capillary pressure and relative permeability expressions in our work were obtained from 3-D microscale simulations. Note that the interrelationship of parameters in a partially-saturated fibrous medium is such that fluid transport depends on capillary pressure and relative permeability, both of which in turn depend on the medium’s microstructure, material of the fibers, fluid properties, and of course, instantaneous fluid saturation. Quantitative knowledge of capillary pressure and relative permeability allows one to solve the so-called Richards equation for diffusive flow in partially-saturated porous media (the macroscale model) to obtain the rate of fluid absorption (Jaganathan et al. 2009 and Ashari et al. 2010) or release (Ashari and Tafreshi 2009a) as a function of time and space throughout the material.

In almost all modeling studies published previously, including those of our group, fibers were treated as impermeable solid cylinders, incapable of absorbing and/or storing the fluid in their internal structure (non-swelling fibers). On the contrary, many fibrous materials used in fluid absorption or release applications are often comprised of fluid-absorbing porous fibers (swelling fibers). Modeling fluid transport in media made up of porous fibers is a challenge. This is because not only is the fluid able to enter the micrometer-sized voids between the fibers (inter-fiber region), it can also penetrate the nano-sized pores inside the fibers (intra-fiber region). Being several orders of magnitude
different in size, devising any direct numerical simulation that simultaneously solves for fluid saturation in both the intra-fiber and inter-fiber regions is almost impossible. Moreover, when a fluid seeps into the pores of a fiber, it often causes the fiber to swell, which in turn changes the morphology of the entire medium, adding further complexity to the modeling task. To circumvent the difficulties involved in modeling the swelling of porous fibers in software, we have conducted a series of vertical height rise experiments, and used the results in our simulations.

The objective of the current study is to present a general semi-analytical technique for simulating fluid absorption and release in composite multi-layered fibrous fabrics made up of swelling and non-swelling sheets. The fibrous sheets and the fluid used in the study are chosen arbitrarily, for model demonstration purposes only. Section 6.2 describes the Richards equation in its general 3-D form. Measurements and discussions related to the changes of a material’s microstructural parameters due to fiber swelling are presented in section 6.3. The capillary pressure expressions required for solving the Richards equation for swelling and non-swelling media are discussed in section 6.4, which also encompasses the use of our height rise test method, which was employed to obtain capillary pressure expressions for swelling fibrous media, and the effective contact angle for non-swelling fibrous sheets. In section 6.5, we discuss the permeability of fibrous media having varying fiber orientations, and present our general expression for relative permeability. We simplify Richards’ equation for 3-D absorption and 1-D motion-induced fluid release simulations in section 6.6, and present our boundary conditions for multi-layered composite fabrics. The simulations are conducted for fluid absorption from a pinhole into
bi-layered three-dimensionally anisotropic dry media, as well as fluid release from the same media when partially-saturated and placed on a moving hydrophilic surface. In section 6.7, we present results of our numerical simulations obtained for a bi-layered composite fabric, and discuss the effects of the order by which the layers are stacked on top of one another. This discussion is followed by our conclusions given in section 6.8.

6.2 Problem Formulation: Richards’ Equation

Two-phase flow in porous media obeys Darcy’s law, which was originally derived for single-phase flow by Henri Darcy in 1857, and was later modified for two-phase flows (Dullien 1991). Darcy’s law relates the average velocity of a liquid to the pressure gradient in a porous medium. Considering two-phase flow of air and liquid at constant atmospheric pressure, the modified Darcy’s law for the fluid phase can be written as (Dullien 1991):

\[
\begin{align*}
\nu_x &= -\frac{1}{\mu} \left( K_{xx}(S) \frac{\partial p_c}{\partial x} + K_{xy}(S) \frac{\partial p_c}{\partial y} + K_{xz}(S) \frac{\partial p_c}{\partial z} \right) \\
\nu_y &= -\frac{1}{\mu} \left( K_{yx}(S) \frac{\partial p_c}{\partial x} + K_{yy}(S) \frac{\partial p_c}{\partial y} + K_{yz}(S) \frac{\partial p_c}{\partial z} \right) \\
\nu_z &= -\frac{1}{\mu} \left( K_{zx}(S) \frac{\partial p_c}{\partial x} + K_{zy}(S) \frac{\partial p_c}{\partial y} + K_{zz}(S) \frac{\partial p_c}{\partial z} \right)
\end{align*}
\]  

(6.1) (6.2) (6.3)

where \(\nu_x, \nu_y, \) and \(\nu_z\) are velocity in the x, y, and z directions, respectively. \(K_{ij}(S)\) and \(p_c(S)\) are the saturation-dependent permeability tensor and capillary pressure term, respectively. Also, \(\mu\) is the viscosity of wetting phase. The continuity equation for incompressible unsteady liquid transport inside a medium is given as:
\[ \varepsilon \frac{\partial S}{\partial t} + \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) = 0 \]  

(6.4)

where \( \varepsilon \) is the medium’s porosity and \( S \) is the saturation of wetting phase. Substituting the velocity from the modified Darcy’s law (Equations 6.1 thorough 6.3) in Equation 6.4, the well-known Richards’ equation can be obtained (Richards 1931):

\[
\varepsilon \frac{\partial S}{\partial t} + \frac{1}{\mu} \left( \frac{\partial}{\partial x} \left( -K_{xx}(S) \frac{\partial p_c}{\partial x} \right) + \frac{\partial}{\partial y} \left( -K_{xy}(S) \frac{\partial p_c}{\partial y} \right) + \frac{\partial}{\partial z} \left( -K_{xz}(S) \frac{\partial p_c}{\partial z} \right) \right) + \frac{\partial}{\partial y} \left( -K_{yx}(S) \frac{\partial p_c}{\partial y} \right) + \frac{\partial}{\partial z} \left( -K_{yz}(S) \frac{\partial p_c}{\partial z} \right) + \frac{\partial}{\partial z} \left( -K_{zx}(S) \frac{\partial p_c}{\partial z} \right) = 0
\]

(6.5)

where the permeability tensor is defined as:

\[
K(S) = \begin{bmatrix}
K_{xx}(S) & K_{xy}(S) & K_{xz}(S) \\
K_{yx}(S) & K_{yy}(S) & K_{yz}(S) \\
K_{zx}(S) & K_{zy}(S) & K_{zz}(S)
\end{bmatrix}
\]

(6.6)

Equation 6.5 is the most complete form of Richards’ equation, and can be simplified depending on the problem under consideration, as will be discussed later in this paper.

### 6.3 Microstructural Properties of Swelling and Non-Swelling Media

As mentioned earlier, the diameter of most porous fibers increases (fiber swelling) as they absorb a wetting fluid. Fiber swelling affects the properties (e.g., porosity, thickness, in-plane dimensions…) of a fibrous sheet. Some of these properties are very hard to measure accurately, especially if soft thin sheets are considered. To demonstrate our semi-analytical modeling methodology in this paper, we have arbitrarily chosen two
different nonwoven fibrous sheets, one consisting of porous Rayon fibers, and the other made of solid (non-swelling) PET fibers. Both sheets have anisotropic in-plane fiber orientations common in hydroentangled nonwoven fabrics (Anantharamaiah et al. 2007, Vahedi Tafreshi et al. 2003 and Hou et al. 2010). Dry and wet characteristic properties of these sheets will be discussed in this section. We have also arbitrarily chosen a commercially available water-like diluted soap-lotion as the wetting fluid in our study (see Table 6.1 for physical properties).

Table 6.1: Physical properties of the water-based lotion used in this study.

<table>
<thead>
<tr>
<th>Property</th>
<th>Water-based lotion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity (Pa.s)</td>
<td>0.00113</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>998</td>
</tr>
<tr>
<td>Surface tension (N/m)</td>
<td>0.0276</td>
</tr>
</tbody>
</table>

To estimate the swelling of fibers in saturated Rayon sheets, diameters of dry and wet Rayon fibers were measured using an optical microscope. Measurement cuts were taken from different parts of a given samples to ensure that the collected data are representative of the whole medium. Forty images were taken of both wet and dry fibers, and the diameters of several fibers in each image were measured using the ImageJ software package. The results of our fiber diameter measurements for wet and dry PET and Rayon sheets are shown in Figure 6.1. Mean diameters of $13.1 \pm 1.87 \mu m$ and $18.1 \pm 1.76 \mu m$ were found for dry and wet Rayon fibers, respectively, indicating a diameter increase of
about 38% \( \beta_d = (d_f^w - d_f^d) / d_f^d = 0.38 \) where \( \beta_d \) is fiber diameter expansion factor, \( d_f^w \) is diameter of wet fiber and \( d_f^d \) is diameter of dry fiber. The statistical modes for the dry and wet fibers were obtained to be 13.2 µm and 18.5 µm, respectively, indicating that dry and wet fiber diameter distributions are almost Gaussian. We also conducted a similar test with our PET sheets and obtained a mean fiber diameter of 12.6 ± 1.12 µm regardless of their moisture content.

Another important effect that has experimentally been observed with Rayon sheets is a change in the macroscopic dimensions (length, width, and thickness) upon wetting.

Conducting 38 trials with our Rayon sheets, we obtained an average Cross Direction (CD),
i.e., lateral direction, expansion of $\beta_{CD} = (l_{CD}^w - l_{CD}^d)/l_{CD}^d = 0.0595$ (where $\beta_{CD}$ is sheet expansion factor in CD, $l_{CD}^w$ is length of wet sheet in CD and $l_{CD}^d$ is length of dry sheet in CD), and an average Machine Direction (MD), i.e., longitudinal direction, expansion of $\beta_{MD} = (l_{MD}^w - l_{MD}^d)/l_{MD}^d = -0.0148$ (length contraction where $\beta_{MD}$ is sheet expansion factor in MD, $l_{MD}^w$ is length of wet sheet in MD and $l_{MD}^d$ is length of dry sheet in MD). The extent of this effect depends on many parameters such as fiber properties, the process by which the fiberwebs were produced, and the fiber-to-fiber bonding technique used in consolidating loose fiberwebs. Therefore, it is very hard to develop a direct relationship between the changes in a given sheet’s dimensions and the swelling percentage of the fibers. Nevertheless, in the absence of a better alternative, and because of the errors involved in accurately measuring the thickness of soft wet and/or dry nonwoven sheets, we assumed that the expansion in the Thickness Direction (TD) is proportional to that of fiber diameter, i.e., $\beta_{TD} = (l_{TD}^w - l_{TD}^d)/l_{TD}^d = 0.38$ (where $\beta_{TD}$ is sheet expansion factor in TD, $l_{TD}^w$ is length of wet sheet in TD and $l_{TD}^d$ is length of dry sheet in TD). No change in the dimensions of the PET sheets was observed. We calculate a medium’s dry Solid Volume Fraction (SVF) $\alpha^d$ using the equation below:

$$\alpha^d = 1 - \varepsilon^d = \frac{W^d}{l_{TD}^d \rho_f^d}$$

(6.7)

where $\alpha^d$ is dry solid volume fraction, $\varepsilon^d$ is porosity of dry sheet, $W^d$ is dry basis weight, and $\rho_f^d$ is bulk density of dry fiber. The above formula resulted in an SVF of about 7.6%
and 6% for the dry PET and Rayon sheets, respectively. For Rayon, in which case microstructural parameters change upon fluid absorption, wet SVF $\alpha^w$ can be calculated via a similar equation:

$$\alpha^w = 1 - e^w = \frac{W^w}{l_i^w \rho^w_f}$$ (6.8)

