A Study on the Structure of Paper: The Links between Paper and Fibre Properties

by

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Abstract

The work shown in this thesis, focuses on the effects of fibre geometry (fibre length, width and coarseness) to the paper strength and bulk. It is believed that fibre networks, for a given furnish, can be optimized through fractionation to create a stronger and bulkier paper. A first set of experiments was performed to determine the correlations among fibre properties of a softwood kraft pulp furnish. The fibre properties were measured using a Fibre Quality Analyzer (FQA). Coarseness ($\omega$) and width ($D$) were found to increase linearly with length ($L_f$). These correlations are thought to be influenced by the tree species and the pulping process. A second set of experiments was aimed to determine empirical expressions of bulk and tensile index ($TI$) in terms of the fibre geometry distribution ($\omega$, $L_f$ and $D$) and the press-drying pressure ($P$). Bulk and $TI$ was measured for handsheets made at different pressures from different size distributions. These distributions were created by a combination of fractionation on a Bauer McNett Classifier (BMC) and fibre cutting. The determined relations show agreement with experimental work from other researchers. In order to provide insight into the causes of such behavior, simulations of two-dimensional (2D) and three-dimensional (3D) random networks were performed. Matlab was used to write the simulation codes. Mechanical response of fibres (affected by the fibre geometry) to the forces induced by drying or pressure is not considered directly in the simulations. However, 2D simulation models are a good representation of high press-drying conditions and high fibre flexibility, whereas 3D models are better predicting air-dried (low pressure) paper made from fibres of high rigidity. Geometric statistics of random networks explain some of the experimental observations. The statistical outputs of the 2D simulations were; network coverage ($e$), network thickness ($\tau_N$), number of fibre crossings ($N_c$) and the relative bonded area ($RBA$). In the case of 3D simulations, only $\tau_N$ was determined. The 2D and 3D outputs were measured for different fibre size distributions ($L_f$, $D$ and $\omega$).
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Nomenclature

\[ A_c \quad \text{Fibre cross-sectional area} \]
\[ A_p \quad \text{Pixel area} \]
\[ b \quad \text{Bond strength} \]
\[ BW \quad \text{Basis Weight} \]
\[ \beta_D \quad D \text{ exponential coefficient (TI fit)} \]
\[ \beta_L \quad L_f \text{ exponential coefficient (TI fit)} \]
\[ \beta_\omega \quad \omega \text{ exponential coefficient (TI fit)} \]
\[ \beta_P \quad P \text{ exponential coefficient (TI fit)} \]
\[ \beta_\sigma \quad \sigma \text{ exponential coefficient (TI fit)} \]
\[ C \quad \text{Pulp consistency} \]
\[ c \quad \text{Coverage} \]
\[ \bar{c} \quad \text{Average coverage} \]
\[ C_B \quad \text{Bulk fit coefficient} \]
\[ CI \quad \text{Curl index} \]
\[ C_f \quad \text{Fibre chord} \]
\[ C_T \quad \text{TI fit coefficient} \]
\[ D \quad \text{Fibre width} \]
\[ \bar{D} \quad \text{Mean fibre width} \]
\[ D_o \quad \text{Wet fibre width} \]
\[ \delta \quad \text{Paper strip width} \]
\[ F \quad \text{Breaking force} \]
\[ f \quad \text{Dried fibre voids fraction} \]
\[ f(x) \quad \text{Probability density function} \]
\[ \tilde{f}(x) \quad \text{Weighted probability density function} \]
\[ \phi \quad \text{Collapse index} \]
\[ g \quad \text{Acceleration of gravity} \]
\[ GSM \quad \text{Paper grammage} \]
\[ \gamma_D \quad D \text{ exponential coefficient (bulk fit)} \]
\[ \gamma_L \quad L_f \text{ exponential coefficient (bulk fit)} \]
\[ \gamma_\omega \quad \omega \text{ exponential coefficient (bulk fit)} \]
\[ \gamma_P \quad P \text{ exponential coefficient (bulk fit)} \]
\[ LWL \quad \text{Length weighted average length} \]
\[ \mu \quad \text{Distribution mean value} \]
\[ N \quad \text{Number of pixels} \]
\[ N_{fc} \quad \text{Number of fibre crossings} \]
\[ N_f \quad \text{Number of fibres} \]
\[ \omega \quad \text{Fibre coarseness} \]
\[ P \quad \text{Press-drying pressure} \]
\[ P_{MAX} \quad \text{Maximum pixel value} \]
\[ P(x_j) \quad \text{Probability of bin } j \]
\[ P(x,y) \quad \text{Pixel value distribution} \]
\[ RBA \quad \text{Relative bonded area} \]
\[ \rho_f \quad \text{Fibre density} \]
\[ S \quad \text{Fibre chord length} \]
\[ \sigma_D \quad \text{Width standard deviation} \]
\[ T \quad \text{Breaking length} \]
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Chapter 1

Introduction

Paper is made mostly from wood fibres. Wood fibres are obtained by the pulping process of wood chips. In the wood chips, lignin, a glue-like substance holds the fibres together. By the use of mechanical forces or chemicals, the chips are converted into individual fibres. Through this process, water is added to form a fibre-water mixture that is dried to make paper. Figure 1.1 and Figure 1.2 show the top view and cross-section of a standard handsheet made from softwood pulp.

