Master Thesis

Modelling Geometries and Simulation of Fluid Flow in Airlaids for Virtual Material Design

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Artwork: Illustration from Simulation Results.
Airlaids are typically used as absorbent materials. The simulation shown here solves the Navier-Stokes equation in a modelled paper-like material made from two kinds of fibres (dark and light grey). The colour across the domain represents a pressure gradient applied, while the lines represent the paths taken by the fluid streamlines. The colours on the lines are a function of the velocity of the liquid at that point.
Modelling Geometries and Simulation of Fluid Flow in Airlaids for Virtual Material Design

Modellierung von Geometrien und Simulation der Fluidströmung in Airlaids für das virtuelle Materialdesign

Master Thesis

Presented by Vedant Prusty
Matric. No.: 374159

The present work was carried out at the:
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and submitted to the:
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Notices & Declarations

The Deutsche Nationalbibliothek (German National Library) has published bibliographic information about this Thesis and lists this work in the Deutsche Nationalbibliografie; the detailed bibliographic data is available on the Internet at http://dnb.d-nb.de.

This master thesis was carried out within the Research & Development function of the Procter & Gamble Company (P&G) and submitted to Institute of General Mechanics (IAM) at the RWTH Aachen University. It has been screened by P&G and does not contain any confidential business-relevant information. It is made available in the public domain and may be used exclusively for academic and research purposes.


The author declares that the present work was carried out independently. Only the sources and resources explicitly mentioned in the work were used. All adopted ideas have been identified literally or analogously.

Der Autor erklärt, dass die vorliegende Arbeit selbständig angefertigt wurde. Es wurden nur die in der Arbeit ausdrücklich benannten Quellen und Hilfsmittel verwendet. Wörtlich oder sinngemäß übernommenes Gedankengut hat er als solches kenntlich gemacht.
Author’s Note

Life lessons are learnt when we are faced with adversity. Since writing this colossal piece of work was no less, the most profound philosophical truths dawned upon the author’s head during the journey. And what better an opportunity to sermonize than the only section of a book which gives absolute discretion to the Author! Of course, the rare super-interested reader’s temper and patience will not be tested, and I shall limit myself to expounding no more than two life lessons.

First, uncertainty can often be the source of the most-unexpected experiences. My journey at P&G always started with me not having an iota of idea about what I would work on. And yet, each of the bold steps (one before starting an internship, and the other before starting this thesis) always led to work on solving problems that I could never have imagined existed. For one, the very application of this thesis in the consumer goods sector is rather astonishing to someone who is not from the area. Never would I have expected to have worked on such a topic, for such an application. And yet taking the step into uncertainty was key. As I learnt recently, in any decision-making process, there comes a point beyond which no new data can add an advantage. It comes down to a gut-feeling… a tide in the affairs of men, which, taken at the flood, leads on to fortune… I dare not say the rest.

Second, in life, like in modelling, there is no point in waiting for the ultimate, perfect, final wonderful, flawless, target. One must work with what one has and keep refining the “model” continuously. Had doctors decided to wait for CT-Scans instead of working with X-Rays, Orthopaedic practice would have been limited to the Clavicle, Radius, Ulna, Femur, Fibula and the Tibia; and I would have been treating people! In writing this Thesis, an earlier start to jotting down ideas instead of waiting for the perfect flow would have gone a long way in preventing my late Zombie nights for over a month. To recognize and accept the limitations, and then march on in pursuit of the goal is the key.

It must now be apparent to the reader what great erudition the author has seen in his own journey. But humour aside, the journey has actually brought me several lessons, for which I am grateful to the ones who shepherded me into making it. Foremost, an acknowledgment of the source of all that I am today - my parents Dr. Gourikumar Prusty and Dr. Mala Chattopadhyay. Next, the evil sibling, Dr. Lydia Prusty, since someone needs to be the recipient of these sermons. I extend my heartfelt gratitude to Mr. Andrea Rossetti for this opportunity and his trust, and Dr. Michael Ban for his serene guidance throughout the time of this project. I am indebted to the support I received from the wonderful people at GMDSO FemCare, Analytical, FEI BabyCare and other departments at P&G - their critical inputs were indispensable for the success of the modeling approach developed. Adrien, Alex, Andrea, Andreas, Cagda, Carola, Elena, Luigi, Martin, Norbert, Paul, Thomas… the list is extensive. I am thankful to all my colleagues at P&G, the fellow interns, and my friends for all the great time we had together, and for their support when I needed it.

MRMK. Vedant Prusty
10th March 2019, Kronberg im Taunus.
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Geometric Modelling and Simulation of Fluid-flow in Airlaids for Virtual Material Design

Vedant Prusty

February 2019
To the Women of the World.
Abstract

This thesis explores modelling and simulation capabilities for the development of new Airlaid materials. The formulation and porous structure of such materials are studied in detail to understand the distribution of fibres in the network. This, along with geometric information about fibres that go into Airlaids, is used to generate artificial domains, on which simulations are setup to predict Permeability and Capillary Pressure. Prediction of these fluid handling properties represents a key insight into the development of new material technologies. The intent is to build fundamental knowledge on the impact of main design and geometric parameters of the feedstock on the fluid dynamic behaviour of the material by numerical analysis, to allow for potential design improvements. This comes as the first step in complete Virtual Material Design.

GeoDict, a design and modelling environment initially developed by Fraunhofer ITWM, was identified and used to model a basic domain of fibres and simulate fluid absorption/flow. The model was then developed iteratively to represent the complex structure of actual Airlaids with pulp and binders. At each iteration, Simulation results were compared with experimental results to assess the possibility of model refinement and reduction, removing parameters that do not have a significant influence on calculations.

The physics and theory behind fluid flow in porous and fibrous mediums are revisited and used as a reference to develop modelling methods. Factors of consideration include selection of relevant Boundary Conditions used for calculations using the Pore Morphology method and for the solution of Stokes equations; The wetting/de-wetting (imbibition and drainage) behaviours and the influence of pore volume distribution on the capillarity/permeability of the structure is analyzed in detail. It is shown that fibre-orientation in the plane of the material impacts the in-plane permeability. Methods are also proposed to model the bonded BiCo fibres inside the Airlaid web structure. The influence of properties like fibre length, width, cross-section, kink, curl, crimp, etc. is elaborated and approaches to model them are discussed. The Aspect Ratio or flatness of Cellulose fibres is found to significantly influence the packing of the Airlaid web structure and in turn the pore volume distribution. The EJ and LIR solvers for the Stokes equation have been validated, alongside sensitivity tests carried out to determine dimensions for a Representative Elementary Volume. The limitations of Capillary Pressure calculations using the pore morphology method have been indicated. The thesis presents approximation methods and simplifications for input data which do not have a one to one mapping with information from fibre specifications.

Results from simulations on the artificially generated domains for a reference Airlaid material compare well both with experimental results as well as simulations run on a CT-Scan of the material. The fluid handling properties are therefore well-predicted, opening up possibilities for modelling and simulation inspired material design, which can be used instead of an empirical one based on trial and error.

Focus Areas / Keywords: Nonwovens, Porous Media, Permeability, Capillarity, Fibre Properties
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Chapter 1

Introduction

Airlaids are textile-like materials categorized as non-woven fabrics, widely used in the areas of Hygiene & Personal Care, Food Packaging, Industrial wipes, and more recently in the Energy industry in solid-state supercapacitors [20]. They are made mostly of fluff-pulp and characterized by their isotropic structural strength and good absorption proprieties. While the chemical, mechanical and thermodynamic properties of other non-wovens have been studied in detail in the textile industry, Airlaids continue to be in a fairly under-explored territory. Compared to other non-woven technologies, these materials have the unique ability to have very short fibres laid down, to form a homogeneous (or also heterogeneous) and continuous web. It is also possible to mix in Super Absorbent Powders or fibres, thereby creating highly absorbent webs. Moreover, the Airlaid web itself can be bonded in several ways. This choice in ingredients allows manufacturers to achieve very specific absorption properties and hence the Airlaid manufacturing industry is now growing rapidly. In fact, a report from Smithers Pira projects global Airlaid manufacturing will grow to over 550,000 tons by 2020 [100]. The global Airlaid Paper market is valued at 1257.79 Million USD in 2018 and is expected to reach 1382.27 Million USD by the end of 2024, growing at a CAGR of 1.59% during 2018-2024 [2].

![Airlaid Sample Image]

**Figure 1** Tomography of a 59 gsm Airlaid RM from Rexcell. A density gradient across the layers is visible.

*Source: P&G*

The sections below give a brief background on Airlaids, how they are made, and what the constituents of its structure are. This provides the reader a better insight into the problem statement that this thesis addresses. A literature survey presents major work done related to this field. A description of the approach taken in this thesis is then presented, followed by a short note on the Airlaid sample used as the subject of study.
1.1 Formulations

Airlaids can be defined based on their formulations. A formulation defines the composition of an Airlaid in terms of its ingredients, or feedstocks in various weight percentages across its layers. Airlaids can be made of 100% fibres, or mixtures of pulp and short cut synthetic fibres (for example, bicomponent or BiCo fibres). As described above, super absorbent powders (SAP) can also be added. The formulation must also mention the target thickness (caliper) and the weight in grams per square metre (gsm). Typically, the bonding method used is also mentioned.

Understanding the geometry of Cellulose and BiCo fibres is relevant to understanding the Airlaid structure. This has been discussed in detail later in this thesis.

Table 1 An example formulation for an Airlaid RM with a single layer.

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Weight (gsm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latex</td>
<td>10</td>
</tr>
<tr>
<td>Pulp Fibres</td>
<td>60</td>
</tr>
<tr>
<td>BiCo Fibres</td>
<td>20</td>
</tr>
<tr>
<td><strong>Total grammage</strong></td>
<td>90</td>
</tr>
<tr>
<td><strong>Target Caliper (mm) under 0.6 kPa</strong></td>
<td>0.1</td>
</tr>
<tr>
<td><strong>tensile strength (N/inch)</strong></td>
<td>20</td>
</tr>
</tbody>
</table>

1.2 Bonding

Bonding refers to the way the fibres in the Airlaid structures are attached to each other. This includes Latex Bonding (LBAL), Thermal Bonding (TBAL), Multi Bonding (MBAL), Hydrogen Bonding (XBAL) and Spunlace or hydroentanglement bonding [25]. LBAL, TBAL and MBAL are relevant to this thesis and are described below:

- In LBAL, a liquid binder is applied to both sides of the web, which is then dried and cured to achieve the dry and wet strength needed. Typical applications include dry and wet wipes, industrial wipes and household products [16].
- In TBAL, bonding fibres, typically bicomponent fibres, are included in the web formation, and the web is heated to activate the melting components of the synthetic fibres to bond the web. TBAL is typically used for absorbent cores, where Super Absorbent Powder can also be present and locked into the web structure by the synthetic fibres.
- MBAL combines both the processes mentioned above using latex as well as thermal properties of BiCo fibres in the bonding process. The inner part of the product is thermal-bonded, and the surfaces have a slight layer of binder to eliminate dust and linting. MBAL is being increasingly used for making absorbent cores, household products, dry and wet wipes. This process can also add Super Absorbent Powders to the Airlaid.

The bonding method used has a direct impact on the structure and mechanical properties of the Airlaid raw-material (RM). This has been considered while studying the fluid dynamics of the RMs.
1.3 Manufacturing of Airlaids

The word “air-laid” is inspired by the associated manufacturing process. A moving line acts as the bed. A vacuum system under this bed pulls down fibres. The feedstocks are added into container-like “forming heads” which deposit the fibres onto the bed below. The airlaid process consists of dispersing the fibres in a stream of air. Fibres are carried and formed to the structure of paper by the airstream. In between two forming heads, the material can also be calendered by rollers, to pre-compress the deposited layers before the next layer of fibres are added. This basic process can have several variations and owing to the large-scale industrial impact of this process, several patents were already floated in the market as early as 1984! [49, 77, 112]

As the fibres are carried onto the bed below, the line keeps moving. Clearly, this influences the orientation of the fibres along the belt. We can think of the process as follows. A fibre falling through the air makes an initial contact at a point with the belt below. As the belt keeps moving forward, this contact point moves along with the belt, and the remaining fibre settles down. It is easy to hypothesize that fibres would tend to be more longitudinally oriented along the moving line (machine direction or MD) as compared to across the belt (cross direction or CD).

Figure 2 The Air-laying principle, showing a single Forming Head. Source: P&G
This intricate structure of Airlaids and the complex manufacturing method with several parameters, make it difficult to predict absorption related properties like capillarity and permeability. Highly empirical, and therefore costly approaches dominate the material design of Airlaids presently. To model airlaids, we must first be able to understand the structure of airlaids, the impact of the manufacturing processes on it, the geometries of the fibres, and the pore distributions. The approach is to use the capabilities within the GeoDict simulation and modelling environment to overcome this challenge.

1.4 GeoDict

GeoDict [1, 114], a design and modelling software was initially developed by Fraunhofer ITWM. It can create virtual 3D material models and also import them from tomography images. From virtual fibre structures, GeoDict is capable of predicting fluid flow properties. It is being widely used in several fields including composites, filtration (gas, liquid and soot), digital rock physics, batteries and fuel cells. Within the context of this thesis, it has been used to study CT scans of Airlaids, create artificial domains (AD) of the Airlaid structure, study pore size distributions, compress domains, as well as carry out simulations to determine permeability and capillarity of structures.

1.5 Literature & State of the Art

The non-woven industry is fast growing with huge profits, and hence has already seen significant scientific work [50, 91]. However, the specific domain of modelling Airlaids remains fairly unexplored. The commercial aspect of this industry has led to more patents being filed than actual freely-accessible research work on Airlaids being published. Over the years research primarily focused on the mechanical, thermal [17, 78, 117, 118] and sound absorption [30, 39, 82, 108] properties of Airlaids.

Fluff pulp remains a critical component in Airlaid structures and in 2011, Lund studied pulp cross-linking and network strength in his thesis [64]. The United States Department of Agriculture showed
that a critical amount of moisture lowers the temperature at which constituent natural polymer-softening initially occurs during the press-drying cycle in airlaids. This enhances web consolidation and results in higher ultimate sheet strengths [14]. Puiu et al. looked at airlaids being used in the electrical industry and proposed a mathematical model for heat transfer through power air-laid cable insulation [87]. In 2017, Çelik determined the air-permeability of Airlaid non-wovens using regression analysis [15]. Interestingly, the air-laying process can be used with metal fibres as well! Applications of metal fibres as related to EMI (electromagnetic interference), ESD (electrostatic discharge) and lightning-strike problems in composite structures, missiles and airframes were examined by Toon in 1990 [106]. Zhu et al. further studied the development of air lying processes using metal fibres [122]. Within the mechanical domain, the tensile strength (wet or dry) has been a popular research area [22, 37, 58, 105].

Closer to the modelling and simulation perspective of this thesis, some of the following works are worth mentioning. Moisture absorption by airlaids (with SAP included) using simulations was studied in detail by Irzmańska and Dutkiewicz in Poland [41]. As early as 1990, David R. Schuchardt and John C. Berg at the University of Washington had studied wicking and liquid transport across cellulose-based materials [94]. In 2003, Pourmohammadi, Leaf, and Lawrence based in the School of Textile Industries in the University of Leeds, studied fibre motion in the complex manufacturing process as described in section 1.3 Manufacturing of Airlaids above [85]. They presented a theoretical model of the fibre trajectories in the transport channel of an Airlaid process [85]. While this was a major step in trying to understand the complex fibre movement, it cannot be correlated directly to the fibre orientation that we see in the finished product. The reason behind this is that the fibres must still be carried by air as they fall on the bed below, and this is affected by several parameters including, the speed of the line, the air velocity around the fibres, and the suction pressure of the vacuum below the bed. A later section in this thesis explains how pore size distribution is the key driver of both capillarity and permeability. Rawal et al. experimentally investigated the effect of fibre orientation on the pore size in non-woven structures including Airlaids [88].

Airlaids can be looked upon as porous media and this work draws from several lessons from porous-media research while making assumptions and establishing ideas. Simulators to determine capillary pressure in porous media have already been proposed [73]. GeoDict was also used to carry out quasi-static imbibition simulations which agreed well with experimental data [12]. It was shown that for modelling relative permeability in imbibition an approach is needed that captures moving liquid-liquid interfaces which requires viscous and capillary forces simultaneously. This is a reason we use only permeability and not relative permeability in this thesis work, by considering fully-saturated flow. The Lattice-Boltzmann method has been used to model pore-scale processes as well as predict capillary hysteresis in porous media [3, 46].

Clearly, the niche focus of this thesis- the structure of an airlaid and an attempt to model it in order to be able to predict its fluid handling properties has not been explored thus far. This underlines the motivation for carrying out this thesis - to generate new knowledge and understanding in the field. While the works mentioned above cannot be picked and placed as reference, they, along with several other pieces of literature have been used in the thesis to base theories and assumptions on. The list above is not exhaustive, and other specific works have been cited in relevant sections later.
1.6 Modelling Approach

It is important to elaborate now on the approach taken by the thesis. Typical of modelling and simulation projects, the work has involved a cyclic process of setting model parameters, running simulations, comparing results, and adjusting the model parameters again to run simulations. However, to keep a clear flow of ideas, the thesis does not discuss the work carried out in the original order or mention all iterations. Instead, the final learnings and recommendations are discussed. The results are ordered by topic and not chronologically as they were achieved. To prevent misunderstanding, the usage of the word *model* is clarified. The word *model* here refers to a set of parameters, algorithms and methods developed to create the artificial domains and simulate their fluid handling properties.

A reference Airlaid material was selected to start with. Experiments were carried out on it to determine its Permeability and Capillary Pressure curves. Also, a set of CT-Scans was taken for samples of this material. The CT-Scan was used as a 3D structure in GeoDict to run simulations for both permeability and capillarity. These results from the experiments and CT-Scan simulations together formed the reference. Meanwhile, data about the material formulations and specifications about its feedstock are used to model an artificial 3D domain of the same Airlaid material. This is also subjected to simulations to make predictions of permeability and capillarity. These predictions are then compared with the references mentioned above. The differences in the results are scrutinized in order to finetune the modelling approach. This process is repeated iteratively until the predictions and results match to a reasonable degree.

1.7 Selection of Raw Material

Virtual Material Design refers to designing nonexistent materials from scratch. However, to begin with, a target Airlaid material was selected to carry out the investigations in this thesis. This material is chosen from Procter & Gamble’s vast Airlaid portfolio and is hereafter referred to as Raw Material 1 (RM1). RM1 is used as an absorbent core and has the primary purpose of sucking in and retaining fluid quickly. This Airlaid was chosen based on the following considerations:

- It was easily available as part of a major product. Physical experiment (used to compare with simulations) results could be obtained readily.
- It has a simple bimodal structure, with only cellulose fibres (pulp) and BiCo fibres. It has a uniform structure across its layers in terms of the weight percentages of the feedstock. The absence of SAP also allows us to neglect the non-uniform expansion that occurs in RMs with SAP, which is difficult to include in static fluid dynamics simulations. The formulation is shown in detail below.
- The simple structure allows a fail-fast & learn-fast method, which could be easily modified continuously with the iterative approach taken.