where $\alpha^w$ is solid volume fraction of wet sheet, $W^w$ is the wet basis weight (i.e., weight of the wet fibers per unit area, excluding the weight of the liquid entrapped between the wet fibers) in kg/m$^3$, and $\rho^w_f$ is the bulk density of the wet fibers in kg/m$^3$ which can be obtained as follows:

$$\rho^w_f = (\rho^d_f V^d_f + m_i) / V^w_f = (\rho^d_f V^d_f + m_i) / (V^d_f R_v)$$ (6.9)

where $V^d_f$ is the dry volume of fibers, which can be defined as

$$V^d_f = 0.25\pi (d^d_f)^2 l^d_f n_f$$ (where $n_f$ is the number of fibers). In Equation 6.9, $m_i$ is the mass of fluid inside the fibers, and can be approximated by

$$m_i = 0.25\pi [(d^w_f)^2 - (d^d_f)^2] l^w_f \rho_i n_f$$, where $\rho_i = 998 \text{kg/m}^3$ is the liquid density, and $R_v$ is the ratio of the fibers’ wet volume to their dry volume. In the absence of any better approximations, we assume $R_v = (1 + \beta_v)^2 (1 + \beta_{MD})$. Knowing $d^w_f = 18.1 \mu m$,

$$d^d_f = 13.1 \mu m$$, and $\rho^d_f = 1530 \text{kg/m}^3$, we obtain a density for wet Rayon fibers of

$$\rho^w_f \approx 1300 \text{kg/m}^3$$. Basis weight of the wet sheets can be obtained as follows:

$$W^w = \rho^w_f V^w_f l(l^w_{MD} l^w_{CD}) = \rho^w_f V^d_f R_v l(l^w_{MD} l^w_{CD})$$ (6.10)
The fibers’ dry volume can be calculated as:

\[ V_j^d = \alpha^d \, V_{sh}^d = \alpha^d \, (l_{MD}^d \, l_{CD}^d \, l_{TD}^d) \]  

(6.11)

Substituting the known values of \( \alpha^d = 0.06 \), \( l_{MD}^d = 0.253 \, \text{m} \), \( l_{CD}^d = 0.205 \, \text{m} \), \( l_{TD}^d = 0.00063 \, \text{m} \), \( l_{MD}^w = 0.249 \, \text{m} \), \( l_{CD}^w = 0.217 \, \text{m} \), \( \rho_f^w = 1300 \, \text{kg/m}^3 \), and \( R_v = 1.88 \) in Equations 6.8 through 6.11, we obtain the SVF for our wet Rayon sheets as being \( \alpha^w = 0.078 \). Note that SVF of dry and wet sheets can also be calculated as \( \alpha^d = V_f^d / V_{sh}^d \) and \( \alpha^w = V_f^w / [V_{sh}^d (1 + \beta_{MD}) (1 + \beta_{CD}) (1 + \beta_{TD})] \). Therefore, one can obtain the SVF of wet sheets as:

\[ \alpha^w = \alpha^d R_v / [(1 + \beta_{MD})(1 + \beta_{CD})(1 + \beta_{TD})] \]  

(6.12)

### 6.4 Capillary Pressure Expressions

As can be seen from Equation 6.5, mathematical expressions for capillary pressure \( p_c(S) \) and relative permeability \( K_y(S) \) are needed for solving the Richards equation. The most popular mathematical relationships for capillary pressure \( p_c(S) \) are the empirical correlations of Haverkamp (1977) and van Genuchten (1980), which were originally developed for granular porous media. Note that unlike permeability, which is strongly dependent on a medium’s microstructure and the direction of flow, capillary pressure is often considered to be identical in different directions.

For fibrous media made up of solid (non-swelling) fibers, we are able to utilize mathematical expressions for \( p_c(S) \) and \( K_y(S) \) obtained via numerical simulations for
different cases of fluid absorption and fluid release, as in our previous work (Ashari and Tafreshi 2009b and Ashari et al. 2010). Landeryou et al. (2005) have recently used an auto-porosimeter to obtain a $p_c(S)$ relationship for needle-felted PET nonwovens. We have previously shown that the above empirical correlations are in more or less good agreement with one another and our full morphology (FM) simulation results (Ashari and Tafreshi 2009a and Ashari and Tafreshi 2009b). The FM technique was originally developed by Hazlett (1995) and Hilpert and Miller (2001), and has also been used by Schladitz et al. (2006) and Schulz et al. (2007) for different porous media. In the FM method, the quasistatic distribution of liquid and gas for different capillary pressures are simulated in a 3-D domain modeled after the microstructure of a given medium. The FM technique is only applicable to media with non-swelling fibers.

Capillary pressure in media with swelling fibers is expected to be higher than that of media made up of solid fibers, due to the nano-sized pores in the intra-fiber region are expected behave as very small capillary tubes which generate additional capillary pressures. Modeling capillary pressure of swelling media is very challenging. We will therefore obtain these relationships experimentally, as will be discussed in the next subsection.

6.4.1 Height Rise Test

A vertical height rise test is used in our work for two main purposes: 1) to obtain an “effective” contact angle between the fluid and fibers, which is needed for our general capillary pressure expressions (the case of non-swelling media), and 2) to obtain a
relationship between capillary pressure and saturation for media made up of porous fibers. While the latter correlation can also be used for obtaining capillary pressure for non-swelling media, the expressions developed using FM simulations require far less time to develop and ascertain.

We designed and built a test rig consisting of a computer-controlled hanging mechanism, on which narrow strips of nonwoven fabrics (5cm × 37cm) can be mounted and vertically moved above a fluid reservoir (a beaker). The beaker is placed on a sensitive scale with a capacity of 120 g and a resolution of 0.001 g for weight measurement (see Figure 6.2). To eliminate the errors caused by fluid evaporation, the entire assembly was placed in a confined environment with approximate height, length, and width of about 0.6, 0.4, and 0.4 m, respectively. To help saturate the air inside the enclosure before running each test, we placed additional fluid containers inside the confinement for almost a day. To start the test, the mounting mechanism lowers the fabric strip until it just breaks the plane of the fluid in the beaker, and then holds it in place for the remainder of the test. The rate of fluid imbibition into the medium is then obtained by reading the changes of the beaker’s weight over time (see Figure 6.3). Additional steps are taken depending on whether capillary pressure or effective contact angle is the parameter of interest, which will be described in the appropriate subsections below.
6.4.2 Capillary Pressure of Swelling Media

Due to the computational difficulty involved with modeling capillary pressure for media made up of porous fibers, we utilize the height rise test as an alternative method. We perform the test as described above, and allow the fabric to stay in contact with the fluid reservoir for at least two hours. We then cut the strip into equal segments and weigh them using a sensitive scale. Knowing the dry weight of the fabric, we obtain saturation using the following equation:

\[ S^w = \frac{(M^w - M^d)}{(\rho_f (1 - \alpha^w)V_s^w)} \]  

(6.13)
\[ S^d = \frac{(M^w - M^d)}{(\rho_f(1 - \alpha^d)V_s^d)} \]  \hspace{1cm} (6.14)

where \( S^d \) is saturation calculated using dry properties of fibrous structure, \( S^w \) is saturation calculated using wet properties of fibrous structure, \( M^w \) is weight of wet segment, \( M^d \) is weight of dry segment, \( \rho_f \) is the density of fluid, \( V_s^d \) is volume of dry segment and \( V_s^w \) is volume of wet segment.

Figure 6.3: A comparison between the weights of the fluid imbibed in the PET and Rayon sheets. The data are obtained from our height rise test. Note that these fabrics have different thicknesses.

Here we use superscripts w and d to distinguish the saturation values calculated using dry properties from those obtained using the fabric’s wet properties. In order to suppress any fluid redistribution, we freeze the samples before cutting using dry ice. Capillary pressure of the media can then be estimated as:
\[ p_c(S) = \rho_c g h(S) \]  
(6.15)

where \( h(S) \) is the height of each segment from the datum.

Results of the capillary pressure measurement conducted for our Rayon sheets are shown in Figure 6.4. Each experiment is repeated at least three times in order to ensure statistical confidence in our measurements. As mentioned earlier, the SVF for the sheet containing swelling fibers changes after wetting, specifically for our Rayon sheets, the SVF rises from about 6% to about 7.8%. In preparing the capillary pressure plots (Figure 6.4a,b), saturation was calculated using dry and wet SVFs. As will also be discussed in the next section, we normally use wet medium parameters for permeability and capillary pressure calculations. However, in our simulations of fluid absorption (Section 6.7) we utilized the capillary pressure expressions obtained using the dry parameters of the material (Figure 6.4). This is justified by considering the fact that during the fluid absorption process, the liquid front penetrating into the dry medium provides the capillary pressure. We curve fit the correlation of Landeryou et al. (2005) to our experimental results obtained from height rise with dry properties. We chose this correlation because it showed better agreement with our experimental data when compared to the correlation of Haverkamp et al. (1977). The empirical correlations of Landeryou et al. (2005) and Haverkamp et al. (1977) are given as:

\[ S = \exp \left( \frac{p_c}{p_c^*} \right) \]  
(6.16)

\[ S = \frac{1}{1 + |p_c|^p / C} \]  
(6.17)
where $p^*_c$, $b$, and $C$ are empirical coefficients that can be obtained from curve fitting.

Here we found a value of $p^*_c = 790.38$ for capillary pressure relationship using the data shown in Figure 6.4b.

### 6.4.3 Capillary Pressure of Non-Swelling Media

We have previously conducted a series of 3-D microscale FM simulations to obtain two general capillary pressure expressions $p_c(S)$ for fluid drainage from non-swelling thin nonwoven sheets (Ashari and Tafreshi 2009b). These expressions were based on the empirical correlations of Haverkamp et al. (1977) and van Genuchten (1980). Either of these expressions can be used here, and so we continue our discussion with the one obtained using the work of Haverkamp et al. (1977):

$$p_c(S) = C_1 \frac{\sigma \cos \theta}{\sigma_w \cos \theta_w} (S^{-1} - 1)^{1/h}$$

(6.18)

where $\sigma_w = 0.073$ N/m and $\theta_w = 80^\circ$ are the surface tension and contact angle of water with a Polyester surface (Zhu et al. 2005). The expression is valid for a fiber diameter range of 10 to 25 µm, a SVF range of 5 to 12.5%, and different surface tensions and contact angles. Constants $C_1$ and $b_1$ are obtained from the plots in Figure 6.5. The contact angle between the fluid and fibers inside a given medium must be found experimentally. We obtained an effective contact angle for our PET sheets using height rise data, as explained in the next subsection.
Figure 6.4: Results of our capillary pressure measurement conducted for the Rayon sheets. Liquid saturation is obtained using wet (a), and dry (b) properties of the sheets. Capillary pressure expressions of Haverkamp et al. (1977) and Landeryou et al. (2005) are fitted into the data.
For fluid absorption in sheets made of non-swelling fibers (PET) we fitted the expression of Landeryou et al. (2005) to our experimental data to obtain $p^*_c = 451.04$ (see Figure 6.6).

**6.4.3.1 Effective Contact Angle from Partially-Saturated Height**

An alternative approach for obtaining an effective contact angle for non-swelling media is to use the experimental capillary pressure values obtained using Equation 6.15, and compare them with those obtained from our general expression given in Equation 6.18. By curve fitting Equation 6.18 to the experimental capillary pressure data, one can obtain an effective contact angle between the fluid and the “pores” in the fibrous sheets (see Figure 6.6).