![Micrograph](image)

**Figure 1.1:** Micrograph (obtained using light microscopy) of the top side of a standard kraft pulp handsheet. The ribbon-like structures are collapsed wood fibres, held together by hydrogen bonds.

1.1 The Structure of Pulp Suspensions, Wet Webs and Paper

A pulp suspension is a mixture of water and wood fibres. Ideally the fibres are sufficiently dispersed so that a small volume of the suspension is representative of the entire mixture. Consistency (C) is
commonly used to describe pulp suspensions. It is defined as the mass ratio of dry wood fibres to the total mass of the suspension:

\[
C = \frac{\text{Dry Fiber Mass Contained in Suspension}}{\text{Total Mass of Suspension}} \times 100
\]  

(1.1)

Even at low consistencies, fibres have a tendency to cluster or flocculate due to fibre-fibre attractive forces. At very low consistencies, fibres (or fibre flocs) do not form a single connected structure. The way to characterize the connectivity or the formation of a fibre network is through the crowding number described by Kerekes and Schell [13].

As consistency is increased (approximately 30%) the mixture is no longer described as a suspension but as a wet web. In a wet web all the fibres are connected. There may not be physical contacts between the fibre surfaces, but the distance is small enough that the surrounding fibres interact constraining the motion of the fibre. However, in wet webs, consistency is low enough so that air and water is still present in the voids between fibres. The forces providing the bonding of the structure are, in this case, from surface tension. Lyne and Gallay [14], found that as water is removed from the web it became stronger. They attributed the increase in strength to the increase of the air-water interface caused by the removal of moisture. Nevertheless, they found that a further decrease in moisture content (approximately 35%), can actually reduce the amount of air-water interface making the web weaker.

At higher consistencies (>90%) the structure can be defined as paper. As was previously stated, an increase in consistency reduces the surface tension bonding forces. However, in the case
of paper, strength increases because the nature of the bonds changes. In paper, distance between fibre surfaces is below 0.2 \( \mu m \). This allows hydrogen bonding, stronger in nature than surface tension, to act as the connecting mechanism between fibres. Hydrogen bonding is what provides the strength of paper and makes it unique from other nonwovens. For example, in fibre glass, fibres do not form hydrogen bonds and need the aid of a bonding substance or glue.

1.2 Fibre Morphology and Fibre Properties

If a piece of paper, or a pulp suspension was observed through a microscope, two different things may be perceived. The observations will depend on the pulping process. There are basically two types of pulping processes; mechanical pulping and chemical (or kraft) pulping. The main difference between the two is that lignin, a substance present in the tree to hold the fibres together, is removed in the kraft process. Kraft pulp fibres tend to have a cylindrical shape with a hollow lumen through its centerline. A dark field micrograph of a kraft pulp fibre is shown in Figure 1.3. As the fibres are conformed into the paper, the hollow cylinders shape into flattened ribbons because of the high flexibility. On the other hand, mechanical pulp fibres present in a suspension may seem more rectangular than cylindrical, yet still having a lumen. This is because of the presence of lignin in mechanical pulp fibres. This compound fills the voids between fibres in the tree making the cross-section rectangular. Furthermore, mechanical fibres being more rigid because of the lignin, remain rectangular after drying. They will only collapse into ribbons if the flexibility is increased through refining or the cell wall is thin enough. Figure 1.4 shows the cylindrical and rectangular fibre models.

![Figure 1.3: Micrograph (obtained through light microscopy) of a kraft pulp fibre. The fibre is in a water solution. At this state the fibre is swollen and has a cylindrical shape. The lumen is irregular in size and changing along the length of the fibre.](image)
Figure 1.4: Fibre geometric models. Kraft pulp fibres in a suspension are cylindrical (left figure). Mechanical pulp fibres tend to remain rectangular (right figure). However, after drying, both can be modeled as rectangular because of the high collapse index ($\phi$) of kraft pulp fibres due to their low lignin content.

The collapse index ($\phi$) characterizes the degree in which fibres collapse after drying. It can be measured using confocal laser scanning microscopy (Jang et al. [7]). It is defined as:

$$\phi = 1 - \frac{LA}{LA_o}$$

where $LA$ and $LA_o$ are the cross-sectional areas of the lumen, before and after drying respectively.

When observing the fibres along their length, it is realized that fibres are not straight but are curled sometimes having kinks. A depiction of a curled fibre is shown in Figure 1.5. A way to characterize the amount of curl of a fibre is by the dimensionless curl index ($CI$) defined as:

$$CI = \frac{S}{C_f} - 1$$

Where $S$ is the curved length and $C_f$ is the chord.