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Weight (gsm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top Layer</td>
<td></td>
</tr>
<tr>
<td>Latex</td>
<td>4</td>
</tr>
<tr>
<td>Cellulose Fibres</td>
<td>42</td>
</tr>
</tbody>
</table>
The values in the formulation have been modified keeping trade secrets in mind. The total grammage of 100 gsm is actual.

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>BiCo Fibres</td>
<td>4.5</td>
</tr>
<tr>
<td>Cellulose Fibres</td>
<td>42</td>
</tr>
<tr>
<td>BiCo Fibres</td>
<td>4.5</td>
</tr>
<tr>
<td>Latex</td>
<td>3</td>
</tr>
<tr>
<td><strong>Total Grammage</strong></td>
<td><strong>100</strong></td>
</tr>
<tr>
<td><strong>Caliper (target) under 0.5 kPa (mm)</strong></td>
<td><strong>0.8</strong></td>
</tr>
<tr>
<td><strong>Density (g/cm³)</strong></td>
<td><strong>0.15</strong></td>
</tr>
</tbody>
</table>

Note the uniform weightage of various feedstocks across the layers. RM1 also has latex sprayed on it from the bottom and the top.

### 1.8 Tomography References

In order to validate the generated artificial domain (AD) qualitatively in terms of the fibre shapes, packing, orientation, etc. and quantitatively through simulations, P&G’s in-house analytical capabilities were harnessed, and micro-computed tomography images were generated for RM1. These micro-CT scans, in the form of 3D models were made using a cone beam x-ray source with a 2D detector array. The radiation is attenuated by the sample or RM. A scintillator converts transmitted x-ray radiation to light and passes it into an array of detectors. A series of projections is acquired as the sample is rotated on a spindle and the projections are 'smeared' back in the direction of the source. The sum of these projections produces the original object. Similar to CAT scans in hospitals but on a small scale with massively increased resolution, these 3D models were used to image the very fine scale internal structure of the airlaid non-destructively.

**Figure 4** The Uniform layers of RM1 with Latex at the top and bottom

**Figure 5** The generation of a micro-CT by revolving an x-ray source around a material. Source: P&G Analytical

Typically, materials to be scanned are cut in circles and placed on a flat surface. However, we intended to view our material in the “virgin” untouched state. Therefore, The RM was mounted in between two foam rings. This allows the RM in the centre of the ring to be free of any contact and the fibres could be
seen as is. In cases where a confining weight was desired (in order to represent conditions under which experiments are carried out to have comparable data), the foam was no longer a ring, but a flat disk placed on the RM.

*Figure 6 Illustration of RM Mounting for Tomography - The RM (blue disc) is mounted in between two foam rings (grey).*

**Post-Processing of CT images**

Thresholding is carried out on the generated raw CT data to define solid areas and pore spaces. A MATLAB script is used which automatically performs clustering-based image thresholding based on Otsu's method [80, 97]. A max filter is applied while downsampling the voxels. It preserves fibre continuity. For example, in a 4 μm thick fibre which is thin at a specific part, with a width of 2 μm, the max-filter, enlarges the resultant voxel to 4 μm and considers it solid, instead of cutting away the fibre at that point. The disadvantage of the method is as follows: The fibres can be dilated on average. This means thicker fibres, smaller pores, the Pore Volume Distribution curve shifted left, higher Capillary pressure (curve shifted right for CT), and possibly lower permeability. As long as these factors are kept in mind while studying simulation data on CT Scan domains, it does not come as a major limitation. The generated images are then filtered to remove artefacts/disturbances (e.g. noise from the foam rings) and cropped to a desired cuboid shape.

The cropping requires special attention. Often, the images include blank spaces above and below the material (see Figure 7). This comes from the machine scanning an entire zone irrespective of the material being present there or not. The blank space needs to be cropped out. While doing so, it is important to consider that stray and lose fibres at the top and bottom surfaces, jutting outwards from the domain mean that there is not a clear boundary where cropping can be done. It is possible to crop the material at different thicknesses. This is shown below in the Scanning Electron Microscope (SEM) views of the CT-Scanned domains in GeoDict (Figure 7, Figure 8, & Figure 9). Even if cropping is done to just include all jutting fibres, we get an “under-cropped domain” with porous space below and above the material. When Pore Volume Distribution (which can be determined using Granulometry explained later in Section 4.3 Pore Volume Distribution using Granulometry) of these domains are studied, it is noticed that the large spaces express themselves as large pores (Pore Diameter 200 μm and above in Figure 10). Such artificial large pores have a direct impact on Capillary Pressure simulations and therefore need to be avoided. It is recommended to over-crop the domain (“super-cropped domain” in Figure 9) so that the non-homogenous layers close to the top and bottom surfaces are completely removed. If the inner
structure then shows the correct Porosity for the given thickness, the domain can be considered representative of the actual raw material.

Figure 7 Raw “Uncropped” RM1 CT-Scan Domain. Porosity 91.38%. 1.424 mm Domain Height. Stray fibres visible.

Figure 8 “Under-Cropped” RM1 CT-Scan Domain. Porosity 84.13%. 0.680 mm Domain Height. Large pore spaces still present at Z+ and Z−.

Figure 9 “Supper-cropped” RM1 CT-Scan Domain. Porosity 82.01%. 0.520 mm Domain Height.

It should be noted that this over-cropping also artificially reduces the caliper of the domain (see Caliper in Figure 9). More cropping leads to a thinner domain along Z-axis. Permeability, a material property is affected by how compressed the material is. We simulate in-plane permeability, with a no-slip Boundary condition applied on the top and bottom surfaces. Therefore, over-cropping also reduces the distance between the two no-slip surfaces and affects permeability. Imagine a fluid flowing through a pipe with a large diameter as compared to flowing through one with a smaller diameter, both packed with the same kind of material (same porosity). Cropping of CT Scans must be carried out keeping these points in mind. It is recommended to crop away the material just until the excessive artificial pores seen on the right side of the PVD curve (see Figure 10) disappear.
Figure 10 PVD for differently cropped RM1 CT Scan domains.

With a comprehensive background on the Airlaid structure and the CT-Scan references of RM1, we now proceed with discussing the physics and theory of two fluid handling properties of interest - Capillarity and Permeability in the next chapter.

The chapters thereon are organized to enable a smooth flow of ideas. With capillarity and permeability revisited in Chapter 2, Chapter 3 (Experiments) will discuss the Experiments used to create references. Chapter 4 (Simulations) then explains the Simulations’ setup (Algorithms, boundary conditions, limitations, etc.), followed by Chapter 5 (Modelling) which describes the modelling approach to create artificial domains of Airlaids. In Chapter 6, the results from simulations on the artificially generated domain are compared with simulations on CT scans of raw materials and the experimental references. The Thesis thus takes the reader through the journey to develop the final modelling method for Airlaids.
Chapter 2

Fluid Dynamics of Airlaids

The primary aim of acting as an absorbent core needs the right mixture of several parameters in Airlaids. We look at two such major parameters - Capillarity, which defines the sponge-like absorbent behaviour of the material, and Permeability, a measure of the ease with which fluid can flow through the material. In general, the smaller the pores in a porous material, the less permeable it is (more resistance to fluid flow), while it can drive more fluid suction though a higher capillary pressure. However, if the permeability remains low, the fluid cannot be taken up quickly despite the high capillary pressure. One can imagine that the zone of fluid entry of the material saturates quickly driven by high capillary forces, while the rest of the material remains free of fluids due to low permeability. Therefore, understanding what drives these parameters at the structural level and striking the right balance between them becomes important. In the sections below we discuss in detail the characterization of porous media, theories and measurement methods with respect to capillary pressure and permeability. The aim of this part is to give the basics on fluid transport in porous media, which includes some backgrounds concerning technical parameters, properties and measurements directly related to this thesis to facilitate the comprehension of the results and the report.

2.1 Fundamentals of Capillarity

Wetting phenomena may be broadly divided into:

➢ The movement of liquid in the microscopic spaces (pores) that porous materials have.
➢ Liquid absorption into a non-porous solid (e.g. absorption into SAP, natural fibres).

This thesis mainly deals with the first effect. Well-known phenomena that occur due to surface energy or capillarity include the tendency of an isolated mass of liquid to minimize its surface area by forming spherical drops, the rise of liquid in narrow tubes or along sharp edges, and the wicking of fluid through fibrous materials.

Interfacial Tension

When a liquid is in contact with another substance (another liquid immiscible with the first, a gas, or a solid), there is a free interfacial energy present between them. The interfacial energy arises from the difference between the inward attraction of the molecules in the interior of each phase and those at the surface of contact. Since a surface possessing free energy contracts if it can do so, the free interfacial energy manifests itself as interfacial tension.

Interfacial tension $\gamma_{ik}$ is defined as the amount of work that must be performed in order to separate a substance $i$ from substance $k$ per unit area (Units: N/m).
The interfacial tension $\gamma_{ik}$ between a substance $i$ and its own gas/vapor phase is called surface tension.

Interfacial free energy has its source in the universally present forces of intermolecular attraction. Large forces between molecules implies high interfacial free energy and surface tension. These forces are generally considered to be of two different types referred to respectively as dispersion forces and polar forces:

- **Dispersion force of attraction** (Van-der Vaals; Lennard-Jones Force) are present between any neighboring pair of molecules regardless of composition/charge distribution (Forces in the distance $\frac{1}{r^{12}} - \frac{1}{r^{6}}$, where $r$ is the molecule radius)
- **Polar forces of attraction** which result from charge localization within the molecules. These include ion-dipole, dipole-dipole, induced dipole or combinations.

Intermolecular forces act both within each phase and across a phase interface. These intermolecular forces are the (microscopic) reason for capillary fluid motion.

**Contact Angle & Young’s Equation for a three-phase system**

Contact angle is the angle at which a liquid/vapour interface meets a solid surface. The contact angle (CA) is specific for any given system and is determined by the interactions across the three interfaces. Contact angle is governed by the interfacial tensions between the three phases described in Young’s equation.

For a three-phase system, the total interfacial free energy is given as:

$$F_{\text{if}} = \gamma_{LV} \cdot \text{Area}_{LV} + \gamma_{SL} \cdot \text{Area}_{SL} + \gamma_{SV} \cdot \text{Area}_{SV}$$

where L, V and S denote the Liquid, Vapour and Gas phases. In equilibrium interfacial energy is minimized ($\Rightarrow dF_{\text{if}}$ tends to 0). For a planar solid surface with liquid on top of the surface, the upper surface of the liquid will take the form of a sphere (all radii of curvature are the same and constant). The relationship among the $\gamma$ values is defined by Young’s equation [23]:

$$\gamma_{SV} = \gamma_{SL} + \gamma_{LV} \cdot \cos \theta$$
where $\theta$ signifies the contact angle of the system in thermodynamic equilibrium. Young’s equation states that $\cos \theta$ is defined by the ratio of the energy released in forming a unit area of interface between a solid and a liquid to the energy required for forming a unit interface between a fluid and a liquid.

![Figure 12](image)

**Figure 12 Illustration of Young’s equation. Blue liquid droplet on green solid; contact angle. Arrows indicate forces proportional to indicated surface energies.**

It is to be noted that there exists no independent method of measuring $\gamma_{SV}$ or $\gamma_{LS}$ yet. Instead, the surface tension of the liquid and the CAs are frequently used to characterize a solid-liquid-gas system. Moreover, CA is always associated to a given solid-liquid-gas/vapour system.

**Use of Hexadecane**

Solids can be Hydrophobic or Hydrophilic. In hydrophobic solids, the CA of the liquid with the surface is higher than 90°, while in hydrophilic solids, the CA is lower than 90°. A 0° CA represents complete wetting. N-Hexadecane ($n-C_{16}H_{34}$) is considered as a fully wetting liquid. Hexadecane is “a nonpolar liquid of low surface tension which is incapable of forming hydrogen bonds and it exemplifies a liquid whose cohesive and adhesive properties are in some ways ideally simple since only London dispersion forces are usually involved.” [98] Studies have not just shown that hexadecane has a very low contact angle [48], but research has already been conducted using the assumption that Hexadecane has a perfect 0° CA with cellulose [18].

For many liquid-solid combinations, there is a noticeable difference between the CAs observed for advancing (wetting) and receding (drainage) liquid. The receding angle is always smaller and the corresponding work of adhesion larger. Reasons for difference between advancing and receding contact angle include:

- Interface is in contact with a pre-wet surface (e.g. wet versus dry fibres). This provides the liquid a channel to crawl along.
- Planar and Homogenous (Theoretically) solid surface has roughness/structure/surface heterogeneity.

Differences between advancing and receding contact angle can be large! Due to a larger advancing CA and a smaller receding CA, based on Laplace equation (explained in the section below titled Capillary
Pressure & Young-Laplace’s Equation), the absorption pressure due to capillary action will be lower than the desorption one.

![Diagram of Pressure & Young-Laplace’s Equation](image)

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**Figure 13** Illustration of Advancing CA (a) and Receding CA (r) in the context of the Tilting Based method used to measure these values. Source: Ramé-hart Instrument Co.

## Fibre Wetting Phenomena at Microscopic Level

Before we can understand absorption due to capillary action, let us look at some typical ways liquids interact with fibres at the microscopic level. Within the structure, the liquid can form films around single fibres or around the overlap region of two fibres. Capillary condensation [38] and Surface wicking also influence how the liquid travels around and through grooves.

Capillary condensation is the "process by which multilayer adsorption from the vapour phase into a porous medium proceeds to the point at which pore spaces become filled with condensed liquid from the vapour phase" [93].

![Diagram of liquid wetting a single fibre and liquid bridge](image)

**Figure 14** Illustration of liquid (blue) wetting a single fibre (Left) and liquid bridge formed between two fibres (Right).

![Diagram of capillary condensation and surface wicking](image)

**Figure 15** Illustration: Left - Capillary Condensation. Water vapour will condensate when water vapour partial pressure is equal or higher than vapour. Right - Surface wicking. The liquid spreads along grooves or rugosities present on the surface.
2.2 Fundamentals of Permeability

Porosity

Pores are void spaces which are distributed extensively throughout the volume of a porous medium. Porosity \( n \) is the ratio of the void space in a porous medium over the total bulk volume of the medium. Porosity is thus a dimensionless quantity between 0 and 1. The fraction of the bulk volume that makes up the solid walls (Solid Volume Percentage or SVP when multiplied by 100) is thus \( 1 - n \). Porosity can be calculated when the caliper \( d \), the basis weight \( BW_i \) and the material density \( \rho_i \) of the material components are known.

\[
n = 1 - \frac{BW_i}{\rho_i \times d}
\]

Saturation is then defined as the volume of fluid in the material divided by the total void volume.

Capillary Pressure & Young-Laplace’s Equation

When two immiscible fluids are in contact, a discontinuity in pressure exists across the separating interface. This difference of pressure from the non-wetting \( P_{\text{non-wet}} \) and the wetting side \( P_{\text{wet}} \), is called capillary pressure \( P_c \).

Capillary pressure is proportional to surface tension and contact angle and inversely proportional to the radius of the pore. This relationship between capillary pressure \( P_c \), the effective radius of the pore \( R \), the resulting surface tension \( \gamma \) and the contact angle \( \theta \) is known as Young-Laplace’s equation.

\[
P_c = \frac{2\gamma \cos \theta}{R}
\]

Capillary pressure is saturation dependent: capillary pressure decreases while saturation increases. Capillary pressure is a fundamental property of any absorbent that does govern how liquid would move inside its absorbent structure.

2.2 Fundamentals of Permeability

Permeability describes the ease with which a liquid is able to flow through a layer. Darcy’s law is a phenomenologically derived constitutive equation that describes the flow of a fluid through a porous medium. The law was formulated by Henry Darcy based on the results of experiments on the flow of water through beds of sand [27]. Although the law was determined experimentally by Darcy, it has since been derived from the Navier-Stokes equations via homogenization [40, 75].

The law describes the liquid flow through a fully saturated porous material driven by a pressure gradient. It says that the flow \( Q \) of a liquid, through a cross-sectional area \( A \) in a porous medium, is directly proportional to the pressure gradient \( \Delta P/L \) applied across it. The proportionality is driven by the permeability of the porous medium \( k \) and the viscosity of the fluid \( \mu \).
Fluid Dynamics of Airlaids

Darcy’s Law

\[ Q = \frac{K \cdot A \cdot \Delta P}{\mu \cdot \Delta L} \]

\( Q = \text{flow (m}^3/\text{s}), \ \Delta P = \text{pressure difference (Pa)}, \ K = \text{permeability (m}^2), \ A = \text{cross section (m}^2), \ L = \text{length (m)}, \ \mu = \text{viscosity (Pa s)}; \)

The pressure gradient includes any driving force, i.e. capillary pressure, gravity, external pressure. Darcy’s law introduces the permeability \( k \) in order to characterize fully the porous medium as a flow resistor (measuring the ease of liquid flow through the material). The permeability is an intrinsic property of the porous medium only and independent of the fluid properties. It considers all the microscopic/structural characteristics of the porous media, such as porosity, pore volume distribution, tortuosity and specific surface area. The unit of the permeability \( k \) is m².

Limitations of Darcy’s Law

Darcy’s law is only valid for a Reynolds number \( (Re) \) much less than 1. The Reynolds number (a dimensionless parameter) for a porous media assesses the importance of the inertial forces versus the viscous forces and is typically expressed as:

\[ Re = \frac{\rho v d}{\mu} \]

where \( \rho \) is the density of the liquid (mass per volume), \( v \) is the specific discharge or the Darcy velocity (not the pore velocity; and is expressed in units of length per time), \( d \) is a representative dimension of the porous medium (for instance, the grain diameter for particles) and \( \mu \) is the dynamic viscosity of the fluid. Liquid flow in Airlaids is assumed to be laminar, smooth and without turbulence. This assumption is made based on the fact that in real applications, fluids are not ‘pumped’ as such into the material. Instead, the material is left in contact with fluids and allowed to absorb it.

A Note on Permeability in Fibrous Media

In Airlaids, as the liquid advances through its porous medium, the small pores with greater capillary pressure will tend to fill first. They will also drain last when liquid is being withdrawn. Since at any location only pores up to a certain size are filled, the local flow is somewhat restricted to those filled pores. It follows that the local permeability would be dependent upon local saturation. Therefore, the
2.2 Fundamentals of Permeability

Permeability of a material depends on the saturation of the material. The concept of relative permeability addresses this and is seen as an extension of Darcy’s Law. However, within the time-scope for this thesis, only flow in fully-saturated media was considered, i.e. the saturation dependency was removed by making sure material was 100% saturated before measurements or simulations are made. This is explained in detail later in the next chapters. Moreover, Berg et al. had already shown that for modelling relative permeability in imbibition, an approach is needed that captures moving liquid-liquid interfaces which requires viscous and capillary forces considered simultaneously [12]!