Note that Equation 6.18 was originally developed for fluid drainage from a fibrous medium in the through-plane direction. However, since the porosity of the fibrous sheets considered in this study is relatively high (87.5 to 95%) capillary pressure values for absorption and drainage are expected to be very close to one another (no significant hysteresis effect) if the fibers are non-absorbing (solid fibers). In addition, our group has shown in a recent study that fiber orientation does not have any significant effect on the capillary pressure values, indicating that our general expression (Equation 6.18) can also be used for fluid transport in directions other than the through-plane direction (Bucher et al. 2011). By fitting Equation 6.18 to the experimental data obtained for our PET sheets, (see Figure 6.6) we obtained an effective contact angle of 72 degrees.
Figure 6.5: Constants $C$ and $b$ to be used in our general capillary pressure equation (Equation 6.18).
Figure 6.6: Results of our capillary pressure measurement conducted for the PET sheets. Our general capillary pressure expression (Equation 6.18) is fitted to the experimental data to find an effective contact angle. The correlation of Landeryou et al. (2005) is also fitted into the data to be used in our absorbency simulations.

6.4.3.2 Effective Contact Angle from Fully-Saturated Height

Mullins et al. (2007) curve fitted different capillary rise models to their experimental data to find that the modified Washburn equation, originally presented by (Reed and Wilson 1993), is the simplest model to be used with acceptable accuracy. The modified Washburn equation is given as:

\[
t = \frac{8 \mu}{g \rho \gamma r_c^2} [(x_\infty + x_0) \ln\left(\frac{x_\infty}{x_\infty - x}\right) - x]
\]  

(6.19)

where \(x(t)\) is the saturated height of the liquid, and \(x_0\) is the length of the capillary completely submerged in the liquid. The quantity \(x_\infty\) is the steady-state height of the liquid column in the capillary as \(t\) approaches infinity:
\[ x_\infty = L_c \sigma \cos \theta / (A_c \rho_f g) \] (6.20)

One can use Equations 6.19 and 6.20 to obtain an equivalent capillary diameter, an effective contact angle, and \( x_\infty \) from height rise data (Mullins et al. 2007).

The Washburn theory and all its modified versions are based on the capillary tube theory in which the tube is divided into two regions of fully-saturated and fully-unsaturated lengths with a distinct interface. To use the Washburn equation, one has to obtain an equivalent fully-saturated height for the fluid distributed within a partially-saturated medium. This can be done using the cross-sectional area and SVF of the medium as follows:

\[ x(t) = \frac{m_\alpha(t) / \rho_f}{A_f (1 - \alpha)} \] (6.21)

As mentioned before, the results of our height rise test with PET sheets are plotted in Figure 6.3. Assuming an immersed length of \( x_\theta = 2 \) mm, we obtained the equivalent saturated height of the absorbed liquid (see Figure 6.7a). As mentioned by (Mullins et al. 2007), Equation 6.19 shows better agreement with the data collected during the early stages of the experiment. Therefore, we fitted Equation 6.19 for a time period of 100 sec (see Figure 6.7c), resulting in \( R^2 = 0.9798 \), a capillary radius of \( r_c = 33.101 \mu m \) and \( x_\infty = 0.0383 \) m. With this information, we determined the effective contact angle between the fluid and the fibers in the PET sheets from Equation 20 to be 77 degrees. The capillary pressure obtained in this way (dash-dot blue curve) is plotted in Figure 6.6 for comparison. Although the resulting capillary pressure does not perfectly match the
experimental data, one should note that unlike the two other correlations shown in Figure 6.6, these results are not obtained via curve fitting to the capillary pressure values obtained experimentally.

Masoodi et al. (2007) presented a different form of the Washburn equation that includes the capillary pressure of the liquid front edge and the medium’s single-phase permeability, along with saturated height:

\[
p_c \ln \left( \frac{p_c}{p_c - \rho g x} \right) - \rho_l g x = \frac{D^2 g^2 K}{\varepsilon \mu} t \quad (6.22)
\]

Neglecting gravity, these authors simplified the Washburn equation to obtain Masoodi et al. (2007) (see also Landeryou et al. 2005):

\[
x(t) = \sqrt{\frac{2K}{\varepsilon \mu}} \frac{p_c}{t} \quad (6.23)
\]

In Figures 6.7a–d we present the saturated height of PET (Figures 6.7a and 6.7b) and Rayon sheets (Figures 6.7c and 6.7d) at different times during the height rise test. Figures 6.7a and 6.7c show the entire duration of the experiment, while Figures 6.7b and 6.7d show only the first 100 seconds for better comparison. We curve fitted Equations 6.19, 6.22, and 6.23 into our experimental data. Since the equations of Mullins et al. 2007 (Equation 6.19) and Masoodi et al. (2007) (Equation 6.22) are essentially different forms of the original Washburn equation, the lines presenting these expressions fall on top of one another.
Figure 6.7: Results of height rise test (saturated height versus time) for the PET (a and b) and Rayon sheets (c and d) for test periods of 7200 s and 100 s. The well-known Washburn equation written in different forms is fitted to the experimental data for comparison.

Note that the Washburn equation is based on the assumption that the fibrous medium is made up of a series of parallel capillary tubes, which are divided between fully-saturated and fully dry regions (i.e., no partial-saturation). Therefore, the apparent height of the liquid inside a medium is not necessarily equal to the fully-saturated height obtained from Equation 6.21 (and the plots in Figures 6.7a–d).
As can be seen in Figures 6.7b and d, the Washburn equation perfectly matches our experimental data obtained during the first 100 seconds of the experiment. It is worth mentioning that the simplified Washburn equation (Equation 6.23), in which the capillary forces are only balanced with the viscous forces, does not seem to show close agreement.

6.5 Relative Permeability Expressions

We have previously shown that saturated (i.e., fully-saturated) permeability of a fibrous medium is a diagonal tensor, i.e., the off-diagonal elements are negligibly small [29-30]. Total permeability of a partially-saturated medium can be considered as the product of saturated and relative permeability tensors (Dullien 1991):

\[
K_{xx}(S) = K_{xx}^{s} K_{xx}^{r}(S) 
\]

\[
K_{yy}(S) = K_{yy}^{s} K_{yy}^{r}(S) 
\]

\[
K_{zz}(S) = K_{zz}^{s} K_{zz}^{r}(S) 
\]

where superscripts s and r stand for saturated and relative permeability, respectively. The relative permeability constants \( K_{xx}^{r}(S) \), \( K_{yy}^{r}(S) \), and \( K_{zz}^{r}(S) \) depend on the medium’s saturation, while the fully-saturated permeabilities are functions of the microstructural parameters of the medium. Calculation of total permeability requires solving the Stokes equations at different states of saturation 0<S<1.

Previous experimental studies have revealed that relative permeability is proportional to saturation via a power law relationship (Landeryou et al. 2005, Wang and
Beckerman 1993). Brooks and Corey (1964) proposed the following equations for relative permeability of the wetting phase:

\[ K_{xx}'(S) = K_{yy}'(S) = K_{zz}'(S) = S^n \]  

(6.27)

The exponent \( n \) has often been reported to be in the neighborhood of 3, but depending on the microstructural parameters of the given medium, it may increase to higher values (Landeryou et al. 2005, Jaganathan et al. 2009, Ashari and Tafreshi 2009a and Ashari and Tafreshi 2009b). In general, the exponent \( n \) for fluid absorption may be different from that for fluid release, as the moisture distribution throughout a fibrous medium can be different during absorption and release, even at identical saturation levels. For the sake of simplicity, and for the lack of a more sophisticated theory, we assume \( n=3.18 \), which was obtained in our previous study on fluid release in the thickness direction (Ashari and Tafreshi 2009b). Such a number is in good agreement with that of Landeryou et al. (2005), which was experimentally obtained for in-plane fluid absorption.

Fully-saturated permeability of media with different fibrous microstructures has been examined in numerous studies (e.g., Spielman and Goren 1968 and Jackson and James 1986). The fibrous media considered in this study are layered (i.e., no significant through-plane fiber orientation) but have some degrees of machine directionality. Here we use the equations of (Spielman and Goren 1968), developed for layered fibrous media with random in-plane fiber orientations. There are many other expressions that have been developed in the past for predicting saturated permeability of fibrous media with different orientations. More information can be found in our previous publications (Jaganathan et al.
2008b, Tahir and Tafreshi 2009, Vahedi Tafreshi et al. 2009 and Hosseini and Tafreshi 2010). Depending on the available information regarding the microstructure of a fibrous medium, one can choose appropriate expressions for the saturated permeability of the medium in different directions.

Expressions of (Spielman and Goren 1968) for layered fibrous media with random in-plane fiber orientations are given as:

\[
\frac{1}{4\alpha} = \frac{1}{2} + \frac{\sqrt{K_{TP}}}{r} K_0\left(\frac{r}{\sqrt{K_{TP}}}\right) \quad (6.28)
\]

\[
\frac{1}{4\alpha} = \frac{1}{4} + \frac{3\sqrt{K_{iso}^{ip}}}{4r} K_0\left(\frac{r}{\sqrt{K_{iso}^{ip}}}\right) \quad (6.29)
\]

We have previously shown that the in-plane orientation of the fibers has no influence on the saturated permeability of a layered fibrous medium in the through-plane (thickness) direction (Tahir and Tafreshi 2009). Therefore, Equation 6.28 can directly be used to predict the through-plane permeability of our PET and Rayon sheets. For in-plane permeability, however, Equation 6.29 needs some modification, as the in-plane fiber orientation in our sheets is not isotropic (see section 6.7).

Calculating relative permeability for swelling media requires special attention. As mentioned before, when a fluid infiltrates a swelling medium, some portion of the fluid enters the nano-pores inside the fibers (intra-fiber region), and some enters the space
between the fibers (inter-fiber region). The fluid that enters the fiber is believed to become trapped inside the fiber, as the friction against fluid motion is greatly higher in the intra-fiber compared to the inter-fiber space. It has been experimentally observed that there is often a saturation threshold below which permeability of the medium tends to zero. This can be due to a variety of reasons, including the fact that the fluid may break up inside the medium, and lose its continuity. We therefore used a saturation threshold of 0.4 for our fluid release simulations (Landeryou et al. 2005 and Haverkamp et al. 1977). For a smooth transition from relative permeability proportional to \( S^{3.18} \) to almost zero permeability, we considered a piecewise function, given as:

\[
K_x^r(S) = K_y^r(S) = K_z^r(S) = \begin{cases} 
S^{3.18} & S \geq 0.4 \\
S^6 & S < 0.4
\end{cases}
\]  

(6.30)

The exponent 6 is chosen arbitrarily, and any other exponent greater than about 6 should suffice as well (see Figure 6.8).

### 6.6 Macroscale Numerical Simulation

In this section, we describe our numerical simulations on the macroscale and their boundary conditions. This section is divided into two subsections. The first subsection describes our modeling approach for simulating penetration and spread of a wetting fluid into a 3-D anisotropic multi-layered fabric, made up of swelling and non-swelling fibers. The fluid is infinite in volume and is released to the material from a pinhole. In the second subsection, we model fluid release from the same anisotropic bi-layered medium when partially-saturated with a fluid. The fluid release is driven by a mass convection boundary
condition, simulating the drainage of fluid due to contacting a hydrophilic surface in motion relative to the sheets.