Another important fibre property is coarseness ($\omega$). It is defined as the ratio of the fibre mass to its length:

$$\omega = \frac{M_f}{L_f} \left[ \frac{mg}{m} \right]$$

The properties described are for a single fibre. Since in a pulp suspension there is a combination
of fibres of different properties, distributions and average values are used. Most of these properties can be measured quickly using a Fibre Quality Analyzer (FQA). However, FQA measurements are for fibres in a suspension. These properties will change when fibres are dried. Accurate, yet time consuming methods exist to determine these properties in the final state of paper (Chinga-Carrasco [1]).

1.3 A Brief Description of the Paper-making Process

A description of the paper-making process is shown in Figure 1.6. The pulp suspension is created by separating the fibres in the wood chips by a mechanical (mechanical pulp) or chemical (kraft pulp) process. After that, paper is made by draining water from the suspension. This is done through a screen or a wire. On a paper machine the suspension flows through a headbox aligning the fibres to some extent followed by a dispersion from a rectangular jet to a moving wire. The result is an isotropic structure due to the preferred fibre orientation (machine direction). In the case of standard handsheets, the procedure is different. Water is drained vertically in a batch process and the fiber orientation is random. However, in both cases, the position of the fibre centers on the wire are not randomly distributed. This is due to phenomena known as flocculation. This is the clustering of fibers caused by electrostatic and possibly other weak fiber attractive forces. It causes an uneven distribution of fibers in the forming wire and is a source of paper weakness. As water is drained by suction and/or gravity the consistency increases to 20% and the force providing the connectivity of the web is mostly surface tension.
Figure 1.6: Flow diagram of the paper-making process (commercial and standard handsheet). After the fibres are separated from the wood chips to form a suspension, water is taken from the mixture by a combination of gravity, suction, pressure and heat.
The process to follow in paper-making is press-drying. In the case of the paper machine, this is done by sets of rolls that apply pressure as the web goes through the gap between the rolls. In handsheet-making, the process is done through a vertical press. Two circular discs remove water by compressing the paper. In the press-drying process, there is further dewatering. The fibers slide and pack to a denser structure. The consistency is increased up to 50% depending on the pressure and residence time. At this stage, it is believed that fibers remain similar to hollow cylinders and that water is still contained inside the lumen.

The final step in the paper-making process is drying. This is done by heated rolls in the paper machine. In contrast, standard handsheets are left to air-dry at a controlled temperature and humidity. After drying, consistency reaches 93% as there is still water contained within the fiber cell wall. At this stage, if the structure is observed in a microscope, many of the fibers will appear similar to flattened ribbons instead of hollow cylinders. Fibres have the tendency to collapse by dewatering and by surface tension forces. The tendency to collapse is a function of the fibre thickness and fibre flexibility (Paavilainen [20]). A similar phenomena is observed when drinking liquid from a very thin wall straw. The low pressure, in this case caused by our lungs, collapses the straw. However, when we stop drinking, the straw recovers to its original shape. In the case of fibers, as the gap between the inner surfaces reduces, hydrogen bonding and other weak bonds (Van der Waals) prevent it from recovering. The outer surface tension acts in a similar way bringing different fibers together followed by hydrogen bonding. As it was stated in the first section of the chapter, the hydrogen bonding is present only when the distances among the surfaces is less than 0.2 \( \mu m \). At consistencies lower than 90%, water surrounds the fibers and the lumen, preventing these types of bonds from forming. Similar to the analogy of the collapsing straw, some fibers may be too rigid to collapse and prevent hydrogen bonding. Thinner fibers collapse easier than thicker fibers. The composition of the fibers also affects collapsibility. Mechanical pulp fibers tend to collapse less because the lignin in the lamellas of the fibers increase rigidity. Kraft pulp, on the other hand, is highly collapsible because of the low lignin content. Another source of collapsibility increase is refining. In this process, fibres are delaminated and fibrillated by the action of rotating discs that compress the fibres as the suspension flows through the discs.

The result of the forming process described is a structure that is mostly two-dimensional. This is because fibers have high aspect ratios and are more likely to lay flat on the mat. Microscopy measurements show that fibres are aligned between 1 to 3 fibres thick along the plane of the mat. Difference between the structure and the two-dimensional approximation is apparent as we increase the basis weight and as the shape of the fibers deviates from the ribbon-like structures of highly collapsible fibers.
1.4 Fibre and Paper Properties

It seems reasonable to say that the properties of paper should depend on the properties of the fibres that constitutes the paper and on the process used to consolidate the structure. The following are common paper properties used in the pulp and paper industry:

1.4.1 Property Distributions

A tree is composed of fibres of different shapes and sizes. The seasons affect the tree growth such that during the winter, fibres grow smaller in length and cross-section than they do during the spring. This is to accommodate the different rates of liquid transport. Furthermore, pulp mills will use wood chips from different species. Fibre properties are known to change among species and by the pulping process used by the mill (USDA [23]). Softwood trees, such as pines, tend to have longer fibres than hardwood trees like birch or maple. When all these fibres are mixed together in the pulping process, the result is a pulp suspension that has a distribution of size properties (length, width and fibre wall thickness). These properties are known to affect the paper properties.