Darcy’s Law for Radial Systems

Here, we give a theoretical background which enables the reader to understand that Experimental setup described later to measure permeability. In the In-Plane Radial Permeability test setup (see section Test Method – Determination of IPRP), the liquid is supplied at a centre point of a circular system. For this case, Darcy’s law can be applied in polar coordinates [8].

![Diagram illustrating the IPRP test method of flow in a radial system. The disc indicates the test-sample. Source: P&G](image)

In the permeability measurement setup, the flux \( q \) is the flow \( Q \) per the cross-sectional area \( A \) (dimension: length divided by time \( L/T \)) and is equal to the hydraulic head gradient (dimension: length/length — where pressure is expressed as height of water). In a system with radius \( r \), and hydraulic head \( h \), this can be expressed (in polar coordinates) as:

\[
q = \frac{Q}{A} = -K \frac{dh}{dr}
\]

At a constant flow \( Q \) through the porous medium, the flux \( q \) will not be constant, as the cross-sectional area \( A \) varies by radius \( r \):

\[
A = 2\pi rc
\]

with \( c \) being the thickness (or caliper) of the sample.

In order to solve the above equations, we substitute the value of \( A \) in the equation for \( q \) and separate the variables \( r \) and \( h \):

\[
\frac{dr}{r} = -K \frac{2\pi c}{Q} \frac{dh}{dh}
\]
and integrate this from the inner boundary (inner radius $r_i$, inner hydraulic head $h_i$) to any radius $r$ and hydraulic head $h$:

$$\int_{r_i}^{r} \frac{dr}{r} = K \frac{2\pi c}{Q} \int_{h_i}^{h} dh$$

$$\Rightarrow \ln \left(\frac{r}{r_i}\right) = -K \frac{2\pi c}{Q} (h - h_i)$$

$$\Rightarrow Q = -K \frac{2\pi c}{\ln(r/r_i)} (h - h_i)$$

If the hydraulic head at a specific radius, for example, at the outer radius of a sample $(r_o, h_o)$ is given, and the flow $Q$ is measured, the hydraulic conductivity $K$ can be determined as follows:

$$K = \frac{Q \ln(r_o/r_i)}{2\pi c (h_i - h_o)}$$

This forms the theoretical background of the test method described in the section Test Method – Determination of IPRP.
Chapter 3
Experiments

3.1 Measuring Capillarity

In a porous media, pores have generally irregular shape and their size has a distribution. Such microscopic structure tends to be rather complicated. This Pore Volume Distribution (PVD) can be measured and provides insights into the structure as explained below.

![Figure 18 Illustration of different kinds of pores in Porous Structures. Source: P&G](image)

In order to adequately determine the impact of pore sizes on material absorption properties, we need to know the distribution of pore ranges, which in some fibrous networks can be quite broad. Essentially pores are sized according to their effective radii and the contribution each has to the total free volume within the sample. This data then is used to study the capillary absorption and desorption (hysteresis) characteristics, i.e. capillary pressure, of the porous material. A porous material is most likely comprised of effective and isolated pores of varying shapes and sizes. Effective pores (shown as a through pore in Figure 18) are those that are interconnected and eventually reach the surface of the structure. These are the pores that contribute to the absorbent capacity of a given porous material. Isolated pores are those entirely surrounded by solid and therefore unable to contribute to absorbent properties directly.

Liquid porosimetry is a procedure for determining the pore size distribution within a porous solid matrix. Each pore is sized according to its effective radius, and the contribution of each size to the total free volume is the principal objective of the analysis. The data can reveal useful information about the structure of a porous network and can also be used to predict the absorption and retention characteristics of a material [72].

For liquid to enter or drain from a pore, an external pressure must be applied that is just enough to overcome the term \( P_c \cdot \cos \theta \) from Laplace’s equation. This is negative when liquid must be forced in; \( \cos \theta \) is positive when liquid must be forced out. If the external pressure on a matrix, having a range of pore sizes, is changed, either continuously or in steps, filling or emptying will start with the largest pore and proceed in turn down to the smallest size that corresponds to the maximum applied pressure difference.
Experiments

Test Method – Determination of Capillary Pressure

The target is to study the imbibition (wetting) and drainage (de-wetting) related saturation with regards to pressure change in Airlaids. Modelling methods and simulation results needed to be validated against real experiments on RM1. While there are several methods to approach porosimetry, we have based our test method on an apparatus developed at the Textile Research Institute in 1993 by Miller and Tyomkin [72]. While the complete setup is described in the cited paper, the paragraph below gives a short description of the same.

The sample to be studied is placed in a measurement cell on top of a thin porous membrane glued to a porous metal support plate (frit). The membrane and frit together are impermeable to air molecules. The cell is connected to the test solution which is in a reservoir, via a tube. The solution reservoir is placed on a balance. The measurement cell is exposed to controlled air pressure which is varied. Changes in air pressure in the measurement cell result in absorption/desorption of fluid by the sample, as detected by the balance. The weight of solution absorbed/desorbed by the sample as a function of applied air pressure is monitored and gives information about the pore size distribution of the sample and absorption capacity of the sample at various pressures. In addition, the thickness of the sample is monitored as a function of air pressure in the cell.

The experiment for this project was carried out by the Analytical division within Procter and Gamble R&D. A pre-selected air pressure was applied to the sample in the measurement cell and the incremental and cumulative quantity of liquid that is absorbed/desorbed by the sample at each pressure, as detected by the balance was determined. The pressure corresponds to the capillary pressure exerted by a capillary of a particular radius: As pressure is decreased, larger pores are filled. At the lowest pressure, all the pores are filled. Pressure steps were decided by the computer based on target pore diameters to be measured.

![Diagram of apparatus](image)

Figure 19 The Apparatus used for PVD experiments, following TRI principle as described in [72].

![Diagram of TRI device](image)

Figure 20 The TRI Device for compressing materials to specified thickness. Source: Miller & Tyomkin, 1994

It should be noted that in our test method, a confining pressure of 0.25 psi (1.724 kPa) is placed on the sample. This pre-compression can already significantly change (compress) the caliper from what was measured under a different confining weight after manufacturing the material. The wet caliper is recorded during the experiment and must be kept in mind while studying results.
n-Hexadecane was used to reduce contact angle hysteresis. This decision has to do with the fact that there is no way of determining specific contact angles of various fibre types with other fluids, and hence the same cannot be replicated in a simulation environment without advancing and receding CA data. From a single lot\(^1\) of RM1, three samples (55 x 55 mm squares) were cut out to carry out three replicates of the experiment. For each sample, the basis weight, caliper, and the liquid uptakes at corresponding pressures were recorded. Surface Tension value 27.2 mN/m, and density 0.77 g/cm\(^3\) was used for n-hexadecane in calculations. The pressure was varied in between 0 to 2000 mm H\(_2\)O (0 to 19613.30 Pa) according to a target Pore Radius. The following target radii (in \(\mu\)m) were used to calculate pressure from the Laplace equation: 5, 10, 15, 20, 25, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140, 150, 160, 170, 180, 190, 200, 225, 250, 275, 300, 400, 600, 800, 1000, 1200, 1000, 800, 600, 400, 300, 275, 250, 225, 200, 190, 180, 170, 160, 150, 140, 130, 120, 110, 100, 90, 80, 70, 60, 50, 40, 30, 25, 20, 15, 10, 5, 10, 15, 20, 25, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140, 150, 160, 170, 180, 190, 200, 225, 250, 275, 300, 400, 600, 800, 1000, 1200.

Saturation in the experiment is defined as liquid uptake by the material at measurement point divided by the maximum liquid uptake recorded.

**Experimental Results - Porosimetry**

![Figure 21 Raw PVD Experiment Results for RM1 using Hexadecane.](image)

In Figure 21, we see the result of the Porosimetry carried out on RM1 (averaged values over three replicates). Initially, we begin with a higher pressure, and start reducing this. As the surrounding pressure falls, the pores in the material which generate the corresponding capillary pressure (and are connected to the wetting phase) absorb the liquid. Measuring the liquid uptake allows us to calculate saturation and plot the imbibition curve (shown in red). After reaching a minimum pressure (45.0125235 Pa), when no further liquid uptake is measured for a given amount of time (Equilibrium Rate of 10 mg/min of liquid absorbed or desorbed), the pressure is increased again. At corresponding capillary pressures, relevant pores will no longer be able to hold fluid and push this out. With this, we get the

---

\(^1\) “Lot” refers to a single sheet or few sheets of material manufactured together as a batch on the line. Using a single lot removes the variations coming from the different manufacturing conditions and parameters that are not considered (example humidity, line speed, etc.).
The drainage curve never returns to 0 saturation. This is attributed to the “residual” liquid that remains trapped in the material as liquid films along the fibre, as liquid absorbed into the cellulose structure through osmosis, and liquid in the pores not drained due to lack of connection to wetting phase.

The hysteresis observed between the imbibition and drainage curves can be attributed to Contact-Angle Hysteresis (as explained in section Contact Angle & Young’s Equation for a three-phase system) as well as the Ink-Bottle effect (explained in the next paragraph). While we have used Hexadecane as the wetting fluid, we cannot completely discount the effect of a slightly higher CA for imbibition as compared to drainage. While this angular difference may be only a few degrees, it will tend to shift the curve slightly left.

The Ink-Bottle effect [26] arises out of the non-uniformity of individual pore geometries: many pores are larger than their openings ($R_t > r_t$) or connections to the wetting phase (see pore throat in Figure 22). The illustrated pore can be filled by liquid during the acquisition process (wetting) only when pores with a radius lower than $R_t$ are already filled (because these smaller pores have higher suction as per Laplace equation). On the contrary, the illustrated pore will remain full of liquid during the dewatering process (drying) until pores with a radius higher than $r_t$ are completely drained (because these pores have a lower draining resistance).

At first glance, one can notice the strange behaviour of the curves at very low pressures. Imbibition (read from right to left, high pressure to low) reaches saturation at about 85% and then sees a sudden rise in liquid uptake. This is unusual and indicates very large pores forming a significant part of the volume of material. Pore radius and capillary pressure are inversely proportional as per Laplace’s equation. These pores must be of the scale of 1100 micrometres. While such large pores may exist, it is unlikely that they form a significant part of the volume of the material (almost 15% of total liquid uptake). This is referred to as the “nose problem”.

Interestingly, this same behaviour is noticed in the capillarity simulations on under cropped CT-San domains of RM1. Below we compare the experimental results with simulation results on an Under-cropped CT domain “CT 2” Under-cropped” (similar to but different from the one mentioned in section 1.8 Tomography References). The same “nose-problem” is seen between about 0 and 500 Pa.
3.1 Measuring Capillarity

Figure 23 Comparison of raw experimental results with Simulations on an under-cropped CT Scan Domain.

“Nose problem” is identified.

On taking a closer look at the Domain SEM view (Figure 24), we notice the large pores at the top and bottom of the material, which come as a result of under-cropping, which is done to consider the jutting-out fibres as part of the domain. Hence it is concluded that the nose-problem in the experimental results arises out of artificial large pores. This might occur when the sample is not sufficiently pushed against the supporting frit, and not sufficiently compressed by the confining weight during the experiment. This would lead to large pores being at the contact of the frit and material, as well as the weight and the material, inside the apparatus. It also explains why the experimental imbibition curve starts at a much lower pressure. This is associated with the large pores at the frit-material interface.

Figure 24 SEM View of Under-Cropped CT Domain of RM1. Porosity 83.19%. 0.620 mm Caliper. Large pores are visible at the top and lower ends along the Z axis.

The “nose” is hence considered an experimental artefact. It is removed by cropping out experimental data for pressures below 196 Pa (corresponds to 86.7% saturation in Figure 23), the pressure at which the sudden jump in saturation starts. The liquid uptake at this Pressure is considered the new maximum liquid uptake with 100% saturation. The remaining saturations are re-calculated, and the following graph is achieved as the reference results to be used from experiments.
The caliper of the sample is also tracked as the experiment progresses. This is shown below. Figure 26 shows how the caliper changes significantly as the material absorbs fluid and then releases it based on the surrounding pressure applied. As imbibition starts (red curve moving from higher pressure on right to lower pressure on left), the caliper starts falling slowly. This might be attributed to fluid filling up air gaps in between the fibres of the material. At a certain pressure, the material caliper has a sharp fall (approximately 1350 Pa), which can be interpreted as wet-collapse. This occurs as the cell walls of the cellulose fibres collapse. The elliptical cross-section with a lumen turns into a flat structure [33]. As we continue to move to lower pressures, there is again a rise in the caliper, which can be attributed to the osmosis process, where the fluid is absorbed into the structure of the fibres themselves. As drainage begins, the fluid in the material continues to fall as the liquid in the pores leaves the material. At one point, air is able to enter the porous structure and allows the material to swell again.

The caliper of the material has a direct impact on its pore volume distribution. Therefore, it is necessary to consider the right caliper to be used for modelling artificial domains and running simulations to get results which can be compared with experimental results. This is not straight forward. As seen in the graph, imbibition and drainage show a significant different in caliper as the experiment progresses.
Simple averages taken individually for imbibition and drainage (shown as cross marks), or further combined into a single average (shown as a green triangle) is not a suitable approach since it takes into account several points which are not representative of the material while it is exhibiting capillary action. The approach taken is to consider an average of caliper across a pressure range which sees the maximum change in saturation (the desired fluid handling property of capillarity is studied is seen in this range). This approach is shown below in Figure 27. For imbibition, caliper is averaged between 0.52 and 83.1% saturation, while for drainage, it is averaged between 12.8 and 81.6% saturation. The points were selected with a target to consider the minimum number of measurement points for the largest saturation change. These two calipers are used to model two different domains as explained alter in section 0.5.1 Domain Size & Resolution.

Figure 27 Caliper change for the largest saturation change in RM1 during PVD

3.2 Measuring Permeability

Permeability is usually measured by constructing a “plug” made of the porous medium of interest. A pressure difference is applied to cause a steady flow through the porous medium. From flow rate measurements, the permeability can be calculated by using Darcy’s law. This approach was modified to meet the needs of understanding permeability along the plane of the Air laid sheet. Given the fact that Latex applied on RM1 might hinder fluid flow through the plane of the sample sheet, the permeability was explored only along the plane of the sheet instead of through it. This is referred to as In-plane Permeability (IPP). Several test methods have been used in the past to determine IPP in the context of porous thin-films [90], paper [4], resin-transfer modeling in composites [52, 63, 65], and wood composites [121]. Here, a method is used where the fluid flows from a central point of a circular sample sheet outwards radially. The permeability value obtained is referred to as In-Plane Radial Permeability (IPRP). The specific test method is patented and well described [110]. In the section below we outline a brief description which should be enough to get a frame of reference while considering the results discussed later. Meanwhile, the methods used by Lundström et al. may also be used to get an idea of other similar experimental methods to get the same results [66].
Experiments

Test Method – Determination of IPRP

The purpose of this method is to determine the IPRP of non-swelling (fully saturated) porous materials under pressure, using a liquid solution. The flow rate through a test piece is determined by gravimetric determination of the quantity of solution flowing through the porous material under constant hydrostatic pressure, as a function of time. Darcy’s law and steady-state flow principles are used for determining the flow conductivity.

A circular patch of material is cut and compressed between two plastic disks of the same diameter. The setup has a hole in between (see Figure 17). Using a known hydrostatic pressure head, the fluid with known density and viscosity, is allowed to flow through the disk-shaped material, from the inner hole toward the outer boundary in the radial direction. The fluid passing through is collected and the flow rate is measured continuously. The following equation (based on Darcy’s Law for Radial Systems described earlier) is applied to get the permeability at time step $i$:

$$k_{r,i} = \frac{(Q_i / \rho) \times \mu \times \ln(r_o / r_{in})}{2\pi \times L_{pi} \times \Delta p_i}$$

where $Q_i$ is the mass flow rate at time $i$, measured from the collected fluid passing through the material, $\rho$ is the density of 0.9% saline (value used here 1.01 g/cm$^3$), $\mu$ is the liquid dynamic viscosity at 20 °C, $r_o$ is the sample’s outer radius, $r_{in}$ is the sample’s inner radius, and $L_{pi}$ is the averaged sample thickness for time $i$, measured over the present and previous time steps. $\Delta p_i$ denotes the pressure drop applied across sample calculated using the value of the hydrostatic head.

The $k_{r,i}$ values are averaged over all data points (which varied with time), and then divided by the viscosity $\mu$ to get K, the IPRP.

The experiment is repeated on 6 replicates cut out from a single lot of RM1. The caliper of the material is tracked before and during the experiment. Also, the material is pre-compressed under a confining weight of 0.25 psi (1.724 kPa) inside the apparatus.

![Figure 28 Sample cut of a material (similar to RM1) cut out for the IPRP test. Source: P&G Analytical](image)

Experimental Results – IPRP

We see below the results of the IPRP experiment carried out on RM1. RSD stands for relative standard deviation. The difference between the lower and upper limits (Rep4 and Rep6) is 19.67% (with respect to the lower limit – Rep6), which is quite large.
3.2 Measuring Permeability

Table 3 Results of IPP test on RM1. IPRP values are given in undisclosed units.

<table>
<thead>
<tr>
<th>Rep Nr.</th>
<th>IPRP [Expt units]</th>
<th>Dry Caliper [mm]</th>
<th>Avg Flow Rate [g/s]</th>
<th>Wet Caliper [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>674</td>
<td>0.677</td>
<td>0.163</td>
<td>0.678</td>
</tr>
<tr>
<td>2</td>
<td>709</td>
<td>0.738</td>
<td>0.185</td>
<td>0.735</td>
</tr>
<tr>
<td>3</td>
<td>702</td>
<td>0.701</td>
<td>0.175</td>
<td>0.699</td>
</tr>
<tr>
<td>4</td>
<td>791</td>
<td>0.683</td>
<td>0.191</td>
<td>0.678</td>
</tr>
<tr>
<td>5</td>
<td>717</td>
<td>0.703</td>
<td>0.179</td>
<td>0.703</td>
</tr>
<tr>
<td>6</td>
<td>661</td>
<td>0.647</td>
<td>0.154</td>
<td>0.653</td>
</tr>
<tr>
<td>AVG</td>
<td>709</td>
<td>0.692</td>
<td>0.174</td>
<td>0.691</td>
</tr>
<tr>
<td>RSD%</td>
<td>6.40%</td>
<td>4.40%</td>
<td>8.00%</td>
<td>4.10%</td>
</tr>
</tbody>
</table>

The first intuitive approach might be to consider the average value of IPRP as the value to be used to validate the simulations. However, given a constant grammage, a changing caliper changes the density in such materials. This impacts the PVD and therefore also permeability. Below we take a closer look at the caliper tracking during the experiment.