Figure 6.8: The general relative permeability expressions used in our study; for the PET ($S^{3,18}$) and Rayon sheets (Equation 6.30).

6.6.1 Modeling Fluid Absorption in Multi-Layered Composite Media

For modeling fluid absorption in multi-layered fibrous media, Equation 6.5 needs to be solved numerically. Our previous studies, in agreement with available information in the literature, indicated that the off-diagonal values of total permeability tensor are about 2 orders of magnitude smaller than the diagonal elements. Neglecting the off-diagonal permeability terms in Equation 6.5 we obtain:
Implementing the chain rule, we get:

\[
\frac{\partial S}{\partial t} + \left( \frac{\partial}{\partial x} \left( D_{xx}(S) \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_{yy}(S) \frac{\partial S}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_{zz}(S) \frac{\partial S}{\partial z} \right) \right) = 0
\]

where nonlinear diffusive coefficient defined as

\[
D_{xx}(S) = -\frac{K_{xx}^s K_{xx}'(S) \frac{\partial p_c}{\partial S}}{\varepsilon \mu}
\]

\[
D_{yy}(S) = -\frac{K_{yy}^s K_{yy}'(S) \frac{\partial p_c}{\partial S}}{\varepsilon \mu}
\] and

\[
D_{zz}(S) = -\frac{K_{zz}^s K_{zz}'(S) \frac{\partial p_c}{\partial S}}{\varepsilon \mu}.
\]

Equation 6.32 is the main governing equation we use in our model to solve for 3-D anisotropic absorption or release in multi-layered fibrous media. In modeling multi-layered media, we use Equation 6.32 for each separate layer, and use their specific diffusive coefficients.

For the interface between of two layers we consider equal saturation flux in the x, y, and z directions:

\[
\begin{bmatrix}
D_{xx} \frac{\partial S}{\partial x} & 0 & 0 \\
0 & D_{yy} \frac{\partial S}{\partial y} & 0 \\
0 & 0 & D_{zz} \frac{\partial S}{\partial z}
\end{bmatrix}_{upper \ layer} \begin{bmatrix}
\frac{\partial S}{\partial x} \\
\frac{\partial S}{\partial y} \\
\frac{\partial S}{\partial z}
\end{bmatrix}_{upper \ layer} = \begin{bmatrix}
D_{xx} \frac{\partial S}{\partial x} & 0 & 0 \\
0 & D_{yy} \frac{\partial S}{\partial y} & 0 \\
0 & 0 & D_{zz} \frac{\partial S}{\partial z}
\end{bmatrix}_{lower \ layer} \begin{bmatrix}
\frac{\partial S}{\partial x} \\
\frac{\partial S}{\partial y} \\
\frac{\partial S}{\partial z}
\end{bmatrix}_{lower \ layer}
\]

It should be noted that no-flow and symmetry boundary conditions

\[
\frac{\partial S}{\partial x} = \frac{\partial S}{\partial y} = \frac{\partial S}{\partial z} = 0
\]

are used on the remaining surfaces as shown in Figure 6.9.
Figure 6.9: The mesh distribution and boundary conditions considered for our absorption simulations.

We coded the Richards equation (Equation 6.32) along with the appropriate equations for capillary pressure (see section 6.4) and relative permeability (see section 6.5) in the FlexPDE program to be solved via the finite element method. FlexPDE is a mathematical program developed by PDE Solutions Inc., designed for solving partial differential equations. We have previously compared the results of FlexPDE with those of the well-known CFD code from Fluent Inc. enhanced with user defined subroutines (UDFs), and obtained superior accuracy for a given number of cells (Ashari et al. 2010). FlexPDE’s better accuracy for a fixed number of cells allows us to complete a given simulation with much shorter CPU time, and therefore, we only use FlexPDE in this paper.
6.6.2 Modeling Fluid Release from Multi-Layered Composite Media

Fluid release in the thickness direction is a 1-D problem. For these simulations, Equation 6.32 simplifies to:

\[
\frac{\partial S}{\partial t} + \frac{\partial}{\partial z} \left( D_{zz}(S) \frac{\partial S}{\partial z} \right) = 0
\] (6.34)

The boundary conditions for fluid release simulations are the same as those shown for absorption (Figure 6.9). However, for the release simulations we have used a mass convection boundary condition (Ashari and Tafreshi 2009b) as:

\[
D_{zz}(S) \frac{\partial S}{\partial z} = -k_f (S_m - S_{out})
\] (6.35)

where \( S_{out} \) is the saturation outside the domain (if any). The coefficient \( k_f \) plays an important role in this boundary condition, and should be found empirically as a function of speed. Here we also set the external saturation \( S_{out} \) equal to zero to simulate the case of a dry target surface. This boundary condition is placed in order to mimic fluid release from the medium as it is moved against a stationary surface. Since the sheet is considered to be thin, for the sake of simplicity, we assume that the fluid release from the bottom boundary is solely due to the relative motion between the sheet and the target surface. In other words, we assume that the thin sheet is not significantly compressed while delivering the fluid to the target surface. Note that surface energy of the target surface is not included in the boundary condition, as we have assumed the target surface to be hydrophilic. For solving Equation 6.32, we simplified our FlexPDE code (see previous subsection) and added
Equation 6.35 as the mass convection boundary condition for the side in contact with the target surface.

6.7 Results and Discussion

Solving the Richards equation, we obtain a medium’s saturation as a function of time and space. Our simulation results obtained for fluid absorption in bi-layered anisotropic sheets and motion-induced fluid release from similar materials are presented in the following two subsections.

6.7.1 Fluid Absorption in Bi-Layered Anisotropic Materials

Our absorption simulations here are performed for a bi-layered composite sheet. The layers are the same PET and Rayon sheets discussed earlier. Here, we simulate fluid absorption in this composite nonwoven fabric, and discuss the influence of the order by which the sheets are stacked on top of one another, i.e., whether the Rayon is placed on the top or at the bottom.

We considered a simulation domain with in-plane (MD and CD directions) dimensions of 1 cm by 1 cm. The SVF and fiber diameter for wet PET and wet Rayon are calculated in section 6.2, and are also summarized here in Table 6.2. With this information, and using the expressions of Spielman and Goren (1968) (Equations 6.28 and 6.29), we obtained the layers’ respective through-plane and in-plane permeability constants $K_{tp}$ and $K_{ip}$ (see Table 6.3). These theoretical values are obtained assuming that the medium is
layered with isotropic in-plane fiber orientation, i.e., $K_{CD} = K_{MD}$. However, thin fibrous sheets, especially those processed via so-called hydroentangling, are often anisotropic, with their fibers predominantly oriented in the machine direction (Anantharamaiah et al. 2007 and Vahedi Tafreshi et al. 2003) for more information on hydroentangling). In a recent study, we simulated saturated permeability of similar fibrous sheets having different in-plane fiber orientations via 3-D microscale simulations (Ashari et al. 2010). We compared the permeability of media with isotropic in-plane fiber orientation with their counterpart having a somewhat MD-oriented fiber orientation, resembling hydroentangled thin sheets. Although the permeability of the sheets simulated by (Ashari et al. 2010) are quite different from those of our PET and Rayon sheets used in this study, it is reasonable to assume that the influence of fibers’ in-plane orientation is similar in both studies. Therefore, ratio of the permeabilities obtained by (Ashari et al. 2010) for in-plane isotropic and MD-oriented media ($K_{MD} / K_{IP}^{iso} = 1.5$ and $K_{CD} / K_{IP}^{iso} = 0.73$) can be used here to calculate the permeability of our PET and Rayon sheets in the MD and CD directions by modifying the in-plane permeability value obtained from the expression of Spielman and Goren (Equation 6.29). Table 6.2 shows these permeability values for PET and Rayon sheets.

As mentioned in section 6.4, to obtain capillary pressure expressions for the absorption simulations, we fitted the equation of Landeryou et al. 2005 to our height rise test results to obtain $p^* = 451.04$ for our PET sheets, and $p^* = 790.38$ for the Rayon
sheets. Note again that we used the dry diameter of the fibers in this curve fitting exercise (see section 6.4.2).

Table 6.2: Dry and wet microstructural properties of PET and Rayon

<table>
<thead>
<tr>
<th>Parameters / Material</th>
<th>PET</th>
<th>Rayon</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dry fiber diameter (µm)</td>
<td>12.6</td>
<td>13.1</td>
</tr>
<tr>
<td>Wet fiber diameter (µm)</td>
<td>12.6</td>
<td>18.1</td>
</tr>
<tr>
<td>Dry SVF</td>
<td>0.076</td>
<td>0.06</td>
</tr>
<tr>
<td>Wet SVF</td>
<td>0.076</td>
<td>0.078</td>
</tr>
</tbody>
</table>

The results of our fluid absorption simulations are summarized in Figure 6.10. Figures 6.10a-e show the configuration in which the PET is placed on top of the Rayon sheet, whereas Figure 6.10f-j illustrate the alternative configuration. Simulations begin at t=0, where both sheets were fully dry, and the saturation contour plots shown here are taken at t=0.4 s. The fluid is introduced from a pinhole with a diameter of 2 mm, which is assumed to be connected to an infinitely large reservoir. As can be seen in Figure 6.10, fluid spread in the Rayon layer is slightly faster than that in the PET layer. Also, fluid penetration through the thickness of the whole fabric is faster when the Rayon is placed on top. This is because the Rayon sheets have higher diffusion coefficient (attributed to both higher capillary pressure and permeability). Note also that the Rayon layer is thicker than the PET, and therefore constitutes a larger portion of the volume of the composite fabric. It can also be seen that the higher permeability in the x-direction for both layers, caused by
the fibers’ in-plane anisotropy, has resulted in a faster fluid spread in the machine direction.

Table 6.3: Permeability values for the PET and Rayon.

<table>
<thead>
<tr>
<th>Permeability×10^{10} (m^{2})</th>
<th>PET</th>
<th>Rayon</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Isotropic In-plane (S&amp;G 1968)</strong></td>
<td>1.89</td>
<td>3.75</td>
</tr>
<tr>
<td><strong>Machine Direction</strong></td>
<td>2.86</td>
<td>5.68</td>
</tr>
<tr>
<td><strong>Cross Direction</strong></td>
<td>1.39</td>
<td>2.76</td>
</tr>
<tr>
<td><strong>Thickness Direction</strong></td>
<td>1.10</td>
<td>2.17</td>
</tr>
</tbody>
</table>

To compare the overall absorption performance of our composite fibrous material, we calculated the rate of fluid absorption for the configurations shown in Figure 6.10. In Figure 6.11, we show the absorbed liquid volume versus time. It can be seen that the configuration in which the Rayon is placed on top reaches the fabric’s maximum absorption capacity in a shorter time.
Figure 6.10: Contour plots of fluid saturation in our bi-layered medium at t=0.4 s. The left column (a to e) shows the configuration in which PET is placed on top. The right column (f to j) shows the alternative configuration. Figures (a) and (f), (b) and (g), (c) and (h), (d) and (i), and (e) and (j), show the isometric view, top view, bottom view, cross direction side view, and machine direction side view, respectively.
6.7.2 Fluid Release from Wetted Bi-Layered Anisotropic Materials

We also studied the fluid release performance of the composite fabric discussed in the previous subsection. All input values for fluid release simulations are similar to those used in the absorbency simulations except those listed here.