The natural question that arises is; what statistical value is a representative quantity to predict the paper behavior? An arithmetic mean of the property distribution does not correlate strongly with the properties. However, length-weighted average, show better correlation. This is because of the strong weight dependency and the fact that the fibre mass for the most part is linearly proportional to its length.

We should now introduce the length-weighted average length ($LWL$):

$$LWL = \frac{\sum L f_i^2}{\sum L f_i} \tag{1.5}$$

where $L f_i$ is the length of the $i$th fibre in the distribution.

Similarly for all other properties $\gamma$, such as width and wall thickness:

$$LW\gamma = \frac{\sum \gamma_i L f_i}{\sum L f_i} \tag{1.6}$$

where $\gamma_i$ is the fibre property of the $i$th fibre in the distribution.

In the case of Probability Density Functions (PDF), we can compute the mean and variance in the following way:

$$\mu = \int_{-\infty}^{\infty} f(x) \cdot x \, dx \tag{1.7}$$
\[ \sigma^2 = \int_{-\infty}^{\infty} f(x) (x - \mu)^2 \, dx \quad (1.8) \]

\( L W L \) can be calculated by applying equation 1.7 to the length-weighted distribution \( \bar{f}(x) \) defined as:

\[ \bar{f}(x) = \frac{1}{\int_{-\infty}^{\infty} f(x) \, x \, dx} \cdot f(x) \cdot x \quad (1.9) \]

The unity-weighted distribution can be calculated from the inverse transformation of the length-weighted distribution:

\[ f(x) = \frac{1}{\int_{-\infty}^{\infty} \bar{f}(x) \, dx} \cdot \frac{\bar{f}(x)}{x} \quad (1.10) \]

The previous equations (1.7 to 1.10) can be used for discrete probability in bins by changing \( f(x) \, dx \) to \( P(x_j) \) and \( \int_{-\infty}^{\infty} \) to \( \sum_{j=1}^{N} \). \( P(x_j) \) is the probability of bin \( j \).

### 1.4.2 Basis Weight

It is the ratio of the dry fibre mass to the flat area that the fibres cover and commonly reported in grams per square meter.

\[ BW = \frac{\text{Total Dry Fibre Mass}}{\text{Area}} \quad \text{[g m}^{-2}] \quad (1.11) \]

### 1.4.3 Paper Strength

The paper strength is usually characterized by the tensile index (\( TI \)). Other measures of strength are the tensile energy absorbed (\( T EA \)) and the breaking length (\( T \)). The tensile index is defined as follows:

\[ TI = \frac{F}{\delta BW} \quad \text{[Nm g]} \quad (1.12) \]

where \( F \) is the breaking force, \( \delta \) is the strip width, and \( BW \) is the basis weight in \([g m^{-2}]\). The testing is performed in a horizontal tester that holds the paper strip with pneumatic clamps. The tester records the force as a standard specimen is pulled apart. A standard specimen has a length of 10 cm and a width of 15 mm.

\( TI \) is divided by \( BW \), since increasing the total fibre mass will increase the strength. In most cases, this division allows comparison of strength of papers with different \( BW \). However, the comparison is not always valid. IAnson et al. [6] has found that for a given furnish, \( TI \) changes
with $BW$, and has an optimal value where it reaches a maximum.

### 1.4.4 Fibre Strength

The fibre strength is usually measured through the Zero Span Tensile Index ($ZI$). The testing apparatus is very similar the one used for measuring $TI$. However, for $ZI$ the initial distance between the clamps is very small ($< 1 \text{ mm}$). Thus, when the strip is pulled apart, the fibres break instead of the bonds. The value is obtained using the same equation for $TI$ (equation 1.12) except that by reducing the span, the recorded breaking force is usually higher. $ZI$ is also affected by the clamping force of the sample. If the pressure is too low, the strip will slide recording a low value. If the pressure is too high, damage will be done to the fibres such as to reduce the required breaking force. Thus, the value that should be reported is the maximum obtained by changing the clamping pressure.

### 1.4.5 Paper Thickness and Bulk

Calliper or paper thickness is measured with a micrometer applying a very low pressure ($< 5 \text{ psi}$). The measurement is done at different points of the sample and an average value is recorded. The bulk of the paper refers to the apparent density of paper. It is calculated as the ratio of the calliper to the basis weight of the sample:

\[
Bulk = \frac{\text{Paper Thickness}}{BW} \left( \frac{\text{cm}^3}{g} \right)
\]  

(1.13)

### 1.4.6 Relative Bonded Area

As was previously mentioned, fibres are joined to others fibres in the network through hydrogen bonding. When the paper is forced in tension, usually the bonds will start breaking before the actual fibres. However, it depends on how the strength of the fibre compares to the strength of the bond. Additionally during breakage, the stress can redistribute in such a way that even though bonds started breaking, the fibres will break as well. A way to characterize the degree of bonding is through the relative bonded area ($RBA$) defined by equation 1.14.

\[
RBA = \frac{\text{Total Bonded Surface}}{\text{Total Available Surface for Bonding}}
\]  

(1.14)
1.5 Brief Summary of Determined Models and Studies on Paper and Fibre Properties

For many years, researchers have tried to relate the fibre properties to the paper properties. Unfortunately, the final product is highly dependent on the complex forming process. Therefore, an applicable model that perfectly relates the paper to the fibres and the process has not been fully developed. Nevertheless, there have been great contributions. A solution to the problem seems closer due to the growing capabilities of computers and simulations.