![RM1 - Caliper Chnage in IPRP Experiments](image)

Figure 29 Caliper Variation with Time for IPRP experiment on RM1

Figure 29 shows that the caliper tends to remain constant once the material is fully wet. The differences seen between the replicates can be attributed to different dry calipers as well as the fact that there are variations in how the material might have been compressed. The initial rise in caliper seen at the beginning of the experiment (between 0 and 2 seconds) represents swelling of the material. A large part of RM1 consists of cellulose fibres (hydrophilic in nature) as seen in the formulation mentioned in section 1.7 Selection of Raw Material. Cellulose is known to absorb large amounts of fluid via osmosis and swell [51, 74, 76]. Overall, the constant caliper is in line with the idea of recording measurements under fully-saturated conditions to avoid caliper changes during imbibition.
But the large variation in wet caliper even between replicates still leaves the question about deciding on a value to compare with simulations open. One would think that lower caliper caliper always leads to smaller pores in the structure and therefore lower permeability, i.e. permeability should vary linearly with caliper. We plot below permeability against the caliper.

![RM1 - Correlation between Caliper and IPRP](image)

*Figure 30 IPRP and Caliper measurements for different test replicates*

We notice that the Permeability value does not vary linearly with caliper. This can arise out of experimental limitations in the way the sample is placed in the apparatus, as well as minor inhomogeneities in the different replicates compared with each other. The Linear regression line fit on these points (indicated by the blue dotted line) has an R-squared value of only 0.0386. The variation in the IPRP value is far too much to use the simple average (indicated by blue diamond). We also recognize that 6 measurement points do not form a good basis for a regression. However, acknowledging these limitations, the approach taken is to identify the point closest to the linear regression and use the corresponding values of caliper and IPP. Replicate 2 with an IPRP value of 709 (only coincidentally equal to the overall average IPRP) is chosen. Its wet caliper is 0.735, its permeability in SI units is $7.09 \times 10^{-11}$ m$^2$. This value is later used as an experimental reference.

**Test Method – Permeability in 1 Dimension**

To explore the idea about Airlaids having possibly different permeabilities in the Machine and Cross-Directions due to the different orientation of fibres in as they are laid down, it is necessary to devise and experiment which can measure IPP in a single dimension or direction (instead of radial as in IPRP). Here, this method which is also proprietary to P&G, is referred to as 1D IPP.

The objective is to measure the flow rate in a specific direction (MD or CD) of the sample. The apparatus and approach are similar to the one used for IPP explained above with some minor changes. Instead of a radial system, a linear one is used. A strip of material is cut out from the sample and compressed in between two plates. The liquid is allowed to enter from one end and exit from the other. The compressing plates prevent liquid from flowing through the plane. The compression is “ideally” enough to prevent parallel liquid flow along the plane of the material in contact with the plates. The liquid exiting the system is collected and weighed. Based on the length of the strip, the pressure applied, dimensions of the system and the volume of liquid collected, the flow rate is calculated.
3.2 Measuring Permeability

![Illustration of the 1D IPP Test Apparatus. Z-Axis represents the material caliper. Flow is allowed only along X.](image)

12 measurements were made using samples cut from a single lot of RM1. 6 were in the Machine Direction, and 6 in the Cross Direction. Each sample strip was 40 mm long and 10 mm wide.

**Experimental Results – 1D IPP**

<table>
<thead>
<tr>
<th>Replicate Nr.</th>
<th>Dry Caliper [mm]</th>
<th>Average Flow Rate [g/s]</th>
<th>Wet Caliper [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Machine Direction</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.458</td>
<td>0.019</td>
<td>0.458</td>
</tr>
<tr>
<td>2</td>
<td>0.42</td>
<td>0.017</td>
<td>0.416</td>
</tr>
<tr>
<td>3</td>
<td>0.421</td>
<td>0.02</td>
<td>0.42</td>
</tr>
<tr>
<td>4</td>
<td>0.431</td>
<td>0.019</td>
<td>0.43</td>
</tr>
<tr>
<td>5</td>
<td>0.417</td>
<td>0.019</td>
<td>0.417</td>
</tr>
<tr>
<td>6</td>
<td>0.394</td>
<td>0.017</td>
<td>0.395</td>
</tr>
<tr>
<td>Average</td>
<td>0.424</td>
<td>0.018</td>
<td>0.423</td>
</tr>
<tr>
<td>RSD%</td>
<td></td>
<td></td>
<td>7.10%</td>
</tr>
<tr>
<td>Cross Direction</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.425</td>
<td>0.021</td>
<td>0.425</td>
</tr>
<tr>
<td>2</td>
<td>0.423</td>
<td>0.019</td>
<td>0.423</td>
</tr>
<tr>
<td>3</td>
<td>0.421</td>
<td>0.018</td>
<td>0.422</td>
</tr>
<tr>
<td>4</td>
<td>0.422</td>
<td>0.019</td>
<td>0.422</td>
</tr>
<tr>
<td>5</td>
<td>0.402</td>
<td>0.016</td>
<td>0.403</td>
</tr>
<tr>
<td>6</td>
<td>0.399</td>
<td>0.019</td>
<td>0.399</td>
</tr>
<tr>
<td>Average</td>
<td>0.415</td>
<td>0.019</td>
<td>0.416</td>
</tr>
<tr>
<td>RSD%</td>
<td></td>
<td></td>
<td>8.00%</td>
</tr>
</tbody>
</table>

The experiment indicates that there is no measurable difference between the two flow directions in RM1. The flow rates and the Relative Standard Deviation (RSD) of the readings are similar for both directions. Based on the accuracy/uncertainties of the experimental setup, the CD average Flow rate of 0.019 g/s should not be read as higher compared to 0.018 g/s in the MD. As a conclusion, within the limitations of the experiment, permeability is seen as isotropic in the X-Y plane.
Chapter 4
Simulations

All calculations and simulations discussed in this thesis were performed on a 64-bit Linux system with 56 cores and about 500 GB of memory. Permeability solvers could harness the parallelization of 20 cores simultaneously. The individual conditions for the different studies were separate. Simulation run-times varied largely between a few minutes to days, depending on resolution/size of the domain as well as boundary conditions and tolerances entered.

4.1 Capillary Pressure

This section describes the simulation setup used to determine capillary pressure for RM1. Within the SatuDict module in GeoDict, simulations were carried out on CT-Scans of RM1, as well as the generated artificial domains (ADs). SatuDict uses the Pore Morphology method (PMM) to determine the distribution of the two phases inside the porous media. The method, introduced by Hilpert [35], and later pursued by Lehmann[3, 54, 109], calculates the stationary distribution of wetting and non-wetting phases for a given capillary pressure [61], and is repeated for a variety of capillary pressures in order to get the capillary pressure curve and saturation. First, each pore voxel is assigned a pore radius. Next, the radius is used to simulate drainage and imbibition. The resulting pore radius – saturation relationship is transformed into a capillary pressure – saturation relationship using the Young-Laplace equation. Phase distribution for both types of phase displacement (Drainage and Imbibition) are calculated. A Drainage displacement occurs where a non-wetting invading fluid enters the porous media and displaces a wetting fluid, which was saturating it. The opposite case, Imbibition, occurs when a wetting fluid invades the space around the material and the material surface, which had been occupied by a non-wetting fluid, displacing it.

Limitations

It is important to highlight the assumptions and limitations of the calculations made in SatuDict. GeoDict considers the porous structure as a non-deformable solid. Therefore, swelling or compression effect cannot be modelled. The structure is described via a binary solid/void voxel grid. GeoDict distinguishes 3 different phases: liquid, gas and solid. Thus, a voxel, shaped like a cube, can be only attributed to one of these phases and shares an edge, vertex or complete face with another voxel-phase. For the calculation of capillary pressure, SatuDict assumes spherical liquid/gas interface. PMM is a quasi-static model which can only describe thermodynamic processes at an assumed equilibrium state. It involves trying to fit spheres into the porous space to determine the radii of the pores, and thereby the capillary pressure associated with these radii. Since the structures are described using cubes, the sphere fitting approach leaves rooms for significant over or underprediction of capillary pressure values. This consideration of perfectly spherical interfaces instead of the actual curvature or meniscus shape of pores
Simulations

is an important shortcoming. Another assumption was that the material is homogeneous, i.e. there exists a well-defined contact angle between material surface and phase boundary (homogeneous wettability properties for the solid through the entire structure) and only a constant contact angle was implemented. While multiple contact angles can be entered as an input (also used in past research coupled with PMM [96]), it was not possible to determine the advancing and receding contact angles for the used fluid with different kinds of cellulose and BiCo fibres in RM1. Therefore, a constant CA of 0 degrees is assumed. The interaction between solid and fluid is also limited to a constant surface tension (of the liquids interface, constant in space and time). The algorithm considers gravity and viscous forces are negligible compared to capillary forces. Importantly, the pore morphology method does not describe film formation arising out of adsorptive forces or evaporation/condensation or wettability effects. Moreover, the liquid could indefinitely wick between two parallel fibres, as described in the section Fibre Wetting Phenomena at Microscopic Level.

The boundary conditions depend on the chosen direction of the flow which will position the wetting (WP) and non-wetting phase reservoirs (NWP) on the structure. In principle, the side boundaries are considered impermeable. However, one could use periodic boundary conditions. For our project, the wetting phase is represented by water and the non-wetting phase will be air.

Set-up and Boundary Conditions

The boundary conditions (BCs) depend on the chosen direction of the flow which will position the wetting (WP) and non-wetting phase reservoirs (NWP) on the structure. Air is considered as the non-Wetting phase (NWP) and Hexadecane as the Wetting Phase (WP) liquid. A constant 0° wetting phase CA is used. Surface Tension value used for Hexadecane is 0.0272 N/m. During imbibition, the WP is set as the invading fluid while the NWP is the replaced fluid. During drainage, the opposite setting is used. The Imbibition process (referred to as Imbibition II in the SatuDict environment) is calculated considering the displacing WP continuously connected to a WP reservoir at a given spatial location. In the Drainage process (referred to as Drainage I in the SatuDict environment) the invading NWP phase is connected to a reservoir and displaces the WP starting at one given spatial location. In our case, the WP reservoir is always located at the Z- (under) face of the material, while the NWP reservoir is located at the Z+ (top) face. This reflects what is used in the experimental setup, with the material kept on a membrane through which liquid (WP) is absorbed from under it, while air (NWP) pressure is applied on top of the material. Along the side boundaries of the domain (X+, X-, Y+, Y-), the domain is not in contact with any reservoir. Here, the algorithm determines pore sizes and checks connectivity using symmetric boundary conditions, i.e. by mirroring the entire domain and pore structure at these sides. All closed pores i.e. pores that are not connected to the domain boundary (without a direct path for the WP or NWP to get in contact), are ignored and considered as solid regions during the simulation.
4.2 Permeability

As early as 1986, Jackson and James at the University of Toronto not only studied, but also worked on predicting the permeability of fibrous porous media [42]. In 1997, Clague and Phillips modelled the permeability of disordered bimodal media in 3-D space [24]. Their work was limited to one specific set of parameters (fibre diameters, and species mass fractions) and did not discuss all influencing parameters, which we try to do later in Chapter 5 Modelling. Within GeoDict, the FlowDict module is used to predict the permeability of both ADs and CT-scanned domains of RM1. Three-dimensional Computational Fluid Dynamic (CFD) simulations are performed on a representative domain. FlowDict has been successfully used in the past to make predictions of permeability in other sectors, especially using CT Scans [5, 47].

Governing Equations Used for Simulating Fluid Flow

The Navier-Stokes equations describe the motion of Newtonian fluids. More specifically, the Navier Stokes equations describe the momentum conservation. Together with the mass conservation,
Simulations

energy conservation and state equation we get a system of non-linear partial differential equations of second order. They form the fundamental base of CFD [62].

\[-\mu \Delta \vec{u} + (\rho \vec{u} \cdot \nabla)\vec{u} + \nabla p = \vec{f}\]  
Navier-Stokes Conservation of Momentum

\[\nabla \vec{u} = 0\]  
Conservation of Mass

Here, \(\vec{u}\) is the fluid velocity, \(\rho\) is the fluid density, \(p\) is the pressure, \(\mu\) is the fluid viscosity, and \(\vec{f}\) is the force density. The simulations compute \(\vec{u}\) and \(p\) for a given pressure drop \(\Delta p\) by converting it into a force density and using specified boundary conditions on the computational domain [5].

The Stokes equations are a simplification of the general Navier–Stokes equations. They are used when the fluid velocity is very slow, i.e., the Reynolds number is low (\(Re \ll 1\)), as in the case of fluid flow through Airlaids when they are used as absorbents. The influence of temperature is neglected, and a constant density is assumed. Therefore, only the pressure and the velocity of the fluid are considered. Moreover, the system is restricted to the steady state case where no unsteady acceleration is present. The convective acceleration is also omitted. Dropping this inertia term (shown in blue above) from the Navier Stokes equation, the Stokes equation is expressed as:

\[-\mu \Delta \vec{u} + \nabla p = \vec{f}\]  
Stokes Conservation of Momentum

\[\vec{u} = 0\]  
No-slip BC applied to the surface of solids

To determine the permeability, the flow of the fluid through the medium is simulated, i.e. Stokes’ equation shown above is solved in the pore space. The resulting velocity field \(\vec{u}\) allows to determine the average velocity \(\vec{u}\), which, together with Darcy’s law can be used to determine the permeability \(k\) [10].

\[\vec{u} = \frac{-K}{\mu} \nabla p\]  
Darcy’s Law

Where \(K\) is a tensor. The effective permeability of a representative periodic volume element in the three-dimensional case is described by the tensor \(K \in \mathbb{R}^{3 \times 3}\). The tensor \(K\) can be determined by applying three axis aligned pressure drops and evaluation of the corresponding mean velocity [62]. In our case, we apply the pressure drop only across specific desired axes as explained below.

**Limitations**

As explained above, Darcy’s law only applies to very slow (so-called creeping or Stokes) flows, with \(Re\) close to zero. The Stokes equations, which are simplified from Navier-Stokes equations by dropping the inertial term, are used to describe the flow. In this regime, changing pressure drop or velocity by a factor, linearly changes the other by the same factor, so that Darcy’s law always predicts the same value for the permeability. Later, the \(Re\) calculated in the simulations are discussed with the results.

The second caveat lies in the definition of length across which pressure is applied in Darcy’s law. This length is meant not to include the inlet and outlet (inflow and outflow regions) that some virtual flow experiments require. Under the assumptions of slow flow and the voids of inlet and outlet, choosing the Stokes flow option in FlowDict and using the computed permeability is valid [60].
Solvers Used – Explicit Jump & LIR

GeoDict provides several flow solvers. The Explicit Jump Stokes (EJ-Stokes or EJ) flow solver, which is based on the immersed interface method [55, 56], is chosen as the primary solver for this project. The jump conditions are solved by adding auxiliary forces on obstacles. The jump corrected standard difference formulae are solved with Fast Fourier Transform [113, 115]. This solver has been shown to perform well for fibrous structures with Solid Volume Percentage (SVP) less than 20 [21], and this is the case with RM1.

GeoDict also provides the Left Identity Right (LIR) solver [62], which uses a non-uniform adaptive grid resulting in very low memory requirements. It coarsens the computational grid inside large pores while keeping a high resolution near the pore surfaces. This makes it much faster and memory-efficient than the EJ Solver for highly porous materials [59] as in the case of RM1. The solver has also been used in porous media applications including for fibrous domains [5] [53]. The LIR solver can be used to solve the Stokes, Stokes-Brinkman, Navier-Stokes, and Navier-Stokes-Brinkman equations [60].

The limitation of the LIR solver though is that it does not provide the option to have different boundary conditions along the two directions tangential to fluid flow. As explained in the section below, our setup requires that there is a no-slip applied on the top and bottom surfaces ($Z^+$ and $Z^-$) and the domain is left periodic along the plane (X or Y). However, in the LIR solver, either both directions are set to periodic or both are set to no-slip. Therefore, the LIR solver cannot be used to produce results which can be compared with experiments.

However, given the long run-times of the EJ solver, the LIR solvers speed is harnessed in studies where two artificially built domains need to be compared with each other only. In such simulations, the no-slip BC is applied along both tangential directions. The obtained difference in permeability is comparable to the difference that is seen using the EJ solver. In Appendix A, the LIR and EJ solvers have been compared for a different set of BCs. For the same BC, both solvers give same results.

Set-up & Boundary Conditions

Solvers need information about the structure beyond the domain boundaries in terms of what happens at the inflow/outflow boundary, what happens at the pore-solid boundary, and what happens at the tangential boundary. The BCs were selected in order to best represent the IPRP experimental conditions, with flow along a single direction along the plane (X or Y), and the material being sealed from the top ($Z^+$) and bottom ($Z^-$).

The porous space of the domain being simulated is considered filled with water with density 998.234 kg/m$^3$ and dynamic viscosity 0.001 kg/(ms). This reflects a fully-saturated condition of the material. Flow was computed along the X and Y directions, or along the plane of the material in MD and CD. Along the direction of the flow, periodic boundary condition is used. This can be considered as the domain being repeated along the direction of flow (see Figure 33 EJ-Stokes Simulation BCs along material plane. Periodicity along X and Y directions, and the added inflow/outflow regions are illustrated. Figure 33). Moreover, along the direction of flow, implicit in-flow and out-flow regions are created for the fluid. This is done by adding a 10-voxel thick porous space (filled with fluid in the fully-saturated condition) at the inflow and outflow faces. It prevents any non-uniformity in the domain geometry from artificially closing flow channels or creating bottlenecks to fluid flow[60]. This is especially important for CT scanned domains, which are periodic only in theory, but not in their actual domains. All ADs that were created...
Simulations

were generated with periodicity in X and Y. Besides, the CT scanned domains represent a small part of a large sheet of raw material, and hence the periodicity boundary condition is satisfied. Along the top and bottom faces of the domain (Z+ and Z-), no-slip BC is considered. This is a replication of the IPRP experimental setup, which presents flow along the top and bottom faces. The no-slip condition is applied to Z+ and Z- by adding a 1 voxel thick solid layer on these domain surfaces. No-slip is also considered at the pore-solid boundaries. This represents the interface of a liquid and solid phase. Since fibres are considered Solids (explained later in section 5.3 Fibres in Airlaids), the no-slip BC was also applied at the surface of each fibre.