For the capillary pressure of the PET sheets we used our general equation (Equation 6.18) which we previously developed for fluid release in the through-plane direction in non-swelling media (see Section 6.4.3). Using the PET’s SVF and fiber diameter, we found the coefficients $C_1$ and $b_1$ to be 510 and 2.56, respectively, with a contact angle of $\theta = 0.5(77 + 72) = 74.5$ (see Figure 6.6 and its associated discussions in section 6.4). For the capillary pressure of the Rayon sheet, we curve fitted the expression of Haverkamp et al. 1977 (Equation 6.17) to our experimental data obtained with the sheet’s wet dimensions (see Figure 6.4a and the discussions in section 6.4.2). The empirical coefficients $C$ and $b$ were found to be 504.18 and 2.08, respectively.

For the fluid release simulations, we considered a dimensionless mass convection coefficient of $k_f = 5 \times 10^{-5}$ (Ashari and Tafreshi 2009a). We also considered a threshold value of 0.4 for relative permeability during the release simulations (see Equation 6.30 and the related discussions in section 6.5). The results of our fluid release simulations are shown in Figure 6.12, where the medium’s saturation is plotted versus normalized distance in the thickness direction. Figure 6.12a is the configuration in which the PET layer is placed above the Rayon (i.e., the Rayon layer is in contact with the moving surface), whereas Figure 6.12b illustrates the alternative configuration. In Figure 6.12 we also
included snapshots of the saturation contours throughout the medium at t=44 s for illustration purposes. Note that the color bars are different for different contour plots.

From Figure 6.12, one can conclude that the rate of fluid release from the whole medium is lower in the configuration in which Rayon is placed on the bottom. This is due to the permeability threshold that we considered for the Rayon sheets at a saturation level of 0.4.

Figure 6.11: Volume of absorbed liquid versus time for the two configurations shown in Figure 6.10.

To compare the overall release performance of our composite fibrous material, we calculated the rate of fluid release for both the configurations discussed above. In Figure 6.13, we show the medium’s average saturation (averaged across the thickness) versus time. It can be seen that the configuration in which Rayon is placed at the bottom releases the fluid at a lower rate.
Figure 6.12: Results of fluid release simulations with the medium’s saturation plotted versus normalized distance in the thickness direction. a) The Rayon is in contact with the solid surface, b) the PET is in contact with the solid surface. Snapshots of the saturation contours throughout the medium at t=44 s are included for illustration purposes.

Figure 6.13: The medium’s saturation averaged over the thickness during liquid release simulations for the two configurations shown in Figure 6.12.
CHAPTER 7 A Diffusion-Controlled Boundary Treatment for Modeling the Motion-Induced Fluid Release from Partially-Saturated Fibrous Fabrics

Content of this chapter is under review (2010) in an article entitled “A Diffusion-Controlled Boundary Treatment for Modeling the Motion-Induced Fluid Release from Partially-Saturated Fibrous Fabrics”, by Ashari, A., Bucher, T., Tafreshi, H.V.

7.1 Introduction

Modeling the release of wetting fluid from a moving fibrous thin sheet onto solid impermeable surfaces with different hydrophilicity is the subject of this paper. The most popular examples of such systems are sanitary wet wipes used for personal/cosmetic hygiene, baby care, and household applications. Developing an in-depth understanding of the problem of fluid transport in fibrous media is crucially important for engineering new products with optimized performance.

Most of the published studies dealing with fluid transport in fibrous media are only concerned with fluid absorption. To the knowledge of the authors, no published study has been dedicated to better our understanding of fluid release from a fibrous fabric, except for those of our group. We started this research by developing a dual-scale numerical simulation framework for modeling the rate of fluid release from moving fibrous sheets upon contacting with a hydrophilic solid surface (Ashari and Tafreshi 2009a). We later extended our work to model multi-layered composite fabrics made up of fluid absorbing (e.g., Rayon) and non-absorbing (e.g., PET) fibers (Ashari et al. 2011). In the present
work, for the first time, we provide experimental data to be used for empirically modifying our numerical formulation, and improve our model’s predictions. Here, we also report our novel diffusion-controlled boundary treatment, which was developed to incorporate the effects of surface hydrophilicity in our model.

The above-mentioned dual-scale simulations have been based on solving the 1-D Richards’ equation (Richards 1931) of two-phase flows in porous media at the macroscale, coupled with the capillary pressure and relative permeability information obtained via 3-D simulations at the microscale. Our microscale simulations are fully described in our previous publications and will not be repeated here (see Ashari and Tafreshi 2009a, Ashari and Tafreshi 2009b).

For demonstration purposes, we have arbitrarily chosen two different nonwoven fibrous sheets, one consisting of porous Rayon fibers, and the other made of solid (non-swelling) PET fibers. Both sheets have anisotropic in-plane fiber orientations common in hydroentangled nonwoven fabrics (Anantharamaiah et al. 2007). We have also arbitrarily chosen a commercially available water-based diluted soap-lotion as the wetting fluid in our study (see Table 7.1 for physical properties). Using the above mentioned microscale simulations; we previously obtained analytical expressions for predicting capillary pressure and relative permeability of the above sheets (Ashari et al. 2011). In this work, these expressions are used in the 1-D Richards’ equation to be solved numerically for obtaining the rate of fluid release from the sheets when tested on surfaces with different hydrophilicity.
Table 7.1: Physical properties of the water-based lotion used in this study.

<table>
<thead>
<tr>
<th>Property</th>
<th>Water-based lotion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity (Pa.s)</td>
<td>0.00113</td>
</tr>
<tr>
<td>Density (kg/m$^3$)</td>
<td>998</td>
</tr>
<tr>
<td>Surface tension (N/m)</td>
<td>0.0276</td>
</tr>
</tbody>
</table>

In Section 7.2, we briefly describe Richards’ equation along with its constitutive equations for capillary pressure and relative permeability. Section 7.3 presents our new treatment for the boundary in contact with the solid surface. Section 4 describes our experiments, and it is followed by a presentation of our semi-empirical simulations and their related discussions in Section 7.5. Finally, in Section 7.6 we summarize our work and draw conclusions.

### 7.2 Problem Formulation: Richards’ Equation

Considering fluid transport in the thickness direction, the 1-D Richards’ equation derived for two-phase flows in porous media can be written as (Ashari and Tafreshi 2009a, Ashari et al. 2011):

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial z} \left( D_{zz}^{fm} (S) \frac{\partial S}{\partial z} \right) = 0$$

with a nonlinear diffusive coefficient defined as:

$$D_{zz}^{fm} (S) = - \frac{K_{zz} (S)}{\varepsilon \mu} \frac{\partial p}{\partial S}.$$
where, $K(S)$ and $p_c(S)$ are permeability and capillary pressure for a given medium, respectively, and $\mu$ is the fluid viscosity. This equation is written for the liquid phase (e.g., water) in the fibrous media (diffusivity of the fibrous media is denoted by the superscript $f_m$). The ambient air outside the fibrous media is not included in the model, and evaporation is ignored because of the fast dynamics of the system. Equation 7.1 is a nonlinear scalar partial differential equation which can be solved numerically. In this paper, we solve this equation to predict saturation of our PET and Rayon sheets with time.

### 7.2.1 Capillary Pressure Expressions

As mentioned earlier, we have arbitrarily chosen two different fibrous sheets, one made of PET (non-swelling) and the other made of Rayon (swelling) fibers. Fiber swelling affects the properties (e.g., porosity, thickness, in-plane dimensions…) of a fibrous sheet. Some of these properties are very hard to measure accurately, especially if the sheets are soft and thin. We have discussed these issues in our previous paper by Ashari et al. (2011), and only summarize them here in a table (see Table 7.2). As mentioned earlier, we have also arbitrarily chosen a commercially available water-based diluted soap-lotion as the wetting fluid in our study (see Table 7.1 for physical properties).

For the capillary pressure of the PET sheets, we have used a general equation which we previously developed for fluid release in the through-plane direction in non-swelling media (Ashari and Tafreshi 2009b) as follows:

$$p_c(S) = C_1 \frac{\sigma \cos \theta}{\sigma_w \cos \theta_w} \left(S^{-1} - 1\right)^{\frac{1}{h}}$$

(7.3)
where $\sigma_w = 0.073 \text{ N/m}$ and $\theta_w = 80$ degree are the surface tension and contact angle of water with a Polyester surface (Zhu et al. 2005). This expression is valid for a fiber diameter range of 10–25 $\mu$m, a SVF range of 5–12.5%, and different surface tensions and contact angles. For PET sheets with a SVF of 7.6%, and a fiber diameter of 12.6 $\mu$m, we found the coefficients $C_i$ and $b_i$ to be 510 and 2.56, respectively, with a contact angle of $\theta = 74.5$ degrees (Ashari et al. 2011).

Table 7.2: Dry and wet microstructural properties of PET and Rayon.

<table>
<thead>
<tr>
<th>Parameters / Material</th>
<th>PET</th>
<th>Rayon</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dry fiber diameter (µm)</td>
<td>12.6</td>
<td>13.1</td>
</tr>
<tr>
<td>Wet fiber diameter (µm)</td>
<td>12.6</td>
<td>18.1</td>
</tr>
<tr>
<td>Dry SVF</td>
<td>0.076</td>
<td>0.06</td>
</tr>
<tr>
<td>Wet SVF</td>
<td>0.076</td>
<td>0.078</td>
</tr>
</tbody>
</table>

For the capillary pressure of the Rayon sheets, we used the expression of Haverkamp et al. (1977) given as:

$$S = \frac{1}{1 + \left| p_c \right|^b / C}$$  \hspace{1cm} (7.4)

where $p_c$, $b$, and $C$ are empirical coefficients, and are found be 504.18 and 2.08, respectively (Ashari et al. 2011).

7.2.2 Relative Permeability Expressions
Total permeability of a partially-saturated medium can be considered as the product of saturated and relative permeability tensors:

\[ K_{zz}^r(S) = K_{zz}^s K_{zz}^{r'}(S) \]  \hfill (7.5)

where superscripts s and r stand for saturated and relative permeability, respectively. The relative permeability constant \( K_{zz}^{r'}(S) \) depends on the medium’s saturation, while the fully-saturated permeabilities are functions of the microstructural parameters of the medium. Calculation of total permeability requires solving the Stokes equations at different states of saturation \( 0 < S < 1 \).

Previous experimental studies have revealed that relative permeability is proportional to saturation via a power law relationship (Landeryou et al. 2005, Wang and Beckerman 1993). Brooks and Corey (1964) proposed the following equations for relative permeability of the wetting phase:

\[ K_{zz}^{r'} = S^n \]  \hfill (7.6)

The exponent \( n \) has often been reported to be in the neighborhood of 3, but depending on the microstructural parameters of the given medium, it may increase to higher values (Landeryou et al. 2005, Jaganathan et al. 2009, Ashari and Tafreshi 2009a, Ashari and Tafreshi 2009b). In general, the exponent \( n \) for fluid absorption may be different from that for fluid release, as the moisture distribution throughout a fibrous medium can be different during absorption and release, even at identical saturation levels. We consider \( n = 3.18 \) and \( K_{zz}^s = 1.1 \times 10^{-10} \) for the PET sheets.
Calculating relative permeability for swelling media requires special attention. When a fluid infiltrates a swelling medium, some portion of the fluid enters the nano-pores inside the fibers (intra-fiber region), and some enters the space between the fibers (inter-fiber region). The fluid that enters the fiber is believed to become trapped inside the fiber, as the friction against fluid motion is greatly higher in the intra-fiber compared to the inter-fiber space. It has been experimentally observed that there is often a saturation threshold, approximately 0.4, below which permeability of the medium tends to zero. This can be due to a variety of reasons, including the fact that the fluid may break up inside the medium, and lose its continuity. We therefore used a saturation threshold of 0.4 for our fluid release simulations. For a smooth transition from relative permeability proportional to $S^{3.18}$ to almost zero permeability, we considered a piecewise function, given as:

$$K^r_{zz}(S) = \begin{cases} S^{3.18} & S \geq 0.4 \\ S^8 & S < 0.4 \end{cases}$$ (7.7)

In our previous study by Ashari et al. (2011), due to the lack of better estimation, we considered an exponent of 6 for $S$ in the above equation for $S<0.4$. Using experimental data, in the current study we found that an exponent of 8 is a better estimation for $S<0.4$. We use a value of $K^S_{zz} = 2.17 \times 10^{-10}$ obtained in our previous study (Ashari et al. 2011).