1.5.1 Experimental Predictions

O’neil et al. [19] studied hardwood fibres and experimentally found that tensile index was linearly proportional to length. They did not find any dependency with other dimensional fibre properties. The explanation of the increase in tensile index was attributed to the increase in probability of the fibre-to-fibre bonds along the length of the fibre. However, the length variation in their study, was less than 200 \( \mu m \).

Clark [2] studied mixtures made from sulphite pulp and viscose fibres and determined through regression that the tensile index and bulk behaved as follows:

\[
TI \sim \omega^{-0.6} L_f^{0.5} \\
\text{Bulk} \sim \omega^{0.15} L_f^{0.05}
\]

(1.15)

(1.16)

where \( \omega \) is the fibre coarseness and \( L_f \) is the length-weighted fibre length (LWL).

1.5.2 The Page Equation for Strength

Page [21] developed a semi-empirical formula to describe the tensile strength of paper. It is known as the Page equation and is shown as equation 1.17.

\[
\frac{1}{T} = \frac{9}{8Z} + \frac{12 A_c \rho_f g}{b P_f L_f (RBA)}
\]

(1.17)

where:
- \( T \) is the breaking length
- \( Z \) is the zero span breaking length
- \( A_c \) is the fibre cross-sectional area
The Page equation can be expressed in terms of the tensile index by multiplying the breaking length by the acceleration of gravity \( g \). This would lead to equation 1.18

\[
T I = \frac{\frac{8}{3} b L_f RBA}{3 b L_f RBA + \frac{4 A_c \rho_f ZI}{P_f}} ZI
\]

(1.18)

where \( T I \) and \( ZI \) are the tensile index and zero span tensile index respectively. Unfortunately, the use of this equation is limited due to the fact that some of the variables are difficult to measure. Additionally, the variables are interdependent in a complex way.

For constant bond force \( b \), and constant zero span tensile index \( ZI \), this is an equation of the following form:

\[
T I = \frac{ax}{bx + cy} ZI
\]

(1.19)

where \( x = (L_f RBA) \) and \( y = \frac{A_c}{P_f} \).

Under the assumption that zero span tensile index \( ZI \) is independent of length, the page equation shows that paper strength increases linearly for small values of length and at a slower rate at higher lengths. It grows with length from zero reaching asymptotically a fraction of the zero span tensile index \( \left( \frac{g}{b} = \frac{8}{3} \right) \). This holds true under the additional assumption that \( RBA \) is independent of length.

A prediction of the behavior of tensile index with coarseness and width is difficult to obtain from equation 1.18 because \( RBA \) is itself a function of the fibre coarseness, width, and collapsibility.

### 1.5.3 Statistical Models and Computer Simulations

If several assumptions and simplifications are made, then the fibre network complexity can be reduced to the point where we can explain the behavior and run simulations to construct a network. More assumptions translates into more limitations in the model.

A network can be considered to be composed of a determined distribution of fibres. They
can be collapsible, flexible and hollow tubes with cross-section varying along the chord of the fibre. A three-dimensional (3D) simulation can then be performed. However, this would take a considerable amount of effort, not only in the code development but also in computer processing time. The simplest of the models would be to consider fibres, rectangles of a constant shape and where all the fibres would have the same shape. The justification of the simplification in shape is the tendency of fibres to collapse into a ribbon-like structures. A two-dimensional (2D) model may seem unrealistic. However, it can predict valuable information on the paper structure.

Additional to the complications arising from the shape and distributions of the fibres, the way in which the network is constructed should also be considered. Deposition of the fibres strongly depends on the flow characteristics and the paper-making process. In a paper-making machine, there is a strong fibre alignment in the machine direction caused by the headbox jet, whereas in a standard handsheet-maker the fibre direction is random because of the vertical drainage. Nevertheless, in both cases there is flocculation effects in which the fibre center positions are correlated. If the suspension is very dilute and the formation process is fast enough, the flocculation effects can be minimized. Under all these simplifications, a fibre network can be considered to be a two-dimensional random network.

Because of the paper’s random nature, it is not surprising that there is considerable amount of work done by mathematicians and statisticians. Kallmes, Benier and Perez have published several technical papers relating fiber geometry and coverage of two-dimensional (2D) networks to statistical values that may be linked to the paper mechanical properties (Kallmes and Corte [10], Kallmes and Bernier [9], Kallmes et al. [11]). Their theory became known as the KBP theory. Related work on the two-dimensional (2D) paper structure can also be found in the book of M.Deng and Dodson [16].