![Periodic Domain BC Along X and Y](image1)

*Figure 33 EJ-Stokes Simulation BCs along material plane. Periodicity along X and Y directions, and the added inflow/outflow regions are illustrated.*

![BCs in EJ-Stokes Simulations](image2)

*Figure 34 BCs in EJ-Stokes Simulations. Figure on left is the domain used. Figure on right shows the pressure field applied across it and velocity streamlines. Blue parts on Z+ and Z- are solid layers for no-slip BC.*

A pressure drop of 980.665 Pa is applied across the flow direction. This is the input to the Stokes equation to be solved for the domain. Internally, the FlowDict solves several equations for values of pressure and velocity at each voxel iteratively. It starts with an initial guess for the unknown values (velocity in this case) and improves the current values in each iterative step. The iterative process is repeated until the stopping criteria is fulfilled. A tolerance value of 0.001 on permeability is used as stopping criteria for the simulation. The solver looks for stagnation in the iterative process. This occurs when from iteration to iteration the improvement in the permeability value becomes 0.001 or less. The solver checks for changes in the permeability after every 100 iterations. If the relative change is smaller than the value entered for Tolerance, the iteration is stopped. The solver stops if the relative difference with respect to the prediction is smaller than the specified error bound. In case of the LIR solver, an Error Bound is used as the stopping criterion. Here, the results of the previous iterations are used to predict the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference with respect to the prediction is smaller than the specified error bound. The error bound value used is 0.01 along the flow direction.
Parallelization options (using MPI for EJ) available within FlowDict have been leveraged using upto 20 processors at a time, depending on the time/memory constraints of simulations required. The structure is analyzed, and the maximum pore diameter is found. For the EJ solver, a grid of voxels with side length 1 μm is used. Some settings specific to the LIR solver are mentioned in Appendix A.

Reynolds number \( (Re) \) is also calculated during the simulations and is an extra output (but not used during the simulations). It serves as a check on the assumption that flow through Airlaids is very slow (and that Stokes’s equation can be applied). Characteristic length of \( Re \) (the variable \( d \) as mentioned in the formula in section Limitations of Darcy’s Law) is calculated as the maximum pore diameter in the domain, or the diameter of the largest through pore. This is since Airlaid domains are extremely porous (about 75% porosity) and the areas to observe turbulences (if any) in the fluid flow would be the largest pores. For simulations run on the CT scanned domains and the ADs, the obtained \( Re \) ranged between 0 and 6. For the results with \( Re > 1 \), the higher value may be attributed to a higher characteristic length considered. The maximum pore diameter might have been much larger than the actual area where the turbulence occurs.

### The Permeability Tensor

Darcy’s coefficient of permeability is a symmetric tensor of second rank [57]. FlowDict provides such a tensor as an output of simulations. The permeability Tensor \( K \) obtained only has components associated with the X and Y components, since flow is not calculated along the Z direction. The challenge is to find a way to compare the obtained 3D permeability values with the Radial Permeability value obtained from experiments. The radial permeability can be considered as a combination of the permeabilities along X and Y, but not necessarily an arithmetic average.

**Table 5 Permeability tensor [sq. m] obtained from Simulation for RM1 AD.**

<table>
<thead>
<tr>
<th>( k_{xx} )</th>
<th>( k_{yy} )</th>
<th>( k_{zz} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.07358e-11</td>
<td>-7.88372e-13</td>
<td>unknown</td>
</tr>
<tr>
<td>-7.27582e-13</td>
<td>5.1519e-11</td>
<td>unknown</td>
</tr>
<tr>
<td>-3.32358e-13</td>
<td>-1.74655e-14</td>
<td>unknown</td>
</tr>
</tbody>
</table>

The diagonal values of the tensor, \( k_{xx} \) and \( k_{yy} \) correspond to the permeabilities in X and Y directions respectively. To map these values to a single in-plane permeability value which can be used to compare with experiments, we consider using a formula for the effective permeability from the context of textile fabrics [43, 120]:

\[
K_{eff} = \sqrt{k_{xx} \cdot k_{yy}}
\]

We see from the simulation results that the values for \( k_{xx} \) and \( k_{yy} \) are not very different from each other. This leads to the value for \( K_{eff} \) being almost an average of \( k_{xx} \) and \( k_{yy} \). For CT-scanned domains, this represents no big difference in between the MD and CD for RM1, which is line with the experimental results discussed in section Experimental Results - 1D IPP. Of course, for ADs, the domain generation process itself has the X and Y directions set to be periodic. This is discussed again in section 5.1 Domain Size & Resolution.
In our setup, the relation between the fluid velocity and the pressure gradient is referred to the principal axes only and therefore the tensor must reduce to a diagonal matrix [57]. The non-diagonal elements of the tensor shown above are of $100^\circ$ order magnitude lesser than the diagonal elements and can be considered as zeroes.

### 4.3 Pore Volume Distribution using Granulometry

Since both Permeability and Capillarity are strongly driven by the PVD, it is important to leverage PVD data from CT-Scanned domains while making the ADs. The PoroDict module within GeoDict provides a granulometry algorithm which can be run on domains to get their PVDs. A morphological fitting of spheres of increasing radius is employed in order to determine the pore size distribution of the ADs [101]. The definition of what is a pore becomes important here. A voxel is part of a pore with a diameter equal or larger than $D$, if it is included in a sphere of diameter $D$, which is completely included in the pore space. The superposition of all spheres with diameter $D$ that can be included in the pore space is equal to the pore volume of all pores of diameter $D$ or larger [83]. In the granulometry calculations, the pores found can be isolated inside the structure, and have no connectivity or accessibility to the top or the bottom of the domain. In other words, there is no connectivity check with the wetting or non-wetting phases, and closed pores are also part of the results. This is different from the PVD that is obtained using SatuDict simulations, which gives only a cumulative PVD of all pores that are saturated at a given pressure (connectivity check performed).

The granulometry simulations are used to compare the CT-domains and the ADs. A bin size of 8 $\mu$m is used. This is because the pores are classified by their diameter into bins. All bins are of equal size and each contains pores with a diameter in the range comprised between $((i-1) \times \text{Bin size})$ and $i \times \text{Bin size}$, where $i$ is the bin number. This bin size is an input and a value of 8 $\mu$m is used. This is based on the resolution of the CT scanned domains, which is 4 microns/voxel and 2 voxels is used as the minimum bin size. Both ADs and CT-Scanned Domains are set as being periodic along the plane. This applies periodicity in the X and Y directions with the effect that the structure’s objects and pores ending on one side of the structure reappear on the opposite side [83]. For the Z direction ($Z+$ and $Z-$ surfaces), the pore sizes are computed with symmetric boundary conditions, a good approximation.
Chapter 5
Modelling

The geometrical properties of airlaids (seen as non-woven fibrous media) are modelled using FiberGeo, a module within GeoDict. ADs are created starting from statistical properties of the Airlaids’s feedstocks, such as the known fibre parameters and the fibre orientation distribution. The digital model is a detailed 3D microstructure of the material that reveals the microstructure and allows comparison with the micro-CT scan of the same material. This comparison gives qualitative clues as to the similarity of the generated AD and the actual RM. The algorithm starts with an empty box (domain) into which fibres are then placed randomly until the desired porosity or grammage (stopping criterion) is reached. Random placement means that the actual fibres added are the result of a random process: the centre may be distributed uniformly in space, the direction distribution may follow a prescribed anisotropy [92], the fibre radius may be Gaussian distributed [10]. Once the voxel mesh or AD is created, the properties of the medium can be calculated numerically. Simulations for Capillarity and Permeability are run on this AD and compared with reference results from experiments as well as results from simulations on the micro-CT domain. The input parameters for the AD generation are continuously refined based on the comparisons between predictions and reference results. This is continued iteratively until the predictions reach a reasonable degree of accuracy, at which point it is considered that the AD is a close enough representation of the actual RM. It should be noted that the mechanical properties of the fibres such as tensile strength, Young’s modulus, etc. are not included within the scope of this thesis.

The chapter below discuss the individual modelling parameters that are used as inputs. The process of determining their quantitative values is explained in detail. Moreover, their effect on the overall fluid handling property is also discussed.

5.1 Domain Size & Resolution

The AD is defined with a specific domain size set as number of voxels in each of the axes. The resolution is defined as the length of each voxel. The domain must function as a Representative Elementary Volume (REV). The idea is that this minimum volume must be able to capture at the macro-scale all the fluid handling properties of the material. The size of the REV is such that parameters that represent the distribution of void and solid within it are statistically meaningful and comparable to the original RM represented by a larger domain size [6]. Having a smaller REV is in the interest of faster domain generation and lower simulation run-times. The approach used for airlaids is to have the domain larger than a minimum sized REV. Test simulations helped verify that the REV selected captures the material properties. (see Appendix B - Sensitivity Test for Domain Resolution)

The voxel size is such that each fibre diameter consists of between 8 to 12 voxels. The length of the AD along the X and Y axes (plain of the RM) is such that Each side it at least two times the thickness of the RM. Also, the domain is set as periodic along X and Y direction, i.e., it repeats itself exactly along these directions. This was done keeping in mind the BCs used for permeability can capillarity simulations
Modelling discussed earlier. The size of the domain in the Z direction corresponds to the thickness of the sheet of RM. RM thickness is always associated with a weight which is placed on it in order to measure it. The ADs used to compare predictions with experimental results cannot all share the same thickness. Material caliper has a significant impact on its PVD and hence its fluid handling properties, as explained in Chapter 3 Experiments. Therefore, different domains are generated for comparing with specific reference results as follows:

- AD for comparison with experimental imbibition results uses average caliper recorded over the largest saturation change during imbibition experiment.
- AD for comparison with experimental drainage results uses average caliper recorded over the largest saturation change during drainage experiment.
- AD for comparison with experimental permeability results uses the recorded wet caliper of the test replicate which comes closest to the regression line fit on a graph of IPRP values vs caliper (as explained in section Experimental Results – IPRP).
- AD for comparisons with all simulations on CT-scanned domain of RM uses the caliper of the cropped-CT domain. The limitation here as the CT-Scan caliper is a result of cropping and not real compression of the material. Therefore, the porosity is higher in the CT-Scan compared to the generated AD for the same Z-Axis length.

Generating different domains with different calipers (Z-Axis lengths) is one way. The other approach is to create a single domain at a large caliper and then compress this domain to different calipers using the ProcessGeo module within GeoDict. The operation compacts the structure in Z-direction by the value entered as a “compression fraction” $CF$, defined as:

\[
CF = 1 - \frac{\text{New target caliper of Domain}}{\text{Original caliper of Domain}}
\]

As an example, to create a 0.68 mm thick (Z-axis length) domain from a 0.8 mm original domain, a CF of 0.15 is used.

### 5.2 Stopping Criterion

Fibres, considered solids, are continuously added to the domain with a given probability distribution until a specific stopping criterion is satisfied. For modelling Airlaids, the grammage of the material is chosen as the stopping criterion. This mimics the actual manufacturing process where fibres are laid down to achieve a specific weight per area in the RM. The Grammage (g/m²) determines the mass per unit area, or weight (in the XY-Plane) of the resulting fibrous structure [89]. The Density (g/cm³) of the fibre material(s) must be defined for each fibre type and the chosen material for the fibres. The temperature of the lay-down process is not taken into account since the thermal properties of the fibre materials are not defined either within the scope of this project.

For RM1, the stopping criterion is determined by subtracting the latex from the formulation. This means removing 4 gsm of Latex from the top layer, 3 gsm of latex from the bottom layer of the 100 gsm material, which gives 93 gsm. It should be noted that the latex is sprayed on the material structure. Therefore, it does not necessarily add to the caliper of the material. Instead, the latex seeps into the structure form the top and bottom. The degree to which this binder penetrates the layers is a research question in itself.
5.3 Fibres in Airlaids

Fibres are the main raw materials for nonwoven products, which determine the basic properties of the final products. Based on how they are manufactured, they may be natural fibres, chemical fibres, modified synthetic fibres, and high-performance fibres [119]. Typically, Airlaids are made of a combination of cellulose (pulp) fibres and BiCo fibres. Of this, cellulose fibres generally make the larger composition. RM1 is a good representation of this with more than 80% pulp. BiCo fibres are added with several purposes. When the material is put inside the oven after the lay-down process, the outer sheath of the BiCo fibres melts into the surrounding and allows the fibres to bond. Moreover, they provide a spring-like effect which adds to the mechanical “springiness” of the material. This prevents the material from getting compressed easily. The size, shape and composition of fibres play a significant role in defining the material properties. For this modelling approach, only the geometrical properties of the fibres are considered. The information for these properties is derived from fibre specifications available from suppliers. For information that is not directly available, qualitative information is derived from the CT-Scan and approximations are made. Sensitivity Tests are carried out to ensure these parameter assumptions do not have a significant impact on simulations results.

![CT-Scan Image](image.png)

**Figure 35** A view of the CT-Scan. Qualitative information about the shape, orientation, distribution. Curl, etc. of the fibres can be derived visually.

The simulations do not take into consideration deformation of the fibres as fluid flows through the material. The following section delves deeper into the characteristics of Cellulose and BiCo fibres. The primary objective here has been to use information available from fibre specification to model the fibre geometry. Later, the effect of different fibre parameters is discussed.

**Cellulose Fibres**

Cellulose fibres are made with ethers or esters of cellulose, and are obtained from the bark, wood or leaves of plants, or from other plant-based material. The fibres may also contain hemicellulose and lignin, with different percentages of these components altering the mechanical properties of the fibres. The chemical nature of these fibres is not of interest in this thesis. Cellulose fibres typically have an
elliptical or rectangular cross-section with a lumen inside. The section between the outer wall and the inner lumen, called the fibre wall, is made up of cellulose cells from the plant. Within the structure of Airlaid, the fibres are distributed in the form of a random network. In general, however, the fibres might be more oriented in the X-Y plane, or the pane of the material. Classically, softwood pulp is used in the paper-making industry. The Table below gives an example of typical pulp characteristics available from suppliers of pulp. The information is gathered using various fibre analysis test methods.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Length</td>
<td>mm</td>
</tr>
<tr>
<td>Length Distributions</td>
<td>mm &amp; %</td>
</tr>
<tr>
<td>Width</td>
<td>mm</td>
</tr>
<tr>
<td>Wall</td>
<td>mm</td>
</tr>
<tr>
<td>Coarseness</td>
<td>mg/100m</td>
</tr>
<tr>
<td>Fines</td>
<td>%</td>
</tr>
<tr>
<td>Kink</td>
<td>%</td>
</tr>
<tr>
<td>Curl</td>
<td>%</td>
</tr>
</tbody>
</table>

These parameters don’t necessarily have a one-to-one mapping with inputs that can be used in FiberGeo to generate fibrous domains. We now take a closer look at the pulp used in RM1, which is a type of slash-pine fibre. Its weight percentage in the material is determined using the formulation for RM1. The software requires a density with which to calculate its weight. This information is not available for the fibre as such. Instead, coarseness, which is a measure of the mass of the fibre per unit length is generally given. Here, an approximation is made based on the density of the wood from which the pulp is taken, i.e. an average density of soft-wood is used, the information for which is available easily. The limitation is that the density of softwood is typically the density of the wooden bark itself and not of the cellulose content in the individual fibres. A wall density (which is the density of the cellulose content in the cells) can also be calculated. However, suppliers in the industry generally do not have this information readily available.

*Length and Width Distributions, & Aspect Ratio*

The fibre length can be measured in several ways using different kinds of optical fibre analyzer setups, which may use image processing to give results [19, 31]. Since natural fibres are never all of the same length, the results are often a set of fibre length ranges and associated percentages of fibres within these length ranges. The percentages are used to create a probability distribution of fibre lengths which is then used as an input.
Table 7 Example of Raw Fiber Analyser Data converted to Probability Distribution of Fibre Lengths

<table>
<thead>
<tr>
<th>Raw Fibre Analyser Data</th>
<th>Length Probability Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length Range [mm]</td>
<td>Percentage [%]</td>
</tr>
<tr>
<td>0.0 - 0.2</td>
<td>13.6</td>
</tr>
<tr>
<td>0.2 - 0.5</td>
<td>6</td>
</tr>
<tr>
<td>0.5 - 1.2</td>
<td>9.2</td>
</tr>
<tr>
<td>1.2 - 2</td>
<td>19.9</td>
</tr>
<tr>
<td>2.0 - 3.2</td>
<td>31.5</td>
</tr>
<tr>
<td>3.2 - 7.6</td>
<td>19.8</td>
</tr>
</tbody>
</table>

Getting relevant data for fibre width gets trickier. Some suppliers also provide data on the average fibre width distribution. It is important to define a major and minor diameter in order to describe elliptical cellulose fibres. Measurement methods can significantly vary and generally give an approximate average of the major and minor diameter [11, 79]. The CT scan was used to manually measure the two diameters on multiple fibres (see Figure 36).

![Figure 36 Manual Measurement of Fibre Widths from SEM view of the CT-Scanned Domain. The images show measurement by zooming, which is inherently error-prone.](image)

Human error in measurement and the possible dilation of fibres in the CT-Scan due to the post-processing method used (Otsu’s method with a max-filter as mentioned in the section Post-Processing of CT images) is kept in mind. The fibre width from the supplier is considered an average of the major and minor diameter. This information is combined to get an approximation for the major and minor diameters. An example of this approach is shown below.

Fibre Width mentioned in Fiber Analysis Data from Supplier = $F_w = 27 \mu m$

The CT-Scanned domain is used to take 5 measurements each of the major and minor diameters to get:

Average Major Diameter from CT-Scan = $D_{CT_{major}} = 42 \mu m$

Average Minor Diameter from CT-Scan = $D_{CT_{minor}} = 12 \mu m$

Therefore, the average fibre width from CT-Scans:

$F_{CT_w} = (D_{CT_{major}} + D_{CT_{minor}}) / 2 = 27 \mu m$

The CT-Scan has dilated fibres, therefore actual fibre width might be lower than this number.
Assumptions are made on the actual Fiber Diameters:

Assumed actual Major Diameter = \( D_{\text{major}} = 40 \ \mu\text{m} \)

Assumed actual Minor Diameter = \( D_{\text{minor}} = 10 \ \mu\text{m} \)

\[
\frac{(D_{\text{major}} + D_{\text{minor}})}{2} = 25 \ \mu\text{m}, \text{ which is similar to } F_w \text{ as well as } F_{-\text{CT}w}
\]

This fibre width of 40 \( \mu\text{m} \) is taken as the mean value in a Gaussian distribution which varies according to an entered Standard Deviation. Along with an Aspect Ratio (which equals the major diameter divided by the minor diameter, both inner and outer), the computer uses the value to create a probability distribution of fibre widths. A Distribution Bound of 40 \( \mu\text{m} \) is used arbitrarily, which corresponds to the interval on both sides of the mean value limiting the random width of the fibre. This allows the fibre widths to vary between 0 and 80\( \mu\text{m} \). The value used as the standard deviation is taken arbitrarily as 10 \( \mu\text{m} \). It is proved later that the Gaussian distribution added to the Fibre Width while generating an AD does not have a meaningful influence on the PVD of the structure. Therefore, the presence or absence of this data from the supplier does not come as a major concern.