### 7.3 Diffusion-Controlled Boundary Condition

The problem of fluid release from a moving partially-saturated nonwoven sheet onto a solid impermeable surface was first studied using a convective boundary condition for the interface between the sheet and solid surface by Ashari and Tafreshi (2009a). In the
convective boundary condition introduced by Ashari and Tafreshi (2009a) the effects of surface hydrophilicity were ignored, for simplicity, leaving the motion to be the only cause of fluid release, with a mass convection coefficient $k_f$ to be found empirically. In the current study, convective outflow of fluid from a moving wet sheet is modeled by a purely diffusive boundary treatment. In this method, we considered the solid surface underneath the sheet to act like a fictitious porous layer with a diffusivity coefficient dependent upon hydrophilicity of the surface as well as the sheet’s speed of motion (see Figure 7.1).

The moisture content of this fictitious layer will periodically be set to zero to resemble motion of the sheet on a dry surface. The resetting period is calculated from the length and speed of the sheet:

$$\Delta t = \frac{L}{V}$$

(7.8)

where $L$ and $V$ are the length and speed of the sheet. The rate of fluid infiltration in our fictitious layer is calculated via Richards’ equation (Equation 7.1) with a diffusive coefficient defined as (diffusivity of the fictitious layer is denoted by the superscript fl):

$$D_{zz}^{fl} = 7.87 \cos \theta_s k_d V$$

(7.9)

where $\theta_s$ is the contact angle between liquid and solid surface, and $k_d$ is a constant to be found from experiment at a given speed (0.127 m/s here). For the interface between of the fibrous sheet and our fictitious layer we consider equal saturation flux in the z-direction:

$$D_{zz}^{fm} \frac{\partial S}{\partial z}_{z=0^+} = \frac{\partial S}{\partial z}_{z=0^-}$$

(7.10)
Figure 7.1: a) Schematic of convective outflow of fluid from a moving wet sheet on an impermeable hydrophilic surface while moving against the surface, b) considering the solid surface underneath as a fictitious porous layer with a diffusivity coefficient dependent upon hydrophilicity of the surface as well as the sheet’s speed of motion.

The fictitious layer should be so large that it always stays partially dry during the above-mentioned $\Delta t$ time interval. For the other boundaries of the solution domain, we considered no-flow boundary conditions ($\frac{\partial S}{\partial n} = 0$, where $n$ is normal to the surface). We coded Richards’ equation (Equation 7.1) with appropriate capillary pressure and relative permeability expressions in the FlexPDE software package to be solved via the finite element method. FlexPDE is a mathematical program developed by PDESolutions Inc., designed for solving partial differential equations. We have previously compared results of FlexPDE software with those of the popular CFD code from Fluent Inc., and obtained superior accuracy for a given number of computational cells (Ashari et al. 2010).
Simulations reported in this paper, are, therefore, performed using the FlexPDE program. Figure 7.2 summarizes the simulation process in the form of a flowchart.

### 7.4 Experiment

As mentioned earlier, an empirical coefficient is required to adjust predictions of our numerical model. We therefore, designed a computer controlled test rig that allows testing a wet sheet of nonwoven fabric on a designated large flat surface. Our test rig is comprised of a sheet holder connected to a mechanical arm that moves the holder on the flat surface. The holder is a rigid panel on which a relatively soft robber pad is mounted. Partially-saturated fibrous sheets are then mounted on the robber pad and tested on the surface (see Figure 7.3). Note that our test setup is designed in such a way that the distance between sheet holder and the solid surface is controlled during the experiment, and therefore, weight of the system has no influence on the test results. We weigh our 0.2m×0.2m sheets before and after the tests using a sensitive scale with 100 microgram resolution to obtain the mass of the fluid released from the sheets. Our system is designed in such a way that the sheets only travel on dry surfaces. This has been achieved by defining a non-intersecting trajectory of path for the sheet holder on the test surface. Our setup allows moving the sheet holder with different speeds and in different directions. The solid surface considered for the tests was a smooth laminated plywood panel (our default test surface).
The sheets are saturated by immersing them in our test fluid for 20 minutes. The extra fluid is then squeezed out of the sheets until a desired weight (corresponding to desired initial saturation) is reached with a margin of error generally less than 5%. To minimize statistical the errors, each test has been repeated five times.
Figure 7.3: Schematic of the designed computer controlled test rig which is comprised of a sheet holder connected to a mechanical arm that moves the holder on the flat surface.

7.5 Semi-Empirical Simulations

In this section, we present our numerical results along with the results of their corresponding experiments for our PET and Rayon sheets. Thickness of our fictitious layer was considered to be almost 1.5 times greater than that of the sheets (large enough to always contain some dry region far from the interface).

Note that the mesh density at the interface between the sheet and the fictitious layer should be relatively high to minimize the numerical error of the calculations. The optimum mesh density was found by simulating a partially-saturated sheet placed on a hydrophobic surface with a contact angle of 90 degrees ($D_z^n = 0$), where no fluid is expected to diffuse into the fictitious layer. The mesh density was continuously increased while we monitored the moisture content of the fictitious layer. Presence of any non-zero saturation at any point in the fictitious layer is an indication of numerical diffusion. We increase the mesh density (especially near the interface) until no considerable non-zero saturation was observed in
the fictitious layer. This mesh density then was used for the rest of simulations reported here.

Experimental results obtained with our PET sheets are shown in Figure 7.4a for five different speeds. As mentioned before, our numerical model needs to be “calibrated” using an empirical coefficient before it can be used for performance (i.e., release rate) prediction. We found, via trial-and-error, that a coefficient of $k_d = 3.5 \times 10^{-11}$ (see Equation 7.9) results in very good agreement between our simulations and experiments with PET sheets at a speed of $0.127 \text{ m/s}$. In Figure 7.4a, we have compared predictions of our calibrated model with experiments conducted at different speeds. Relatively good agreement between our predictions and experiment is evident. We also conducted similar experiment with our Rayon sheets (see Figure 7.4b). Note that microstructural parameters of the Rayon and PET sheets (e.g., fiber diameter, porosity, thickness…) are quite different from one another, and this leads to different capillary pressure and relative permeability values. However, with the same empirical coefficient $k_d = 3.5 \times 10^{-11}$, obtained for PET sheets at a speed of $0.127 \text{ m/s}$, our simulations have produced reasonable predictions for the Rayon sheets at speeds other than $0.127 \text{ m/s}$. This indicates that our semi-empirical model can be used to predict the rate of fluid release from thin fibrous sheets at different speeds. These sheets can have reasonably different microstructural parameters (i.e., porosity, thickness, fiber material, fiber diameter…), such as the sheets often used for producing sanitary wet wipes.
For completeness of study, we have also compared fluid release performance of our PET and Rayon sheets at different speeds. Since these two sheets have different moisture holding capacities, we presented the results in terms of sheets’ normalized weight during the tests. It can be seen that Rayon sheets release their moisture with a lower rate. For example, it takes about 155 seconds, for the Rayon sheets, and about 80 seconds, for the PET sheets, to reach 71% of their initial weights at a moving speed of 0.084 m/s (see Figure 7.5). The slower rate of fluid release from the Rayon sheets is because of the fact that Rayon fibers can trap some part of the sheet’s moisture content within their internal porous structures.

In developing our simulation scheme, we incorporated the surface contact angle in the diffusive coefficient of our fictitious porous layer (see Equation 7.9). For demonstration purposes, we have simulated the release of our water-based soap lotion from the PET sheets when used on surfaces with different contact angles of 10, 35, 65, and 90 degree, at a speed of 0.127 m/s (see Figure 7.6).
Figure 7.4: Comparison of simulation results and experimental results of release performance for different wiping speeds of 0.084, 0.127, 0.212, 0.296 m/s for a) PET sheets and b) Rayon sheets. The constant coefficient of $k_d = 3.5 \times 10^{-11}$ is obtained as the best fit of simulation and experimental result based on wiping velocity of 0.127 m/s.
Figure 7.5: Experimental wiping results based on normalized weight. Comparison is made between PET and Rayon sheets at different velocities.

It can be seen that rate of fluid release decreases with increasing the contact angle. As expected, our simulations show no fluid release from the sheets, when the surface contact angle is 90 degrees. To validate this, we covered our test surface with commercially available wax papers (hydrophobic surface), and repeated our test with pure water using our PET and Rayon sheets at a speed of 0.296 m/s (see Figure 7.7a). We also repeat these experiments on our original laminated surface using pure water for comparison. The contact angle between pure water and our laminated surface and wax paper were measured optically to be about 40 and 90 degrees, respectively. Results of
similar experiment using Rayon sheets are given in Figure 7.7b. It can be seen that fluid release is reduced almost when experiment is conducted on the wax paper. Such a remarkable reduction in the rate of fluid release from sheets tested on wax paper indicates that capillary effects are the dominant mechanisms of fluid release from a wet fibrous sheet. Note in Figure 7.7 that the initial drop in the sheets’ saturation is believed to be due to unavoidable experimental errors.

Figure 7.6: Effect of surface hydrophilicity having different contact angles on the release performance of PET sheet in wiping velocity of 0.127 in/min.
Figure 7.7: Saturation data obtained for Rayon sheet on original surface (no-wax), and wax paper at wiping speed of 0.296 m/s for a) Rayon sheets, and b) PET sheets.
CHAPTER 8 Overall Discussion and Conclusion

As the outcome of our research we developed a mathematical model which can be used to study the performance of porous fibrous media in the absorption and release process. Media can have different microstructural properties, can be composed of solid or porous fibers, can be composed of different layers and can also be anisotropic. Our model is able to predict the rate of release from fibrous samples with the abovementioned properties when moving against a surface having different hydrophilicity. In addition, the technique of dual-scale modeling was employed in our mathematical model (see chapter 3).