In order to understand the modeling of paper as a 2D random fibre network, we must introduce some concepts from the literature that define the random network.

**Coverage**

Coverage ($c$), as shown in equation 1.20, is defined as the ratio of area covered by the fibres projected into the sample sheet, to the area of the sample sheet. It is important to notice that coverage includes the total area of fibres, not only the projected area. Hence, a coverage value greater than unity is possible.

\[
c = \frac{\text{Fibre Area}}{\text{Sample Sheet Area}}
\]  

(1.20)
The basis weight, \( BW \), and the coverage, \( c \) are easily related:

for a sample made from fibres of the same thickness, \( \tau_f \):

\[
BW = \frac{\text{Fibre Area} \ \tau_f (1 - f) \ \rho_f}{\text{Sample Sheet Area}}
\]  \hspace{1cm} (1.21)

where \( f \) represents the voids fraction of the fibre and \( \rho_f \) the fibre density. A common practice is to assume a fibre density of 1200 \( \text{kg/m}^3 \) instead of 1500 \( \text{kg/m}^3 \), and a value of zero for the voids fraction.

Equation 1.21 can be written in terms of the coverage using equation 1.20 as follows:

\[
BW = c \ \tau_f (1 - f) \ \rho_f
\]

\[
c = \frac{BW}{\tau_f (1 - f) \ \rho_f}
\]  \hspace{1cm} (1.22)

It should be noted that \( f \) and \( \tau_f \) are functions of the fibre cross-section in the wet state (\( \omega \) and \( D_0 \)) and the fibre flexibility. Decreasing coarseness, \( \omega \), will result in reducing fibre thickness, \( \tau_f \), (if fibres are collapsible) or increasing the voids fraction, \( f \) (if fibres do not collapse). Thus, regardless of fibre collapsibility, reducing the fibre coarseness will increase the coverage.

One important relation shown by the KBP theory and also by M.Deng and Dodson [16] is that \( RBA \) of a random 2D network depends only on the average coverage (\( \hat{c} \)). They showed that it can be approximated by the following equation:

\[
RBA = 1 - \frac{(1 - e^{-\hat{c}})}{\hat{c}}
\]  \hspace{1cm} (1.23)

Another important parameter of a 2D network is the number of fibre-to-fibre contacts or crossings. The expected density of crossings, \( \mu \), for low coverage is given by M.Deng and Dodson [16]:

\[
\mu = e^{-\hat{c}} \frac{\pi \hat{c}^2}{4 D^2} \left( \frac{1}{2} + \frac{\hat{c}}{3} \right)
\]  \hspace{1cm} (1.24)

where \( \hat{c} \) is the average coverage and \( D \) is the fibre width.

In three dimensions (3D), Gates and Westcott [4] using a orthogonal fibre model, estimated the
bonded area in terms of the fibre coverage and flexibility. One of the most common 3D models mentioned in literature, was developed by Nilsen et al. [17] and coding of a similar model is explained by Conceio et al. [3]. It consider fibres to have a flexible parameter. Fibres are deposited vertically and as the fibre encounters the network, they bend following a flexing rule.

### 1.6 Research Purpose

It is believed that, if it is possible to determine the effect of fibre geometry to the paper properties, the fibre network can be optimized. Paper properties can then be enhanced by fractionation. The objective of the work presented in this thesis is to determine the effects of fibre geometry on the paper strength and bulk. The methods used to determine this relation will be experimental and by computer generated simulations.

Predicting the properties of paper experimentally is proven to be a very difficult task. The difficulties arise from the numerous fibre properties (dimension and shape, flexibility, collapsibility, bond strength, pulp freeness) and process variables (flocculation, pressure, jet and wire speeds, etc.) that affect the final paper product. Other studies have determined fibre geometry effects by using different pulps. However different types of pulp differ in other properties besides shape, such as flexibility and chemistry, that can affect bond strength and collapsibility and therefore affect the results. This may be the reason why the literature is not consistent as to the effects of the fibre geometry to the paper properties. Furthermore, the closest empirical formula (Page equation) is an expression that requires knowledge of properties of the final paper. Experimentally we will study a single pulp furnish so that the differences in behavior can only be attributed to the difference in geometry and process variables.

Experimental results are supported by computer simulations. There have been simulations done by other researchers, using a Lagrangian approach to solve the motion of fibres constructing the fibre mat. However, fibre-to-fibre effects are usually neglected because of the complications in the differential equations. A complete simulation considering the fibre to fibre effects has great computational costs. In the simulation studies presented here, the goal was to determine the statistics of fibre networks without involving the mechanics of the process.
Chapter 2

Predicting Bulk and Strength of Paper

In this chapter, the relations of bulk and strength to fibre geometry (length, width and coarseness) and press-drying pressure are determined. This is done by producing handsheets from different fibre geometry at different pressures. The pulp used was softwood kraft pulp. This type of pulp provided a broader range of lengths compared to hardwood pulps. Kraft pulp was preferred because of the lower presence of fines.