![Capillary Pressure - Simulations - RM1](image)

Figure 37 Sensitivity Test - Effect of having a Gaussian Distribution of Fibre Widths on Capillary Pressure. Both Imbibition and Drainage curves almost overlap. Therefore, the effect can be considered negligible.
5.3 Fibres in Airlaids

Figure 38 Elliptical Cross-Section with a lumen, used to model Cellulose Fibres

Lumen

The lumen size is given by entering an “inner diameter fraction” or IDF:

\[
IDF = \frac{\text{Inner Minor Diameter}}{\text{Outer Minor Diameter}} = \frac{\text{Inner Major Diameter}}{\text{Outer Major Diameter}}
\]

 Suppliers may provide an average Fibre Wall thickness which measures the difference between the outer and inner diameters. Again, this is generally an average value for the elliptical cross-section of the fibre, and the measurement method used must be kept in mind while making an approximation. In reality, the lumens probably collapse as the fluid comes in contact with the fibres. In simulations however, the lumens manifest as small pores. This can be left as it is and the excess water absorbed in lumens can be accounted for as the water that would have been absorbed due to osmosis. However, a residual as seen due to osmosis will not be seen since the simulations can empty all pores at infinite pressure during drainage.

Figure 39 ADs made of Cellulose fibres with Elliptical (a) and Hollow (b) Cross-Sections. Red represents cellulose fibres and green are BiCo fibres. In (b), on viewing closely, one can notice the small yellow coloured lumens visible in on the fibre end faces.

A simplification may be applied by simply considering the cellulose fibres as elliptical and without lumen. This has the effect that the smaller lumen pores (which make up only about 1.23% of the porous space in the structure) are now replaced by the large void spaces in between fibres in order to maintain the same Porosity. Therefore, there are more large pores with smaller capillary pressures, and the capillary pressure curve shifts left (see Figure 40). With more pore space, the simulated permeability saw an increase of about 19% in the case of Elliptical Fibres.
Modelling

Capillary Pressure - Simulations - RM1
Effect of Cellulose Fibre Cross-Section

![Diagram showing capillary pressure simulations with different cross-sections of fibres.](image)

*Figure 40 Sensitivity Test - Effect of Cellulose Fibre Cross-Section on Capillary Pressure. In the case of Elliptical fibres, MAP reduces by about 4% and MDP reduces by about 5%, compared to the Hollow Fibres with Lumens.*

**Kink & Curl**

![Image of kinked fibre](image)

*Figure 41 Kinks at nodes in commercial dried bleached sulphite pulp. Source: [81]*

Kink and curl define how a fibre’s general direction changes along its length. There are several ways to measure these. The data however from different suppliers are not reliably comparable due to lack of standardization. In fact, Hirn and Bauer appropriately point out the inconsistency and lack of standardization in the measurement methods, approaches and ideas used widely in the market today [36].

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5.3 Fibres in Airlaids

Figure 42 Illustration of Curl & Kink. Source: [81]

A curled cellulose fibre is modelled/constructed using straight segments of a specified length. The angle between the two straight segments is the result of a random process. Let $d^n$ and $d^{n-1}$ be the directions of the last two fibre segments. Then, the next segment direction $d^{n+1}$ is found using three Gaussian distributed random numbers $N_i^{G_\sigma(0)}$, $i \in \{1,2,3\}$ and

$$(d_i^{n+1} - d_i^n) - (d_i^n - d_i^{n-1}) = N_i^{G_\sigma(0)} - \alpha(d_i^n - d_i^{n-1}) - \beta(d_i^n - d_i), \quad i \in \{1,2,3\}$$

with parameters $\alpha$ and $\beta$ in $[0,1]$ and a main fibre direction given by $d$. $\alpha$ can be read as a measure of “local straightness”, $\beta$ a measure of the tendency to maintain general direction or the “global straightness”, and $\sigma$ a measure of “randomness”. With $\alpha, \beta = 0$, fibre segments keep their previous curvature. With $\alpha=1, \beta=0$, the change in the segment direction is Gaussian distributed around 0; and with $\alpha, \beta = 1$, fibres keep the main direction. Full anisotropy can therefore be achieved here by setting $\alpha, \beta, \sigma \in \mathbb{R}^{3 \times 3}$. This fibre generation algorithm is briefly explained by Becker [9].

The curl and kink of the cellulose fibres for RM1 were not readily available. A segment length of 100 microns was used by deriving qualitative information from the CT-Scan of RM1. The following parameters were chosen by visually comparing the generated AD with the CT-Scan: $\alpha = 0.4$, $\sigma = 0.1$, and $\beta = (0.1, 0.1, 0.5)$. The anisotropic $\beta$ ensures a higher probability that fibres are oriented in the X-Y plane. This decision is explained later in the section Fibre Orientation. The value 0.5 along Z for $\beta$ means that fibres have a higher tendency to maintain their original set orientation along Z, instead of deviating randomly.

While these parameters do influence the mechanical properties of the material [45, 81], it is proved (see Appendix C - Effect of Cellulose Fibre Curl Parameters) that their effect on the fluid handling properties of the RM is not of sufficient magnitude (only of order $0.1e-10$ sq.m on Permeability, no effect on Capillarity). Moreover, in the section Fibre Orientation, it is shown that as long as the fibres are sufficiently oriented along the X-Y plane (in-plane), the curl parameters do not have a significant influence.
**Modelling**

**Torsion**

![Figure 43](image1.png)

*Figure 43* Domains of Cellulose fibres shown without (left) and with (right) torsion. Fibres are unidirectional to have them discernible.

Cellulose fibres are seldom flat along their entire length. Other than bending or curling along their length, they also turn around the length of their axis. This is referred to as the torsion in the fibre and the data is not typically available. Torsion is handled inside of one straight segment. The orientation of an elliptical fibre is described by the direction of the fibre and the two perpendicular directions of the ellipse axes (see Figure 38). For torsion ≠ 0, the perpendicular axes are rotated around the fibre direction by Θ degrees from the beginning to the end of the segment. The torsion angle Θ is assigned randomly to each. For RM1, each starting segment is kept at Θ = 0, while the maximum torsion changes from one segment to the next is a random value between 0 and 360°. The torsion change between different segments is uniformly distributed. Torsion does not largely influence capillarity, or permeability (see Figure 44).

![Figure 44](image2.png)

*Figure 44* Sensitivity Test on Capillary Pressure for Torsion in Cellulose Fibres and Crimp in BiCo fibres added to a reference domain (REF). The shift in MAP is about 10% while the shift in MDP is about 6%.

**BiCo Fibres**

Bi-Component or BiCo fibres, as the name suggest are made up of two components. They come in several types of cross-sections including “side-by-side”, sheath-core with concentric and eccentric
configurations, “islands-in-the-sea”, “pies”, “tipped trilobal”, etc. [28] The Sheath-Core configuration has a structure with an outer layer (sheath) having a lower melting temperature than that of the core [29]. In thermal bonding of such fibres, as the fibre web is exposed to a heated environment, bond spots are formed by melting of the sheath material [71]. The molten sheath material acts as an adhesive while core parts of the fibres remain fully intact in the bond spots. For bicomponent fibres, polyethylene (PE) is frequently used as sheath material, whereas polypropylene (PP), polyamide 6 (PA6) and polyethylene terephthalate (PET) are the most commonly used polymer core material [91]. RM1 uses sheath-core BiCo fibres with a PET core and a PP sheath.

Figure 45 Structure of a Core/Sheath type BiCo Fibre. Source: [29]

Figure 46 SEM pictures of bicomponent nonwoven fiber cross-sections: a PET/PE, b PA6/PE, c PA6/PP, and d PP/PE (50/50 wt/wt%). Source: [28]

The round profile of BiCo fibres makes it easier to model them as compared to pulp fibres. Typically, suppliers provide the following information as specifications for BiCo fibres:
Table 8 Specification for BiCo fibres used in RM1. Values shown are examples only.

<table>
<thead>
<tr>
<th>General Product Data:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polymer Core</td>
</tr>
<tr>
<td>Polymer Sheath</td>
</tr>
<tr>
<td>Melting Point Core</td>
</tr>
<tr>
<td>Melting Point Sheath</td>
</tr>
<tr>
<td>Cross Section</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Physical Properties</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fibre Fineness</td>
<td>dtex</td>
<td>2.2</td>
</tr>
<tr>
<td>Staple Length</td>
<td>mm</td>
<td>4</td>
</tr>
<tr>
<td>Tenacity</td>
<td>cN/tex</td>
<td>30</td>
</tr>
<tr>
<td>Elongation at Break</td>
<td>%</td>
<td>10</td>
</tr>
<tr>
<td>Shrinkage, hot air</td>
<td>%</td>
<td>--</td>
</tr>
<tr>
<td>Crimp</td>
<td>Crimps/cm</td>
<td>5</td>
</tr>
<tr>
<td>Finish level</td>
<td>%</td>
<td>0.22</td>
</tr>
</tbody>
</table>

To generate a domain with BiCo fibres in it, FiberGeo needs information on the amount of fibres required and the density of these fibres. The formulation for RM1 gives the amount of BiCo fibres to be added in grams per square metre. The density of the BiCo fibres still needs to be calculated. This is shown below.

Calculation of Average Density of Bi-Component fibres

Depending on the type of BiCo fibres, the mass of the two components may be different. RM1 uses a sheath-core type of BiCo fibre with approximately equal masses of sheath \( M_S \) and core \( M_C \) material.

We consider a cross-section of the BiCo Fibre. The masses of the two components are equal.

\[
M_S = M_C (= M)
\]

The density of the BiCo fibre is given by

\[
\rho = \frac{\text{Total Mass}}{\text{Total Volume}} = \frac{M_S + M_C}{V_S + V_C}
\]

Where \( V_S \) and \( V_C \) represent the volumes of the two components making up the Sheath and the Core. Representing the volumes of the two components in terms of their masses and densities (\( \rho_S \) for the Sheath and \( \rho_C \) for the Core), we get:

\[
\rho = \frac{M_S + M_C}{M_S/\rho_S + M_C/\rho_C}
\]

Since \( M_S = M_C = M \), we get:
5.3 Fibres in Airlaids

\[
\rho = \frac{M + M}{\frac{M}{\rho_S} + \frac{M}{\rho_C}} = \frac{2}{\frac{1}{\rho_S} + \frac{1}{\rho_C}} \Rightarrow \rho = \frac{2 \rho_S \rho_C}{\rho_S + \rho_C}
\]

The densities of the individual components are available and can be used to get the average density of the fibre as shown above.

BiCo fibres provide two main properties to the raw material they are added to. First, they change the mechanical properties of the material. Due to their higher flexural strength, as compared to cellulose fibres, they tend to keep the material swollen and prevent it from collapsing (or flattening out). Second, the outer coating or the sheath of these fibres melts into the surroundings and creates bond spots which hold the loose cellulose fibres together. The bond formation can be conceptualized as follows:

- In the Air-laying process, the cellulose fibres and BiCo fibres are randomly distributed in the form of a network in the plane of the raw material.
- When the material is exposed to heat either in an oven or between hot calenders, the outer sheath of the BiCo fibre starts melting. If the temperature is high enough, the outer sheath melts completely and diffuses into the surrounding fibre network. In this case, the BiCo fibre is left only with the resultant inner radius, which is the radius of the Core.
- In the event that the temperature is raised just high enough so that the sheath does not melt completely, the sheath material enters a semi-solid phase temporarily. At this time, the fibres which are in contact with the sheath can merge into it, and as the material cools down, the fibres are left overlapping each other.

![Figure 47 A scanning electron micrograph of an airlaid (100 gsm) thermally consolidated with PE/PP bicomponent fibres. The bonding of the BiCo fibres is apparent. Source: [116]](image-url)
The air-laying process is not simulated. Hence only the final radius of the BiCo fibres in the raw-material is relevant to this modelling approach. Information about the difference between the temperature the material is exposed to and the melting point of the sheath can be used to determine if the BiCo fibres should be modelled in the AD with their inner core radius or original radius (with the sheath). In case the temperature in the oven or hot calendar is not high enough, the overlap between the BiCo fibres and other fibres needs to be defined. This can be considered in the form of a random overlap between fibres, with a maximum overlap distance. The overlap distance is the distance that a fibre merges into the BiCo material. Since only the sheath of the BiCo becomes temporarily semi-solid, the maximum overlap distance is taken as the BiCo Fibre radius $R_S$ minus the Inner Core Radius $R_C$. In all cases, the inner radius, or the radius of the core material becomes important. This information about the inner radius is not typically provided by suppliers and can be calculated as shown below.

![Diagram](Figure 48 Illustration of the Overlap made between a BiCo Fibre and a Cellulose Fibre. Overlapped Region is hashed.)

**Calculation of the Inner Core Radius in Sheath-Core BiCo Fibres**

Consider a Sheath-Core BiCo fibre with an arbitrary length $l$, outer radius $R_S$, and inner core radius $R_C$. Refer to Figure 48. The densities of the sheath and core are given by $\rho_S$ and $\rho_C$ respectively. As in the previous calculation for the average density, the masses for the components making up the sheath and the core are equal.

$$M_S = M_C$$

Representing the masses in terms of the volumes and densities of the components for the given fibre length $l$,

$$\rho_S V_S = \rho_C V_C$$

The volumes can then be written in terms of the effective radius if the cross-sections. The Volume of the Sheath is the volume of the Core subtracted from the volume of the Fibre.
\[
\rho_S \left( \pi R_S^2 l - \pi R_C^2 l \right) = \rho_C \left( \pi R_C^2 l \right)
\]
\[
\Rightarrow \rho_S \left( R_S^2 - R_C^2 \right) = \rho_C \left( R_C^2 \right)
\]
\[
\Rightarrow \rho_S R_S^2 = R_C^2 (\rho_C + \rho_S)
\]
\[
\Rightarrow R_C^2 = \frac{\rho_S R_S^2}{\rho_C + \rho_S}
\]
\[
\Rightarrow R_C = R_S \sqrt{\frac{\rho_S}{\rho_C + \rho_S}}
\]

The overlap distance (the distance in the sheath of the BiCo fibre into which another fibre may merge in) is given by \( R_O \). The maximum overlap distance is given as

\[ R_{O-max} = R_S - R_C \]

As the domain is generated, the fibres are allowed to merge into the BiCo fibre randomly up to this maximum overlap distance.

---

**Figure 49 Crimp in BiCo Fibres.** In the CT-Scan image on the left, a BiCo fibre is traced out in blue. On the right, a single BiCo fibre is highlighted in an AD made completely of Red BiCo fibres.

**Crimps**

BiCo fibres may be made to have crimps in their shape. The degrees of freedom of the crimp, i.e. the crimp amplitude, crimp frequency, and shape (wavy vs erratic, or 2D vs 3D), all play a role in the processability and finished material properties. Crimps in fibres have been characterized in detail and their effect on non-woven materials has been studied [13, 67]. Here, crimps are modelled as curves (different compared to cellulose) in the shape of the fibre. The BiCo fibres are considered to be sinusoidally curved, having two independent frequencies and amplitudes perpendicular to each (in the direction of the main axis) other along their length [89]. The value of the frequency is determined by finding the length of a single crimp from information about the crimps-per-cm in the fibre specification.
The “fibre fineness” as shown in Table 8 is a measure of the mass in the individual fibres. Dtex or deci-tex is a direct measure of linear density and is the number of grams of material in 10 km of the fibre. Along with the fibre length and average density, either the fibre diameter or the fibre fineness is enough to characterize the basic fibre geometry completely.

**Fibre Orientation**

The orientation of fibres affects the fluid handling properties of the raw material. This is not just intuitive, but several studies have been made to understand the case specific to non-wovens. Mao and Russel produced pioneering work in 1999-2000 and showed that fibre orientation is a major factor influencing the anisotropy of permeability in fibrous media with both low or high porosity [69, 70]. Stylianopoulos et al. re-emphasized that in three-dimensional isotropic and oriented fibre networks, permeability has a strong dependence on fibre orientation [102, 103]. However, Rawal et al. took a closer look at the effect of fibre orientation on the PVD (which affects capillarity as well) of non-woven structures and stated that Airlaid nonwovens tend to be more isotropic than those produced by carding and therefore do not have a high directional parameter in their Pore Size Distribution model [88]. Tahir & Tafreshi at Virginia Commonwealth University modelled through-plane permeability in fibrous structures and demonstrated that the transverse permeability of a fibrous medium is independent of in-plane fiber orientation but increases with increasing deviation of the fibers’ through-plane angle from zero [104]. They admit that their results are a contradiction to the conclusions made by Stylianopoulos et al. mentioned above. In a study specific to power-law fluids, Tafreshi’s team found that while the permeability of a fibrous material hardly depends on the in-plane orientation of the fibres, it increases with increasing the fibers’ through-plane orientation [32]. But Tafreshi et al. looked only at through-plane permeability. In this case, the liquid flows perpendicular (along Z-Axis) to the general fibre orientation (X-Y Plane) and therefore it doesn’t matter if the fibres are isotropic along the X and Y Axes or not. Our hypothesis is that in-plane permeability must be dependent on the in-plane anisotropy of the fibres. In Appendix C - Effect of Cellulose Fibre Curl Parameters, we study the effect of fibre curl parameters $\alpha$, $\beta$ and $\sigma$ on the permeability, PVD and Capillarity of the RM and prove that these parameters do have a linear influence on the permeability of the RM. However, the magnitude of this effect was extremely low for the AD we considered. Moreover, PVD and Capillarity were not meaningfully affected by changing the curl parameters.
5.3 Fibres in Airlaids

We now reason the case for Airlaids. During the air-laying process, some fibres may settle down with their lengths oriented along the Z-Axis. However, as the material passes between the rollers, they are flattened and take an X-Y orientation. It was explained in section 1.3 Manufacturing of Airlaids that fibres may, in fact, be more oriented along the MD as compared to the CD. However, the deviation of the fibre orientations from the X-Y plane must be low. Specific to RM1, we had to ascertain that the anisotropy of fibres in the X-Y plane was low enough to not affect the IPRP. The results of the 1D-IPP experiments carried out as part of this thesis show that permeabilities in the X and Y directions of the RM could not be differentiated, i.e. the tendency to orient in MD is not significantly higher than that in CD for RM1. Therefore, while the fibre laying procedure may affect the in-plane orientation of the fibres in Airlaids, the fibres can be considered simply isotropic in the X-Y plane for modelling purposes.

The AD consists of a large number of cellulose and BiCo fibres randomly distributed in the domain to build up a 3-D geometry. The fibre orientation distribution can be controlled by a density function \( p(\theta, \varphi) \) in polar coordinates, in which \( \theta \) is the through-plane angle and \( \varphi \) is the in-plane angle [107].

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

where \( \beta \) is the anisotropy parameter and is equal to 1 for the case of a 3D-isotropic system. This algorithm has been fully described by Schladitz et al. [92], Schulz et al. [95], and Ohser and Mücklich (2000) [44]. \( \theta \in [0, \pi] \) is the through-plane angle and \( \varphi \in [0, 2\pi] \) is the in-plane angle. It should be noted that due to the assumed isotropy in the X-Y plane in Airlaids, \( p(\theta, \varphi) \) is independent of polar coordinate \( \varphi \). By increasing \( \beta \), fibers tend to become parallel to the X-Y 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 its value controls the number of fibers oriented in the z-direction.