Even though the main target of this dissertation was modeling absorption and release in fibrous samples, the introduced modeling technique can be implemented in other similar applications. A broader impact of the work can be seen in modeling the two-phase gas and oil transfer in soil which is a well known application in oil and gas industry. Soil is a famous porous media and predicting an accurate two-phase flow regime in oil wells has always been a high demand in oil and gas industry. There are many existing literary works in which the similar techniques have been implemented in this regard. However, in the majority of the applications in the oil and gas industry, the flow regime can not be considered as laminar due to high pressure and high velocity profile that exists for both gas and oil phases. Therefore in many cases the modified Darcy equation with inclusion of
inertia term is considered. Additionally, there are other cases in which the momentum
equations of gas and oil phases separately are coupled with continuity equation in order to
find the appropriate velocity and pressure profile in the porous media. Nevertheless, the
dual-scale modeling technique used in our work can be merged to existing modeling
techniques in oil and gas problems in order to increase the accuracy of the calculations.
With dual-scale modeling one can obtain more accurate capillary pressure-saturation and
permeability-saturation constitutive equations in soil especially for the anisotropic media.
Moreover, the techniques that we used for modeling the multi-layered fibrous samples can
be used in soil having different properties in different layers. Another application is
modeling two-phase moisture (sweat) and air transport in human tissue (skin). Skin is
another well-known porous medium. Our modeling technique in both absorption and
release can be introduced into modeling the transport of sweat in human skin. However,
existing pores in skin are on a smaller scale than fibrous media and modeling technique
might be involved with higher level of complexity than what exists in fibrous media.
Furthermore, our fully diffusive modeling technique (see chapter 7) in release process can
be implemented in modeling the rate of drug release from drug delivery patches into the
human skin. Due to the analogy that exists between laminar fluid transport in fibrous
media and conduction/convection heat transfer in solid materials, the employed dual-scale
modeling technique in our work can be extended to model the heat transfer inside the solid
materials having anisotropic conductivity. In section 8.1 we discuss the analogy that exists
between studied problem and heat transfer in more detail.
It should be noted that in modeling the release process we neglected the effect of pressure in our model. In fact we modeled the rate of liquid release from the fibrous sample while sample is placed on the surface with zero external pressure and moves with different speed on the surface. We believe that thin fibrous samples (such as wipes) are almost incompressible as they are made of un-crimped fibers. Of course, excessive external pressures can cause deformation in the cross-sectional shape of the fibers, leading to some additional fluid release, however, that is beyond the scope of our work. In addition, it is extremely difficult to experimentally compress a fibrous sheet as thin as 0.35 mm to different thicknesses (say, 0.3, 0.2, and 0.1 mm) and run the fluid release test. Needless to say that, simulating two-phase fluid transport in fibrous media in presence of an external pressure is an additional challenge.

8.1 Analogy with Heat Transfer

Analyzing the governing equation for the fluid transport inside fibrous samples, Richards’ equation (Equation 8.2), along with our convective boundary condition (Equation 8.3) shows that the increase in the release rate is due to either an increase in the Diffusive coefficient, \( D \), or an increase in our mass convection coefficient, \( k_f \), in the boundary condition. As will be shown later in this section, increasing the Solid Volume Fraction (SVF) causes an increase in the sample’s capillary pressure, and the diffusive coefficient, \( D \), (see Equation 8.3). This conclusion can be verified using our previous results obtained in a study conducted for studying the influence of microstructural
parameters on capillary pressure-saturation relationship (Ashari and Tafreshi 2009b).

Increasing the SVF of a sample increases the moisture diffusivity, and reduces the media’s resistant against fluid transport. Therefore, a higher rate of fluid release should be expected if the mass convection coefficient, \( k_f \), is kept constant.

We introduce a new dimensionless number, \( Bi_s \), which is the ratio of resistance against the fluid diffusive transport within the media to that against fluid convective transport outside the media:

\[
Bi_s = \frac{R_d}{R_c} = \frac{k_f t_s}{D}
\]

(8.1)

where \( R_d \) is the resistance against the fluid diffusion inside the media, \( R_c \) is the resistance against the outgoing fluid from the boundary due to the sample motion against the surface, \( k_f \) (Equation 8.6) is the mass convection coefficient at the boundary, \( t_s \) is sample’s thickness, and \( D \) is the moisture diffusivity coefficient inside the sample (Equation 8.3).

In general, higher rates of drainage are concluded from the higher diffusivity coefficients in the Richards’ equation written for fluid transport in the thickness direction:

\[
\frac{\partial S}{\partial t} + \frac{\partial}{\partial z} (-D \frac{\partial S}{\partial z}) = 0
\]

(8.2)

where the Richards’ diffusive coefficient \( D \) defined as:

\[
D = \frac{K(S) \frac{\partial p_c}{\partial S}}{\mu \varepsilon \frac{\partial S}{\partial z}}
\]

(8.3)

where \( \varepsilon \) is the porosity (1-SVF), \( \mu \) is viscosity, and \( p_c \) is capillary pressure (from Equation 8.4) and \( K \) is the total permeability as a function of saturation.
We use our previously-developed constitutive general capillary pressure expression (Ashari and Tafreshi 2009b), \( p_c(S) \), which can be used to model fluid release from a sample without the necessity of conducting computationally-expensive microscale simulations:

\[
p_c(S) = C \frac{\sigma \cos \theta}{\sigma_w \cos \theta_w} (s^{-1} - 1)^{\mu/b} \tag{8.4}
\]

where \( \sigma \) is the surface tension between the wetting (lotion) and non-wetting (air) phase, \( \sigma_w = 0.073 \text{ N/m} \) is the lotion surface tension (considered to be the same as that of water) and \( \theta \) is the contact angle between the wetting phase (lotion) and the fibers. Note that here we have assumed \( \theta_w = 80^\circ \) based on some limited studies in the literature, as no better option was available.

Dependency of relative permeability on saturation is incorporated in our macroscale model via the general expression that we previously developed in the course of this research (Ashari and Tafreshi 2009b). Our general relative permeability expression, \( K(S) \), is given as:

\[
K(S) / r_f^2 = a S^n \tag{8.5}
\]

where \( r_f \) is the fiber radius, \( a = 2.23 \), and \( n = 3.18 \).

Our mass convection boundary condition is given as:

\[
-D \frac{\partial S}{\partial z} \bigg|_{z=0} = k_f (S_{in} - S_{out}) \tag{8.6}
\]
where \( k_f \) is the mass convection coefficient (m/s), \( S_{in} \) is the saturation at the bottom boundary, and \( S_{out} \) is the saturation outside the domain (considered to be zero here).

We found certain analogies between our problem and thermal conduction the solids (see Figure 8.1). In Figure 8.1 a schematic of the transient heat release from a solid wall due to convection (moving air) from the boundary walls are presented. The conduction inside the solid resembles the lotion diffusion inside our fibrous samples, while the heat convection outside the wall is analogous to our mass (lotion) convection from the samples as a result of the wiping action. Unfortunately, the fluid release problem is more complicated than heat conduction. This is because unlike the case of heat conduction, the fluid diffusivity coefficient, \( D \), in porous media is not a constant. This makes the Richards’ equation nonlinear, and therefore more difficult to solve.

![Figure 8.1: Transient temperature distribution for different Biot numbers in a plane wall symmetrically cooled by convection (Incropera et al. 2005).](image)

The equation of transient heat conduction is given as:

\[
\frac{\partial T}{\partial t} + \frac{\partial}{\partial x} \left( -\alpha \frac{\partial T}{\partial x} \right) = 0
\]

(8.7)
where $T$ is temperature and $\alpha = k / \rho c_p$ is the thermal diffusivity ($m^2/s$), which is analogous to the mass diffusion coefficient, $D$ ($m^2/s$), in the Richards’ equation and $k$ is the solid’s thermal conductivity (W/m.K). As mentioned above, thermal diffusive coefficient $\alpha$ is a constant property of the material, while the mass diffusion coefficient $D$ is a nonlinear function of saturation, fluid viscosity, and the media’s relative permeability.

Equation 8.7 can be rewritten as:

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0 \quad (8.8)$$

The heat convection boundary condition has the following form:

$$-\alpha \left. \frac{\partial T}{\partial x} \right|_{x=L} = \frac{h}{\rho c_p} \left[ T(L,t) - T_\infty \right] \quad (8.9)$$

where $h$ is termed the convection heat transfer coefficient ($W/m^2.K$), $\rho$ is the solid material density ($kg/m^3$), $c_p$ is the specific heat of the material (J/kg.K), and $T_\infty$ is the temperature outside the solid. The similarity between Equation 8.9 and Equation 8.6 is evident.

In transient conduction, the dimensionless Biot number, $Bi$ is defined as the ratio of the thermal resistance against conduction to that against external convection:

$$Bi = \frac{R_{cond}}{R_{conv}} = \frac{hL}{k} \quad (8.10)$$

where $R_{cond}$ and $R_{conv}$ are resistance against thermal conduction and thermal convection, respectively, and L is the thickness of the solid. Our abovementioned dimensionless
number, $Bi_s$, (Equation 8.1) is actually inspired from the Biot number used in the heat transfer context.

The linear nature of the above heat conduction problem (Equation 8.8) allows for obtaining an analytical solution for the temperature inside the solid as a function of time and space (Incropera et al. 2005):

$$\theta^* = \sum_{n=1}^{\infty} C_n \exp(-\zeta_n^2 F_0) \cos(\zeta_n x^*)$$

(8.11)

where $F_0 = \frac{\alpha t}{L^2}$, $\theta^* = \frac{T - T_\infty}{T_i - T_\infty}$, $x^* = \frac{x}{L}$ and the coefficient $C_n$ is:

$$C_n = \frac{4 \sin \zeta_n}{2\zeta_n + \sin(2\zeta_n)}$$

(8.12)

and the discrete values of $\zeta_n$ (eigenvalues) are positive roots of the transcendental equation:

$$\zeta_n \tan \zeta_n = Bi$$

(8.13)

However, a similar solution does not exist for the case of fluid transport in porous media (Equation 8.2-8.6) due to the nonlinearity of the Richards’ equation. Therefore, the only viable approach for the case of fluid transport is numerical solution as described in our previous reports.

In Figure 8.1, we can notice that there are three separate regimes of transient thermal conduction in a solid. When $Bi<<1$, the resistance against heat flow (conduction) is much smaller than that in the fluid thermal boundary layer outside the medium (convection). This results in a uniform temperature profile in the solid. On the other hand,
when $Bi=1$, resistance against conduction is about equal to that against convection. In this case, temperature profiles start to form within the solid. Finally, when $Bi>>1$, conduction is very weak compared to convection, which results in strong temperature gradients across the thickness of the solid medium. In the next section, we will conduct a similar study for fluid release from fibrous samples as a function of $Bis$ number.

8.1.1 Fluid Transport in Different $Bis$ Number Regimes

In this section we study the effect of dimensionless number $Bis$ on regime of fluid transport in fibrous media. To start our study, we consider a typical case with

$\varepsilon = 0.94 \, , \, t_r = 1 \, mm \, , \, r_f = 6.5 \, \mu m \, , \, \sigma = 0.073 \, N / m \, , \, \theta = 80 \, ^{\circ} \, , \, \mu = 0.001 \, Pa.s$ is considered and assumed to be saturated with lotion up to an initial saturation of $S_i = 0.6$. For this case, we calculated our mass convection coefficient $k_f$ as presented in Table 8.1. Note that we use the following equation for obtaining the Richards’ diffusive coefficient $D$ by combining Equations 8.3-8.5 to use in calculating $Bis$ from Equation 8.1:

$$D = \left( \frac{ar_f^2}{\mu} \right) \left( \frac{\sigma \cos \theta}{\sigma_w \cos \theta_w} \right) \left( \frac{C}{b \varepsilon} \right) \left( \frac{1}{S_i} - 1 \right)^{(1/b-1)} S_i^{n-2} \quad (8.14)$$

where $a = 2.23 \, , \, n = 3.18 \, , \, C = 410 \, , \, and \, b = 2.47$. Coefficient $C$ and $b$ obtained from our previous study (Ashari and Tafreshi 2009b).