2.1 Experimental Procedure

Three hundred (300) grams of softwood kraft pulp was fractionated using a Bauer Mcnett Classifier (BMC) into five fractions (M14, M28, M48, M100 and M200). The coarseness, length, width and curl index of all fractions and feed pulp was measured using a Fibre Quality Analyzer (FQA). Only the M14, M28 and M48 fractions together with the feed were used for making handsheets as the mass of the collected samples of the finer screens (M100 and M200) was not enough to make handsheets. The handsheets were made at different press-drying pressures while others were air-dried. Some of the air-dried handsheets were cut using a guillotine into small squares and repulped. The cutting was done in a 1 mm and 3 mm grid pattern to reduce the fibre length. By doing this different values of fibre length were obtained at a constant coarseness. Length, width and curl index of the cuts was measured. From the repulped cuts, handsheets were made at different press-drying pressures. The residence time in the drying press was five (5) minutes for all samples. After handsheets were air-dried at controlled humidity and temperature, they were tested for bulk and tensile index. Figure 2.1 shows a diagram of how the pulp was fractionated and cut to prepare the handsheets.
Figure 2.1: Flow diagram of experimental procedure. The original feed pulp was separated into five fractions. Handsheets were made at different pressures from some of the fractions (Feed, M14, M28 and M48). Air-dried samples were cut and repulped to create new handsheets. Tensile index and bulk for all handsheets was recorded and fibre properties were measured for all fractions.

2.2 Assumptions and Limitations

The results obtained from the experimental procedure described here are valid under certain assumptions.

- By air-drying the handsheets there should be no drying effects (Jentzen [8]) since the drying is done under minimum load. Therefore, after cutting, fibres have the same properties as before being cut except for the decrease in length.

- Fibre size distributions are assumed to be sufficiently narrow so that the average values can be representative of the distribution.

- The pulp used is a mixture of softwood species. It is assumed that during the fractionation
process, the species are not separated as to affect the data by a difference in flexibility, or any other property that may differ from one species to the other. Thus, the observed differences account exclusively for changes in the geometry.

- A minimum of three (3) handsheets were prepared for the evaluation of handsheet properties. The errors for bulk and strength were calculated, assuming T-Distribution and propagation of error.

Table 2.1: Size and ω measurements of different pulps obtained from FQA. Errors are from standard deviation between FQA measurements. The table shows consistent correlations among all properties (increasing $D$ and $ω$ with $L_f$) except for CI. Fibre cutting or fractionation did not affect CI significantly.

<table>
<thead>
<tr>
<th>Mesh Size</th>
<th>Length, $LWL$ (mm)</th>
<th>Fibre Width ($μm$)</th>
<th>Curl Index</th>
<th>Average Coarseness ($mg/m$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original Pulp</td>
<td>2.4 ± 0.2</td>
<td>28 ± 1</td>
<td>0.17 ± 0.01</td>
<td>0.20 ± 0.01</td>
</tr>
<tr>
<td>-(coarse cut)</td>
<td>1.50 ± 0.08</td>
<td>-</td>
<td>0.105 ± 0.007</td>
<td>-</td>
</tr>
<tr>
<td>-(Fine cut)</td>
<td>1.2 ± 0.1</td>
<td>-</td>
<td>0.10 ± 0.01</td>
<td>-</td>
</tr>
<tr>
<td>14 Mesh</td>
<td>3.66 ± 0.03</td>
<td>31.5 ± 0.3</td>
<td>0.186 ± 0.006</td>
<td>0.257 ± 0.004</td>
</tr>
<tr>
<td>-(coarse cut)</td>
<td>2.33 ± 0.07</td>
<td>-</td>
<td>0.124 ± 0.004</td>
<td>-</td>
</tr>
<tr>
<td>-(Fine cut)</td>
<td>1.51 ± 0.02</td>
<td>-</td>
<td>0.092 ± 0.004</td>
<td>-</td>
</tr>
<tr>
<td>28 Mesh</td>
<td>2.54 ± 0.04</td>
<td>29.2 ± 0.7</td>
<td>0.17 ± 0.02</td>
<td>0.203 ± 0.003</td>
</tr>
<tr>
<td>(coarse cut)</td>
<td>2.01 ± 0.03</td>
<td>-</td>
<td>0.157 ± 0.004</td>
<td>-</td>
</tr>
<tr>
<td>(Fine cut)</td>
<td>1.33 ± 0.03</td>
<td>-</td>
<td>0.117 ± 0.004</td>
<td>-</td>
</tr>
<tr>
<td>48 Mesh</td>
<td>1.65 ± 0.03</td>
<td>26.7 ± 0.8</td>
<td>0.139 ± 0.009</td>
<td>0.184 ± 0.004</td>
</tr>
<tr>
<td>(coarse cut)</td>
<td>1.4 ± 0.1</td>
<td>-</td>
<td>0.14 ± 0.07</td>
<td>-</td>
</tr>
<tr>
<td>(Fine cut)</td>
<td>1.2 ± 0.3</td>
<td>-</td>
<td>0.12 ± 0.06</td>
<td>-</td>
</tr>
<tr>
<td>100 Mesh</td>
<td>0.941 ± 0.008</td>
<td>24.6 ± 0.4</td>
<td>0.108 ± 0.001</td>
<td>0.160 ± 0.007</td>
</tr>
<tr>
<td>200 Mesh</td>
<td>0.57 ± 0.02</td>
<td>22.8 ± 0.3</td>
<td>0.127 ± 0.001</td>
<td>0.136 ± 0.002</td>
</tr>
</tbody>
</table>