Since fibre orientation data is not readily available for raw materials, the Anisotropy Parameter may be set qualitatively using the CT-Scans of the material as a reference. Methods are also available to measure fibre orientation in non-woven fabrics (as well as other fibrous composites) from CT-Scan or SEM images [34, 99]. The alternative is to simply orient the fibres along the X-Y plane randomly. A Fibre Orientation Tensor \( \Omega \) (explained by Barocas and Tranquillo [7]) is provided as input to the FiberGeo module which described the general anisotropic orientation of the fibres in the domain. \( \Omega \) is a symmetric second-order tensors calculated as the dyadic product of the unit vectors representing the orientation of single fibres in the domain [111]. The trace of \( \Omega \) is always 1. For an isotropic structure, \( \Omega_{xx} = \Omega_{yy} = \Omega_{zz} = 0.33 \), while for aligned networks, the values of the diagonal components are a measure of fiber alignment in the principal directions.
This method is preferred due to its simplicity. For Airlaid, the tensor values as shown below are chosen such that fibres have a high probability of orientation along the X-Y plane and a low probability of orientation along the Z-plane.

\[
\Omega = \begin{bmatrix}
0.45 & 0 & 0 \\
0 & 0.45 & 0 \\
0 & 0 & 0.1 \\
\end{bmatrix}
\]

The off-diagonal components indicate orientation in a direction other than a principal axis. \(\Omega_{zz} = 0.1\) along the Z-Axis for Cellulose fibres, combined with their global straightness or \(\beta\) value of 0.5 as they are generated results in them remaining oriented along the X-Y plane. The combination of the curl parameters for cellulose fibres and the general fibre orientation tensor needs to be handled carefully in order to avoid values which nullify each other’s effects (e.g. having a low value for \(\Omega_{zz}\), but a high value for \(\sigma\) (or \(\sigma_{zz}\) if \(\sigma\) is anisotropic) will result in the fibres starting with the first segment oriented along the X-Y plane, but randomly changing direction, including towards the Z-axis as segments are added. In order to prevent undue effects on the PVD and permeability, the anisotropy in orientation must be carefully restricted to the X and Y directions only. Of course, as used here for RM1, the fibres may be set to isotropic along the X and Y directions, but not along Z.
Since RM1 has a uniform structure across its layers, the fibre centres in the domain are uniformly distributed across the whole structure.

ADs can be generated with the setting that cellulose fibres do not overlap with each other. For BiCo fibres, the maximum overlap distance can be set using the method described above. However, generating such an AD takes a lot of time and computing power. A simplification of allowing the fibres to overlap. The computer faces the question that what is the material ID of an overlapped volume region when two different fibres overlap there. This information is required in order to calculate the density of the material in this region, and thereby the achieved grammage of the domain.

Therefore, “overlap rules” are defined as follows: If two cellulose fibres overlap, the overlapped region is cellulose. If two BiCo fibres overlap, the overlapped region is BiCo material. If a BiCo fibre and a cellulose fibre overlap, the region is set as BiCo material. The reason behind this is that BiCo fibres can be seen as melting into the surrounding fibre network to create bond spots. When this happens, the material of the BiCo sheath engulfs the cellulose surface around the bond spot. Since the BiCo material has a higher density as compared to cellulose, the bond spot can be considered BiCo material. Of course, in reality, inside the RM, these bond spots will have a density higher than that of cellulose, but lower than that of the BiCo fibres. Also, the algorithm now tries to substitute the artificially missing cellulose content of the overlapped region (now defined as BiCo) by adding the necessary amount of Cellulose fibres to achieve the required Cellulose grammage. But since Cellulose has a lower density than BiCo fibres, it will not need to add a lot of material (as compared to adding BiCo material in case overlapped region would be defined as Cellulose, and a higher amount of missing material would need to be

\[ \text{Explanation of Image: Clockwise from top left, domain starts with unidirectional fibres with torsion in (a), and } \alpha, \beta \text{ and } \sigma \text{ are set to 0, and } \Omega_{yy} \text{ is set to 1. In (b), } \alpha \text{ and } \sigma \text{ parameters are set to 0.4 and 0.1 respectively. In (c), isotropic } \beta \text{ value of 0.1 is set, and fibres segments orient randomly in any direction. In (d), } \beta \text{ is made anisotropic with its } Z \text{ value 0.5. This prevents segments from growing towards the } Z \text{ direction. In (e), fibre orientation is made fully isotropic with } \Omega_{xx} = \Omega_{yy} = \Omega_{zz} = 0.33. \text{ Finally, in (f), } \Omega_{xx} = \Omega_{yy} = 0.45 \text{ and } \Omega_{zz} = 0.1 \text{ in order to have in-plane orientation. Note: this is an illustration of the anisotropy effects and not the sequence of steps in which anisotropy was added.} \]
substituted). A sensitivity test is carried out to ensure that this simplification does not have a meaningfully large impact on the fluid handling properties.

5.4 Binders in Airlaids

Binders are added to Airlaids to help hold the network of fibres together. Hence the word “Binder”. Latex is sprayed onto RM1 from the top and bottom in the Airlaid manufacturing process. As a Binder, Latex occupies the pores and clings to the intersection points of the fibres in the network (see Figure 53). Such a distribution ensures that the total free surface energy of the system is minimized. The effect of adding latex is the filling up of open space to create smaller pores, shift the PVD curve left, and the Capillary Pressure curves right. The permeability should be reduced as well due to the smaller pores. However, these effects depend on the degree of penetration of the latex (sprayed on the RM surface) into the structure of the material. In case the latex remains only in the upper and lower layers of the material, the in-plane permeability should not be affected since the fluid flows parallel to the blocked pores on the top and bottom surfaces. The challenge comes from the fact that there is no easy way to identify this degree of binder penetration into the material.

![Binder in Airlaids: (a) Illustration of Latex being sprayed onto the top and bottom of the RM in the manufacturing line. (b) Binder distribution in a fibre network. Source: P&G.](image)

The Latex in RM1 totals less than 8 gsm. This means a possibly low degree of penetration as well as a rather small change in the PVD. When comparing the PVD curves for the Super-Cropped and Un-Cropped CT-Scans for RM1 (see section 1.8 Tomography References), there was no difference noticed. This means the top and bottom layers were not substantially affected by the latex, to the extent that their pore distribution would be changed. The latex did not block pores sufficiently to shift the PVD curve. Therefore, binder was not added to the RM1 ADs generated for this study. Nevertheless, some exploratory studies were carried out with regards to binders as discussed below.

Binder Contact Angle

The Binder makes contact with the fibres in the network in such a way that the total free surface energy of the system is minimized, just as in the case of Interfacial Tension as explained earlier. The
angle at which the binder meets the fibres, in the form of a concave meniscus, is referred to here as the binder contact angle (BCA) and is a measure of the wettability of the fibres. This BCA is required to model the Airland structure. Several studies have been performed to better understand wettability in non-wovens. Because Airlands have porous, heterogeneous, and anisotropic structure, the reliability of the measurement of the contact angle is always a concern, especially when the fabric/paper is hydrophilic. Although the contact angle can be measured by using either goniometer or other indirect methods, there is no standard method to measure the contact angle of nonwoven fabric; the difficulty is always to obtain reliable measurements [68]. For low binder content materials like RM1, it is not possible to visually identify the binder in the fibre network using CT-scans in order to determine the BCA. Added to this is the complexity of the Binder having different BCA for Cellulose and BiCo fibres, i.e., different BCAs is Bimodal/Polymodal fibrous media. Therefore, it is important to understand if the BCA has any real impact on the fluid handling properties of the material. The effect of Binder addition, as well as the effect of BCA, is explored and presented in Appendix D - Effect of BCA on Fluid Handling Properties.

![Binder Contact Angle showing Concave Meniscus formed at Interface with Solids. Red: solid Cylindrical Fibres. Grey: Binder. Source: [84]](image)

**BCA 0°**  
**BCA 45°**

**Binder Distribution**

Algorithms to distribute the latex in-homogenously across the RM cross section were explored. Figure 55 below illustrates different methods for distributing the binder. The most straightforward method is to distribute the binder homogeneously throughout the domain. Only information about the density of the binder and its contact angle is needed. The BCA may be assumed since it does not have a considerable influence. A limitation is that binder density information provided by the supplier is generally for a specific temperature. Simply setting this as binder density does not take into account the structural changes in the binder that may be brought about when the binder is initially heated and then sprayed onto the RM. Moreover, as the binder seeps into the fibre network, its adhesion to the fibre walls may leave some stress in the system and lead to a different final density on cooling down. Therefore, assumptions need to be made.
The three different binder distribution methods. The red cellulose is made semi-transparent. BiCo fibres are invisible. Yellow represents Latex. From the left, homogenous distribution (a), layered distribution (b), and density profile gradient based distribution (c).

The second method is to assume that the binder infiltration into the RM fibre network is limited to a specific depth from the top and bottom surfaces onto which it is sprayed. Specific distances can be defined, and three different ADs can be made as layers. The binder is added to the top and bottom layers. The three layers are then combined by stacking them on top of another. The disadvantage of this method is the fibre and binder discontinuity at the interface of the joined layers (see Figure 56).

The third method involves setting up a density probability distribution of the binder. This is done by creating a single domain and defining a table of values with probability distribution or relative density distribution of the binder. A macro is then written which slices up this domain into layers along the Z axis. The number of layers is determined by the number of points defined in the probability distribution table. In each layer, the binder is added as a percentage of the total grammage required in the domain based on the relative binder density defined for that layer. The different layers with binders are then stacked upon one another. Since the layers were created from a single continuous domain, stacking them up does not create a discontinuity in the fibres. (There may be binder added non-uniformly at the interfaces. But this effect can be neglected since its no a discontinuity as such). It leads to a smooth gradient structure where the binder distribution can be better controlled.
To replicate binder being sprayed on the domain, a relative density function $f(a)$ can be chosen appropriately. The Binder added to each layer is then given as:

$$\text{Binder Added to Each Layer} = \frac{f \left( x_i - \frac{c}{2} \right)}{\sum_{i=0}^{c} f \left( x_i - \frac{c}{2} \right)} \times BA$$

where $c$ is the Caliper of the material, $x_i$ defines the distance of the layer being considered from the bottom surface of the material along the $Z$-axis, and $BA$ is the total amount of Binder to be added to the system. The division of the caliper by 2 shifts the function to align its graphical center with the central layer of the domain. The denominator in the equation sums up the values of the relative density function. This way, the binder is added to each layer as a fraction of the total binder to be added, based on $f(a)$. Figure 57 shows two different $f(a)$s considered in this study. The idea is to choose the function in such a way that the binder is distributed with high probability along the top and bottom surfaces of the domain, and its presence falls significantly as we move inwards into the material. If a method can be devised to examine the penetration of the sprayed binder in actual RMs, this approach can be validated. Until then, these functions provide an approximation, and may be useful in modelling Airlaids with high Latex mass.

![4 gsm Binder Distribution across a 0.8 mm AD using Relative Density Functions](image)

*Figure 57 Binder Distribution along the height of an AD using Relative Density Functions $f(a)$.***
Figure 58 Binder distributed in two ADs. Red Cellulose fibres are made transparent for better visibility. Green fibres are BiCo. In (a), the relative binder density falls linearly from the top surface. In (b), the relative density function $f(a) = a^4$ is used.

The studies on binders were exploratory only. Since RM1 does not have significant amounts of latex in it, the final domains created do not have binder in them.

The domain finally generated for RM1 is illustrated in Figure 59 and can be compared with the formulation shown in section 1.7 Selection of Raw Material for a better understanding.

Figure 59 Illustration of final AD for RM1 considered/modelled. Grey fibres represent Cellulose and Magenta are BiCo fibres.
Chapter 6
Results & Conclusion

The structure of RM1 was successfully replicated to a degree that fluid handling properties could be predicted. Visual comparisons between the CT-Scan Domain and the AD were crucial as the modelling method was refined iteratively through this thesis. As mentioned earlier, the CT-Scan gave important visual hints about parameters such as fibre curl, kink, ordination, distribution, etc. Therefore, a qualitative similarity between the two domains gives the first hint of success for the modelling approach developed. The comparisons shown here are with the “Super-Cropped” CT-Scan Domain as mentioned in section 1.8 Tomography References.

![Figure 60 Comparison of CT-Scan and Artificially Generated Domain for RM1 - SEM views. The slices shown for these tomography images were chosen to avoid any agglomerates in the CT-Scan domain. The Depth of the visible volume was chosen qualitatively for comparison of the fibres here. All fibres or solids are shown in white, while porous space or air is black.](image1)

![Figure 61 Comparison of the CT-Scan and Artificially Generated Domain for RM1 - 3D view. All solids or fibres are red.](image2)
6.1 Comparisons with References

The geometrical similarity between the structures can be verified by comparing the PVD achieved from simulations on the CT-Scan of RM1 and the AD for RM1.

![PVD - RM1 - CT vs AD](image)

*Figure 62 PVD for the CT-Domain and AD for RM1 showing a good overlap.*

A good overlap is seen for the PVD curves indicating that the modelled AD replicates the actual RM well. The micro-CT domain still shown some large pores, which the AD does not capture. However, these form less than 1% of the material and can, therefore, be ignored.

![Capillary Pressure - RM1 - Expmt vs AD Sim](image)

*Figure 63 Capillarity Comparisons - Experiments vs Simulations on AD*

Since PVD drives both Permeability and Capillarity, the first step to be taken in the Virtual Material Design journey is considered taken. Simulations were run on the different generated ADs and the results compared well with the references. We begin by taking a closer look at the Results of simulations on and AD compared with experiments. As mentioned earlier, in the section 5.1 Domain Size & Resolution, ADs with different calipers were generated to run simulations for imbibition and drainage on, in order to reflect the material's state in the during the experiments. This is seen in Figure 63. Since the pressure values are scaled, we focus here on the general shape of the curve and not the exact fit itself.
At higher saturations, the AD seems to behave exactly like the RM, with a low slope at 90% saturation and above. The first most striking difference is seen at the different imbibition start points for the AD and the experiments. In experiments, the imbibition starts much later at a lower pressure. This can be understood as follows: During the experiments, as the RM is kept on the semi-permeable frit, it is not laid absolutely flat despite the confining weight on it. There may be gaps in between the sample being tests and the frit which manifest as artificial large pores. This hypothesis was later verified by considering a Micro-CT domain with artificial large pores at the bottom surface instead of on the top, similar to the one discussed in section 1.8 Tomography References. Simulations on such a domain showed a similar imbibition curve starting late at a lower pressure. Moreover, in experiments, only a finite pressure can be applied to the system. In simulations, however, an infinite pressure can be considered for the system. This can fill up pores of any possible size, which might not be possible in experiments. Therefore, both imbibition and drainage curves in simulations approach zero saturation at much higher pressures. In other words, the RM's PVD from the CT-Scan also shows the presence of extremely small pores with very high capillary pressures that may not reflect in experiments.

The hysteresis seen in experiments between imbibition and drainage is also much higher. As explained earlier in this thesis, there are two sources of Hysteresis: a difference in the ascending and receding Contact Angles, and the Ink Bottle Effect. The first is ruled out. Hexadecane is used in the experiments. It might be that despite Hexadecane’s properties, it might not be 100% wetting. However, this cannot be the source of such large hysteresis. Test Simulations were carried out for Hexadecane with a Drainage CA of 0° and an extreme Imbibition CA of 30°. The Hysteresis observed was hardly enough to account for the difference seen in experiments. This leaves only the Ink Bottle Effect which may arise out of inhomogeneities in the structure. The low hysteresis in the AD then indicates that the AD is far too homogenous with the uniform fibre distribution across its thickness, i.e. perfect distribution of all pore sizes. The PVD comparison with the CT-Scan would not show the spatial distribution of the pores, but only the fraction of pores of each size in the domain. However, when the capillary pressure curves are compared later with the simulations on CT-Scan we see a better fit and therefore attribute the hysteresis seen in experiments to experimental limitations.

The last point of difference is the residual saturation seen in the drainage curve in experiments. Since in simulations, the pressure can be increased to any value, the smallest pores can be emptied out. Moreover, thee simulations do not consider processes like osmosis and film formation, where fluid may be trapped inside the cellulose structure of the fibres or may leave a coating on the fibre surfaces in the form of a liquid film.
The validity of the interpretations above can be verified on comparing simulations run on the AD and the CT-Scan Domain (see Figure 64). Here, the same AD was used for both imbibition and drainage since a single CT-Scan domain is being considered for both simulations. The curves not only fit well, but also show very good similarity in elements of shape, i.e. - similar slopes at different saturations. In fact, the AD provides a hysteresis slightly more than that provided by the CT-Scan domain. Therefore, the question of the generated AD being too homogenous across its thickness is removed.

For comparing permeability predictions with experimental results, it is not enough to have a single RM. A second Airlaed RM, referred to here as Raw Material 2 (or RM2) is considered. RM2, like RM1, is a bimodal fibrous material, with cellulose and BiCo fibres, and with latex sprayed on it from the top and bottom. The formulation, however, is different from RM1, with a non-homogenous distribution of the feedstock across the layers. The layered or gradient structure is generated by centering the fibres with different relative densities across the Z-Axis. The computer adds the first fibre segment randomly using an input of these relative densities.
For both RM1 and RM2, GeoDict (using the EJ Solver) consistently under-predicts IPRP by about 25-28% as compared to experiments. Given that experiments themselves have a variation of 19.67%, the predictions from simulations are considered good. The results of permeability simulations on the CT-Scan domain of RM1 however, gives a value much higher than those from experiments and the ADs. This is not fully explained. But we hypothesize that since the sample is scanned in its virgin state without any confining weight, it is not subject to any compressions and allows fluid to flow easily through its larger pores. This is also indicated by its larger porosity. The AD, on the other hand, is generated compressed. This was explained in Section 5.1 Domain Size & Resolution.

The results show that the modeling approach developed here can be used to generate ADs of RM using only geometric properties of the feedstock, and then predict the fluid handling properties successfully. Parameters for which information is not readily available can be either approximated using the method discussed or neglected due to their marginal influence. This opens up several possibilities for applying Virtual Material Design to drive decisions about formulations of different Airlaid as well as other non-woven materials.

6.2 Applications

Modelling Airlaids opens up the possibility to analyze parameters which have thus far not been studied in detail. As an example, since information regarding the aspect ratio or AR of cellulose fibres had to approximated for RM1 (see Section Length and Width Distributions, & Aspect Ratio), a sensitivity test was carried out to understand its impact on fluid handling properties. Interestingly, it turned out that the AR had the largest impact among the parameters studied in this thesis. It indicates a necessity to not just look at fibre length and coarseness while choosing the pulp but also assessing its flatness since this has a direct impact on how closely packed the structure is. In Figure 66, we see two domains based on RM1 with the same porosity and yet completely different characteristics due to different ARs. This difference notably shifts both the capillary curves (see Figure 67) as well as the permeability value (see Figure 68).