<table>
<thead>
<tr>
<th>$Bis$</th>
<th>$10^{-5}$</th>
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</tr>
</tbody>
</table>
Saturation profiles corresponding to each Bis numbers shown in Table 8.1 are presented in Figures 8.2 and 8.3. Saturation profiles across the thickness for Bis > 0.1 are presented in Figure 8.2. It can be seen that decreasing Bis number results in a more uniform distribution of moisture across the thickness. We found Bis = 0.1 to be a critical Bis number below which one can assume a uniform saturation profile across the sample’s thickness. Figure 8.3 shows the saturation profiles for Bis < 0.1. It can be seen that for any Bis < 0.1 saturation profile remains uniform. It should be noted that the typical range of wiping speeds and sample’s properties result in higher values of Bis > 0.1.
Figure 8.2: Saturation profiles for different Bis numbers of a) Bis=10^5, b) Bis=10^3, c) Bis=1, and d) Bis=0.1.
8.1.2 Effect of Liquid’s Surface Tension on Release Performance in Different Bis Number Regimes

In this section we study the effect of fiber diameter on the release performance of nonwoven samples. We consider sample with $\varepsilon = 0.9$, $t_s = 1 \text{mm}$, $\theta = 75^\circ$, $d_f = 15 \mu m$. 

Figure 8.3: Saturation profiles for different Bis numbers of a) $\text{Bis} = 5 \times 10^{-2}$, b) $\text{Bis} = 10^{-2}$, c) $\text{Bis} = 10^{-3}$ and d) $\text{Bis} = 10^{-5}$.
\[ \mu = 0.00113 \text{Pa.s} \] and \[ S_i = 0.6 \] but liquid has different fiber surface tension of \( 0.25\sigma_w \), \( 0.5\sigma_w \), \( \sigma_w \), \( 2\sigma_w \) and \( 4\sigma_w \) where \( \sigma_w = 0.073 \text{ N/m} \) is the surface tension of water. We consider the typical rage of \( Bis > 0.1 \), we obtain the corresponding mass convection coefficient \( k_f \) by assuming \( Bis = 10 \) for surface tension of \( 0.25\sigma_w \) using Equation 8.1. With a fixed value for \( k_f = 6.93 \times 10^{-2} \) we then extend our calculations by obtaining \( Bis \) numbers for surface tension of \( 0.25\sigma_w \), \( 0.5\sigma_w \), \( \sigma_w \), \( 2\sigma_w \) and \( 4\sigma_w \) (see Table 8.2).

### Table 8.2: Parameters used in studying effects of surface tension on sample’s release performance at different \( Bis > 0.1 \)

<table>
<thead>
<tr>
<th>( \sigma - N/m )</th>
<th>( D - m^2/s )</th>
<th>( Bis )</th>
<th>( k_f - m/s )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 0.25\sigma_w )</td>
<td>( 6.93 \times 10^{-6} )</td>
<td>10</td>
<td>( 6.93 \times 10^{-2} )</td>
</tr>
<tr>
<td>( 0.5\sigma_w )</td>
<td>( 1.385 \times 10^{-5} )</td>
<td>5</td>
<td>( 6.93 \times 10^{-2} )</td>
</tr>
<tr>
<td>( \sigma_w )</td>
<td>( 2.772 \times 10^{-5} )</td>
<td>2.5</td>
<td>( 6.93 \times 10^{-2} )</td>
</tr>
<tr>
<td>( 2\sigma_w )</td>
<td>( 5.544 \times 10^{-5} )</td>
<td>1.25</td>
<td>( 6.93 \times 10^{-2} )</td>
</tr>
<tr>
<td>( 4\sigma_w )</td>
<td>( 1.109 \times 10^{-4} )</td>
<td>0.62</td>
<td>( 6.93 \times 10^{-2} )</td>
</tr>
</tbody>
</table>

We use these values in our numerical simulations to obtain the release performance of each of the samples described in the above Tables. Note that coefficients \( C \) and \( b \) are obtained from our previous study (Ashari and Tafreshi 2009b) as \( C = 540 \) and \( b = 2.5 \). The simulation result is presented in Figure 8.4. It can be seen that when \( Bis > 0.1 \), surface tension is an effective parameter influencing the rate of fluid release in a sample, i.e., increasing surface tension increases the rate of release from a wet sample.
8.2 Overall Conclusion

A two-scale two-phase modeling of motion-induced fluid release from thin fibrous sheets was presented for the first time in this dissertation. The macroscale model is based on the Richards’ equation of two-phase flow in unsaturated porous media. Constitutive relationships necessary for relating the medium’s saturation to the relative permeability and capillary pressure were obtained through microscale modeling and were implemented in our macroscale model. Such two-scale modeling allows for the sheets microscale properties such as fiber diameter and fiber orientation to be included in the macroscale analysis. Microscale properties are important because they can bridge between the conventional macroscale modeling and media’s internal structure – parameters that are
necessary for new product design and development. In addition, a mass convection boundary condition is considered to allow the release of fluid from the bottom boundary of the solution domain, emulating the fluid transfer caused by the relative motion between the fibrous sheet and the target surface. It was shown that the rate of fluid release decreases by decreasing the convection coefficient, $k_f$. We demonstrated that a convection coefficient in the range of $10^{-6} < k_f < 10^{-9}$ is expected to result in a realistic prediction, while the accurate value depends on the properties of the materials involved remains to be determined experimentally for each case.

Forging on, in the next step, we developed general mathematical relationships for capillary pressure and relative permeability in terms of saturation for fibrous sheets. These relationships are needed for studying through-plane fluid transport in fibrous media. Our expressions are based on the empirical correlations of Haverkamp et al. (1977) and Van Genuchten (1980), for capillary pressure, and Brooks and Corey (1964) for relative permeability developed originally for granular porous media. Our generalized expressions are valid for the most practical range of fiber diameters (10–25µm) and SVFs (5–12.5%), and can be directly implemented in the Richards’ macroscale equation. We presented a parameter study for capillary pressure and relative permeability and investigated the effect of fiber diameter, SVF, and thickness of the medium as well as the surface tension and contact angle of the fluid.

Continuing, the model’s ability was extended to simulate moisture absorbency in thin fibrous sheets. Such simulations can be utilized to study the influence of fiber...
diameter, medium’s porosity and thickness, as well as fluid surface tension and contact on the rate of imbibition. It was demonstrated that the wetted region forms an elliptical shape in the case of sheets with anisotropic fiber orientation. More importantly, it was revealed that the rate of liquid imbibition increases by increasing the fiber orientation anisotropy. This is believed to be due to the fact that isotropic media have higher capillary pressures and lower permeability constants. Richards’ equation was numerically solved using both finite volume (Fluent-UDF) and finite element (FlexPDE) methods and good agreement was observed indicating insignificant numerical error in the macroscale simulation results presented here. Moreover, we have compared our results with the analytical expression derived by Marmur (1988), and observed similar trends in the way the wetted area advances in isotropic media. The pore size in our isotropic sheets was found to be about 20µm according to the Marmur’s equation.

Furthermore, a methodology to predict the fluid absorption and release characteristics of multi-layered composite fibrous materials composed of swelling and non-swelling layers with different microstructural properties was developed. Two different fibrous sheets composed of non-swelling (PET) and swelling (Rayon) fibers with different SVFs and thicknesses were arbitrarily chosen in this study in order to demonstrate our semi-analytical modeling approach. Capillary pressure and relative permeability for these fibrous sheets were obtained via a combination of numerical simulations and experiment, and fed into a macroscale model that we developed based on the Richards equation for two phase flows in porous media. Our macroscale model was shown to generate quantitative predictions for fluid saturation as a function of time and space for any composite multi-
layered nonwoven fabrics made up of swelling and non-swelling sheets. For demonstration purposes, we considered a bi-layered composite fabric consisting of the abovementioned two fibrous sheets. We simulated the spread of fluid from a pinhole connected to the top side of the fabric, and observed a higher rate of absorption when the fluid entered the fabric through the swelling layer. A similar study was conducted for the same fabric when partially-saturated with a fluid and brought in contact with a moving hydrophilic surface. It was found that the rate of fluid release is less when the swelling sheet is placed on the bottom where the fabric contacts the surface.

As the concluding action, we reported on a diffusion-controlled boundary treatment which we have developed to simulate fluid release from partially-saturated fabrics onto surfaces with different hydrophilicity. With this new boundary treatment and with an empirical coefficient that we obtained from our experiment, we completed development of a dual-scale semi-empirical model (started originally by Ashari and Tafreshi 2009a) that can be used to predict the rate of fluid release from a moving wet sheet of nonwoven fabric onto a solid surface with a given hydrophilicity. The empirical coefficient used in our model was obtained by testing PET sheets at a speed of 0.127 m/s on an arbitrarily chosen smooth laminated surface and with a water-based soap lotion as the wetting fluid. The resulting model can effectively be used for fibrous sheets with somewhat similar, but not necessarily identical, microstructural parameters (similar to those often used in producing sanitary wet samples), on surfaces with different contact angles, and at different speeds. With every new different wetting fluid (pure water, for instance), a new empirical coefficient has to be found, although the modeling technique remains unchanged.
8.3 Future Plan of Work

Understanding two-phase fluid flow in nonwoven fibrous materials is of great importance in the design and optimization of a variety of products, which are extensively used in our daily life. In this thesis, we focused on developing a mathematical framework to predict the rate of absorbency and release of liquid in fibrous structures. Even though our developed modeling strategy and framework added a very novel and useful tool to the literature, it can be considered as a contributing source to the development of future studies.

Several unsolved problems which are of great interest in nonwoven industry still remain unanswered. In the future, the continuation of the current study which has been discussed throughout this dissertation should involve the study of two-phase flow in fibrous media made up of permeable/swelling (porous) fibers. Our semi-empirical model is dependent on experimental approaches for obtaining the necessary capillary pressure-saturation of the sample. Currently the combination of very small scale pores inside the porous fibers, occasionally in nanoscale, and microscale pores between the fibers make it almost impossible to be modeled numerically. We believe that more works in the future should be focused on finding new computationally affordable techniques to simulate the two-phase fluid transport between and also inside the porous fibers.

Our study also was limited to samples made up of porous fibers having limited amount of swelling such as Rayon (swell around 38% in fiber diameter). However, there are new Super Absorbent Polymers (SAP) which are granular and not a fiber-like, that recently have been used in baby diapers and have the potential of 500% swelling of their
initial diameter. These granular materials have completely different behavior of two-phase fluid flow inside and also in-between them in comparison with Rayon. This will open a completely new direction where our current modeling framework can be extended to.

We developed a general capillary pressure-saturation and permeability-saturation expressions which are valid for the most practical range of fiber diameters (10–25μm) and SVFs (5–12.5%) for the samples made up of slid fibers. However, new studies should be done to find these general equations for multi-component samples made up of different fibers of different materials, and different fiber diameter in blended form. Moreover, our study may also be expanded to bi-component samples made up of blend of porous and non-porous fibers. Obtained general equations afterwards can be used in simulating two-phase flow in macroscale of mentioned fibrous samples.
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- **A. Ashari**, T. M. Bucher, and H.V. Tafreshi, A Diffusion-Controlled Boundary Condition for Modeling the Motion-Induced Fluid Release from Partially-Saturated Fibrous Fabrics, (under review).
- **A. Ashari**, M. Bucher, and H.V. Tafreshi, A Semi-Analytical Model for Simulating Fluid Transport in Multi-Layered Fibrous Sheets Made up of Solid and Porous


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**Conference Proceedings:**