Figure 66 Illustration of Domains considered in this study. Both have the same porosity and formulation. Only the Aspect Ratios vary.
Similarly, modelling can also be used to single out a parameter to study its effect. We illustrate the case for fibre length. The effect of having two different lengths of cellulose fibre, 2.6 mm and 3.1 mm are studied and the results on capillarity are shown in Figure 69. The permeability on increasing the fibre length increased by less than 2%. Such quick studies don’t just help validate expectations from the changing of different parameters, but also give insights into the magnitude of the effects.
6.3 Summary & Outlook

To begin with, an overview of the structure and principle of manufacturing Airlaids was explained in order to better understand the approach developed to model them. The formulations of Airlaids are fundamental in defining how they handle fluids. A reference Raw Material was selected due to its simple formulation and readily available feedstock information. The similarity Airlaids have with other porous media and non-wovens allowed the borrowing of scientific ideas from these other fields. Understanding the distribution of the feedstock inside the Airlaids is important to interpret the pore distributions in the structure. The inherent challenges of taking CT-Scans and trying to analyse such structures was discussed. It was proposed that samples need to be scanned in their virgin state without weight, and the fibres jutting out at the top and bottom surfaces need to be effectively cropped out without compromising on the thickness of the domain, which might affect permeability calculations. An outline of important concept required about the physics of capillarity and permeability in porous non-woven fibrous media was given in order to form a bedrock. Phenomena both at the micro and macro scale which influence fluid handling in Airlaids were discussed. Special considerations for the directional permeability in Airlaids were highlighted. The differences between measuring in-plane and in-plane radial permeability were explained in reference to the experiments that were carried out. Following these fundamentals, the details of the experimental set-ups and procedures were shared. Specifically, the tracking of caliper was highlighted as a major point. The caliper of the material during the experiment is important since it directly changes the porosity. A method to determine the right caliper to be considered was proposed. A test method to understand the degree of fibre orientation along MD/CD in Airlaids was developed and used. The experimental results along with the CT-Scan domains formed references or benchmarks for comparisons. Following this, the experimental setup was interpreted to the right set of boundary conditions for simulations. The solution methods and their limitations were discussed in detail. Two solvers, the LIR and EJ were validated for use in this context. The LIR solver may be used for quick comparisons between two simulations but not with experimental results since it employs different BCs. With the Simulations methods explained, the next step was to dive into the modeling approach.
Parameter reduction was key here. There are several variables that go into generating artificial domains, and they were studied to gauge their influence on fluid handling properties. Parameters with marginal influence were approximated. The right selection of an REV with relevant resolution has been explored. Given BiCo fibres have created the threshold in fibre diameters, a safe 1μm to 2μm resolution is recommended. Both length and width distributions do not influence fluid handling properties much. A method to approximate Aspect Ratios is presented and it is shown that the “flatness” of cellulose fibres has a large impact on the PVD of the material, and hence the fluid handling. Therefore, A simplification may be applied to Cellulose fibres by considering an elliptical cross-section without lumen. The effect of different parameters used to model curl in Cellulose fibres was investigated. We presented calculation techniques to find the average density in BiCo fibres and also the overlap distance with other fibres where bond points are created. A simplification by simply allowing fibres to overlap and then defining the overlapped material is recommended. A detailed consideration is given to the effect of fibre orientation in such domains, especially on permeability. Literature is compared with the experiments and calculations made in this thesis to reason the following: The in-plane anisotropy in orientation of fibres does have a linear impact on the permeability. However, the magnitude of this effect should be considered when making comparisons. Finally, multiple methods for distributing binders in layered non-homogenous formulations were investigated and the use of a relative density function is recommended.

The results of predictions made from the artificially generated domains compared well with the references, both experimental and the CT-Scans. The implications of this thesis extend to a better understanding of general porous media as well as nonwovens specifically. RM1 has a homogenous formulation. Next steps may include exploring gradient structures with different kinds of fibres to achieve specific fluid handling properties. Sensitivity tests carried out in this project help eliminate geometric properties which do not significantly contribute to the PVD. Moreover, the most critical geometric properties were also identified. Airlaids tend to have agglomeration of fibres at certain points inside their structures, a modelling concept for which was not probed here. The inclusion of mechanical properties will come as a major step which will allow a better understanding of material behaviour under loads as fluid flows through it. The thesis work also underlines the need for more standardized fibre analysis methods and fundamental data on the fibre geometries from suppliers in order to support modelling for a complete material design process. The limitations of the pore morphology method were also stressed, and methods may be developed to take into consideration the non-uniform pores shapes in the fibre networks. There is scope for improvement in the fibre generation algorithms allowing more control as well as in the BC options available for solvers. It is hoped that the work may help advance the cause of more efficient materials reaching end-users at lower costs in the fast-growing Airlaids and non-wovens industry.
References & Bibliography


References & Bibliography


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Appendix A - Comparison of EJ and LIR Solvers

Domain considered for simulation was 600 x 600 x 400 voxels, 2 μm resolution, with Cellulose and BiCo fibres as in RM1. Permeability Tensors shown below have values in sq. metres.

For the LIR solver, a “relaxation” value of 1 is used, which is a measure of balance between solution stability and speed. “Grid Refinement” is enabled to allow the solver to analyze the velocity and pressure field during the computation and improve the adaptive grid in places where more accuracy is needed. The solver is optimized for speed instead of memory, since memory was not a concern given the computer used for simulations. Permeability Simulations used a 64-bit Linux system with 56 cores, 20 of them running parallelly, with about 500 GB of memory.

<table>
<thead>
<tr>
<th>Error Bound 0.01 on Flow Permeability. No-Slip on Tangential BC</th>
<th>Tolerance 0.01 on Permeability, No-Slip BC along Z, Periodic BC along material plane (Mixed Tangential BCs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LIR Solver</td>
<td>EJ Solver</td>
</tr>
<tr>
<td>2.41129e-10</td>
<td>2.55303e-10</td>
</tr>
<tr>
<td>-4.15563e-13</td>
<td>-6.54774e-12</td>
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<tr>
<td>1.24601e-13</td>
<td>unknown</td>
</tr>
<tr>
<td>-2.2043e-13</td>
<td>unknown</td>
</tr>
<tr>
<td>2.28824e-10</td>
<td>2.3966e-10</td>
</tr>
<tr>
<td>total Run Time: 397.122 s</td>
<td>total Run Time: 8742.926 s</td>
</tr>
<tr>
<td>Error Bound 0.01 on Flow &amp; Tangential Permeability. No-Slip on Tangential BC</td>
<td>Tolerance 0.01 on Permeability. No-Slip on Tangential BC</td>
</tr>
<tr>
<td>2.41104e-10</td>
<td>2.41444e-10</td>
</tr>
<tr>
<td>1.61649e-15</td>
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<td>8.70382e-14</td>
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<td>2.29403e-10</td>
</tr>
<tr>
<td>unknown</td>
<td>unknown</td>
</tr>
<tr>
<td>unknown</td>
<td>unknown</td>
</tr>
<tr>
<td>total Run Time: 772.556 s</td>
<td>total Run Time: 3505.674 s</td>
</tr>
</tbody>
</table>

Take-aways:

- When EJ uses mixed Tangential BCs, LIR predicts permeability about 4% less than the EJ solver. This is because the no-slip BC along the extra pair of surface slows down the fluid flow in the LIR solution.
- For no-slip BC applied along both the tangential directions, the EJ and LIR solvers give similar results.
Appendix B - Sensitivity Test for Domain Resolution

The study aimed to find out if the assumptions made about the minimum required length for the REV hold. Two ADs were made, one at 1 μm/voxel resolution (Reference Domain or RD) and another at a lower resolution of 3 μm/voxel (Test Domain or TD). The TD has the same length as the RD, but with a different number of voxels. In case the TD is of insufficient resolution or length, it should have significantly different results compared to the RD. Also, the study attempted to see the effect of having a lower number of voxels per fibre diameter. Here the BiCo fibres with 15 μm diameters were considered the bottleneck.

Both Domains were built using the RM1 formulation, with a 96 gsm target and dimensions 1.2 x 1.2 x 0.8 mm. No Gaussian Distribution was applied to the fibre widths in the generation process. Permeability Simulations used the LIR solver, with 20 cores running parallelly. Tensors shown are in sq. metres. Other permeability related result values are averages for simulations along both X & Y directions.

<table>
<thead>
<tr>
<th>TD</th>
<th>RD</th>
</tr>
</thead>
<tbody>
<tr>
<td>400x400x267 voxels – 801 μm thick,</td>
<td>1200x1200x800 voxels – 800 μm thick,</td>
</tr>
<tr>
<td>Resolution 3 μm per voxel</td>
<td>Resolution 1 μm per voxel</td>
</tr>
<tr>
<td>Approx. 5 voxels per fibre diameter (BiCo)</td>
<td>Approx. 15 voxels per fibre diameter (BiCo)</td>
</tr>
<tr>
<td>Domain generated in 22.984 s</td>
<td>Domain generated in 294.518 s</td>
</tr>
</tbody>
</table>

Permeability Simulations Results

<table>
<thead>
<tr>
<th>TD</th>
<th>RD</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.17019e-10</td>
<td>1.45422e-13</td>
</tr>
<tr>
<td>-1.72442e-13</td>
<td>2.20131e-10</td>
</tr>
<tr>
<td>-4.90024e-14</td>
<td>-6.3454e-14</td>
</tr>
</tbody>
</table>

| 2.36362e-10 | 1.00688e-12 | unknown |
| 1.29777e-12 | 2.4733e-10 | unknown |
| -6.21792e-14 | -1.56234e-13 | unknown |

Reynolds number 14.8629 for characteristic length 8.33547e-5 m.
Avg Run Time: 58.86 s, 200 iterations
Avg Memory Usage: 1.404 GB

Reynolds number 17.2751 for characteristic length 8.7456e-5 m.
Avg Run Time: 632.03 s, 250 iterations
Avg Memory Usage: 12.765 GB
For Capillarity, only Drainage simulations were carried out since the drainage curve is typically the one changing the most based on changes in the AD.

**Takeaways:**

We don’t see a significant difference in results from TD. Therefore, the assumptions made for the RD are considered valid to use it as the REV. Most studies in this thesis used dimensions and resolution as in the RD here.
Appendix C - Effect of Cellulose Fibre Curl Parameters

The equation (shown below) presented in the section Kink & Curl is studied to determine the effect of the parameters on the fluid handling properties of the material. The parameters $\alpha$ (Local Straightness or LS) and $\beta$ (Global Straightness or GS), and $\sigma$ (standard deviation or a measure of “randomness”) are all defined in $[0,1]$.

$$(d_i^{n+1} - d_i^n) - (d_i^n - d_i^{n-1}) = N_i^{G_o(0)} - \alpha(d_i^n - d_i^{n-1}) - \beta(d_i^n - d_i), \quad i \in \{1,2,3\}$$

The study uses multiple 96gsm, 1000x1000x230 voxel ADs with resolution 3μm/voxel. Formulation from RM1 is used with both cellulose and BiCo fibres. The fibre orientation tensor $\Omega$ as shown in the section Fibre Orientation is applied ($\Omega_{xx} = \Omega_{yy} = 0.45$, $\Omega_{zz} = 0.1$). BiCo fibres are straight or without crimp. For cellulose fibres, given constant values for $\Omega$ and $\sigma = 0.1$, the effect of varying $\alpha$ (LS) and $\beta$ (GS) on the In-Plane Permeability is discussed below. The LIR solver was used for permeability simulations.

![Images of ADs with different fibre straightness](image)

$\alpha = 0.3$

$\beta = 0.3$

Increasing Fibre Straightness and Permeability

Figure 71 ADs identical in all respects except the values entered for Local and Global Straightness. Domains with straighter fibres (B and D) will create less tortuous paths for fluid flow and are therefore more permeable. (Cellulose Fibres are shown in Red. Straight BiCo fibres are shown in Green)
Maintaining a constant non-zero LS value and increasing the GS value increases the permeability. The increasing GS value makes fibres maintain their original orientation as per the defined $\Omega$, so the domain becomes more isotropic in-plane. At the same time, the fibres bend less. During the generation process in simulations as segments are added, the fibres cannot curl around in the network to fill up empty areas easily (see Figure 71). The larger pores therefore allow easier and less tortuous fluid flow. The same effect can be seen when a constant GS value is maintained and fibres are allowed to curl locally by varying the LS value (see Figure 73). Higher local curling leads to a more packed structure (but same porosity and PVD) and lower permeability.

![Permeability - Simulations - GS variation with const. LS](image1)

*Figure 72 Effect of Global Straightness $\beta$ in Cellulose Fibres on Permeability. Increasing Global Straightness leads to higher Permeability.*

![Permeability - Simulations - LS variation with const. GS](image2)

*Figure 73 Effect of Local Straightness $\alpha$ in Cellulose Fibres on Permeability. Increasing Local Straightness leads to higher Permeability.*

However, this linear dependency of permeability on fibre curl breaks down at extreme values of LS and GS. When these parameters are set to 0 or 1, the permeability no longer increases linearly with increasing straightness (see Figure 74 and Figure 75). The extreme value of any one parameter nullifies the effects of any variation made on the other parameter. As an example, with GS set to 1, changes in the local curvature of the fibres do not meaningfully affect the structure. The same behaviour is observed with LS
set to 1 and GS varied (shown in Figure 76). Of course, the extreme case of both LS and GS being 1, or the cellulose fibre being perfectly straight does not exist in nature.

Interestingly, the fibre curl has almost no effect on the PVD of the structure at constant $\sigma$ (see Figure 77), and therefore the Capillary Pressure curves are not affected either (see Figure 79). However, in the exceptional case of the both $\alpha, \beta = 0$, where fibre segments maintain their previous curvature, the PVD is significantly different compared to other structures. The extremely curled up fibres behave almost like spherical particles, and lead to a higher number of large pores in the space around them. This difference reflects both in the permeability as well as the capillarity of the material. The capillary curve is left shifted (larger pores, lower capillary pressure). The permeability, not shown in the comparative figures above is well above all other structures at $2.23 \times 10^{-10}$ sq. m.
Figure 76 GS varied at an extreme LS value of 1.0 does not meaningfully change the straight cellulose fibres in the domain. (Red: Cellulose, Green: BiCo)

PVD - Effect of LS and GS in Cellulose Fibres

Figure 77 PVD for variations in Local Straightness (ls) and Global Straightness (gs) in Cellulose Fibre. All cases seem to have overlapped curves except where LS and GS are both set to 0.
Appendix C - Effect of Cellulose Fibre Curl Parameters

Figure 78 The Extreme Curly Fibre Case with both LS and GS set to 0. Red: Cellulose, Green: BiCo

Figure 79 Effect of fibre straightness parameters on Capillary Pressure curves of the RM. LS is Local Straightness, GS is Global Straightness. Some extreme values are shown here. Interim LS/GS values in the range [0,1] behave similarly. Imbibition and Drainage Curves for the same LS/GS set are shown with a common colour.

Changing the Standard Deviation or Randomness value $\sigma$ applied to the domain generation process distributes the possibility of the fibres curling up. However, since this distribution is in both the positive and negative directions around a common mean value, the net result on the structure is no change. The fibers are able to change their direction from one segment to the next during the generation process. But this change is isotropically distributed in-plane based on the Fibre Orientation Tensor $\Omega$. 
Figure 80 Minimum effect of Randomness (R) as the Fibre Curl Parameter on the Capillarity of the RM. LS - Local Straightness, GS - Global Straightness. 0.1 and 0.9 are applied as Randomness values to 2 domains identical in all other respects.

Takeaways:

➢ Global and Local Straightness are pure simulation parameters lacking any direct physical meaning. However, in order to reliably generate virtual domains close enough to the RM, it is important to understand their effect on the fluid handling properties. Cellulose fibres which are curly in general can also flatten out as part of the manufacturing process. It would be interesting to explore if curly fires, in general, remain curly within the RM once it is air laid.

➢ The curl parameters do have an influence on the in-plane permeability of the material. In other words, the curliness of the fibre influences the IPRP. Importantly, varying the parameters $\alpha$ and $\beta$ can be seen as a way to influence the permeability of the raw material without affecting its PVD and capillary pressure curves. This translates to selecting between straight or curly fibres. However, it should be kept in mind that the changes in permeability arising out of this approach might be extremely low. In this study, the differences were in the order $0.1 \times 10^{-1}$ sq.m.
Appendix D – Effect of BCA on Fluid Handling Properties

The effect of having different Binder Contact Angles or BCAs is studied. 4 ADs identical in all respects are generated with the following configuration: 500 x 500 x 500 voxels, 1 μm/voxel, 90 gsm, made purely from curved cellulose fibres. To 3 of these domains, 10 gsm of Binder was added using the Add Binder function within the ProcessGeo module in GeoDict. The material is added in the shape of a concave meniscus in locations where surfaces in the structure’s material get close together [84]. Based on analytic data available to the computer, the algorithm can discern the lumens of cellulose fibres from normal pore spaces and does not add binder inside them. The density of the binder material is taken as 1.7 g/cm³ from information provided by the Latex supplier for RM1. Binder is distributed uniformly throughout the structures using BCAs of 0 (perfectly wetting), 30 and 60 degrees.

In case of the domain with BCA 0°, there was an error and the binder addition process did not properly converge. 12.56 gsm of binder was added instead of the target 10 gsm. The problem was not solved despite multiple binder addition iterations.

![Capillary Pressure - Simulations - Effect of varying BCA](image)

Figure 81 The effect of varying Binder Contact Angles on Capillarity. Imbibition and Drainage have the same colour for each domain. Two abnormalities are noticed – the 90% saturation limit in imbibition curves, and the deviating Imbibition curve for BCA0.

At 10 gsm of Binder in an AD, the effect on Capillarity only seems to be at lower saturations (50% and below). As Binder is added to the domain, the curves shift left. This can be understood as the binder filling up small pores and leaving only larger ones which have a lower capillary pressure. The limitation here is the way the computer interprets the pores as per the Pore Morphology Method explained in section 4.1 Capillary Pressure, by attempting to fit spheres in open spaces. Unlike when new fibres are added, the binder does not create new small pores at its interface with the fibre surfaces. The specific variation within capillarity at lower saturations with varying BCA could not be fully understood. Moreover, the imbibition calculations seem to have a bug – they stop at about 90% saturation of the wetting phase. This could not be fully explained.
For permeability, the effect is simpler to interpret. Adding binders reduces the in-plane permeability of the material. It should be noted that the binder here is distributed uniformly throughout the material and not just on the top and bottom surfaces. The different contact angles do not seem to affect permeability substantially.

The singular case of the AD with BCA 0° can be seen as a deviation due to the errors in the binder additions process. The higher binder added to the domain leads to a lower permeability as compared to other domains with binder. Denoted by blue capillary pressure curves in Figure 81, its behaviour deviates slightly during imbibition at low saturation.

**Takeaways:**

- Addition of binder to the domain closes the small pores and tends to shift the Capillary Pressure curves left (a larger fraction of big pores overall in the PVD)
- Binder Contact Angle has no major influence on MAP and MDP. Its effect on capillary simulated pressure curves at low saturation remains to be investigated.
- Binder addition reduces the permeability of the material. The effect is not very different for the different BCAs.