2.3 The Fiber Distributions

In this section, the measurements of fibre size ($L_f$, $D$ and CI) and $ω$ are described.
2.3.1 Length-Weighted Average Values

Using BMC and FQA, size distributions and coarseness of the different fractions and their respective cuts were measured. Table 2.1 shows length-weighted averages of these measurements. The errors were obtained from analysis of different FQA measurements of the same sample. This error is not to be confused with the deviation or narrowness of each distribution.

2.3.2 Property Distributions

The data from FQA measurements yields the length-weighted length distributions presented in Figure 2.2. The recorded distributions appear to be Gaussian. The literature (M.Deng and Dodson [16]) shows that fibre length distributions from the tree tend to be log-normal. However, perhaps from the pulping process, length-weighted distributions shift to Gaussian. Furthermore, Fig 2.2 shows that as the mesh turns finer, the distribution is narrower. This is commonly observed in multi-stage fractionation. It is due to the effect of the probability screening. Even though the grid openings are always larger than the fiber width, it is easier for shorter fibers to pass through the screen and long fibers to be rejected. Gooding and Olson [5] analyzed the fractionation process and proposed a plug flow model. They found that for a given type of screen aperture geometry (slots, holes, etc), the passage of long fibres cannot be reduced without reducing the passage of short fibres as well. Thus, by making the downstream distribution narrower the upstream distribution grows wider by the short fibres retained. The effect is consistent through each stage of the screening process. Another important observation of Fig 2.2 is, that even though Mesh 28 has a length-weighted average length ($LWL$) very close to that of the feed pulp, the distributions are different. The feed pulp distribution, being a mixture of all the mesh sizes, is very wide compared to the Mesh 28 distribution. Figure 2.3 displays the length distribution for Mesh 28 and the two cuts. The figure shows that for the coarse cut, $LWL$ reduces but the standard deviation increases when compared with M28. In the fine cut, the distribution is narrower. This shows that for the coarse cut there are two effects occurring simultaneously. In the cutting, there is a reduction in length of some of the fibres but the rest of the fibres remain unchanged. Thus, it is as if short fibres were added to the uncut distribution. This is why the coarse cut is wider. In contrast, in the cutting process for the fine cut, length for all fibres is reduced. This creates a narrow distribution. Since the size of the cuts was the same for all fractions, the cutting effect is lost as we decrease the size of the mesh opening. This is shown in Figure 2.4.
Figure 2.2: Length distributions (length-weighted) of different fibre fractions obtained from a BMC fractionation. The mean of each distribution shifts as the mesh is finer. All appear to have Gaussian behavior, with a consistent reduction in standard deviation as the mesh fineness increases.

Figure 2.3: Length distribution (length-weighted) of a BMC fraction and its respective cuts. Fibre cutting was effective by reducing LWL of each fraction, shown here as shifts in the distributions. Furthermore, they remain Gaussian without considerably increasing standard deviation.
Figure 2.4: Length-weighted pulp distributions for different cuts (in sequential order: M14, M28, M48 and Feed Pulp). As the mesh is finer the cutting effect is lost and the resulting distribution is wider.

Figure 2.5 shows the scatter plot of length and width of each fiber obtained from FQA data. It can be seen that, even though the range is broad, there is a relation among width and length for each fibre. Madani [15], separating the scatter values into bins and averaging the values in each bin, proposed a relationship (implying length being linear to the fibre aspect ratio) of the form:

\[
D = \frac{L_f}{a_0 L_f + a_1}
\]  

(2.1)
Figure 2.5: Scatter plot of width $D$ and length from fibres for different distributions (Feed Pulp, M14, M28, M48, M100 and M200 in sequential order). Although there is a broad range of width for fibres at certain length, there is a higher concentration at a given value. This is an indication that the width and length are correlated. This is regardless of the fibre fraction. Thus, there is a relation among fibre properties, that may be unaffected by the fractionation process.
2.4 The Natural Links in Fiber Properties

It has been found that fiber properties are linked (Madani [15], Karenlampi and Suur-Hamari [12]). Length, coarseness and width are usually correlated. Longer fibers tend to have a higher coarseness and a larger width. Figure 2.6 shows the relation found between coarseness and length. FQA does not measure coarseness of each fibre but total length of a distribution. By knowing the dry weight of the FQA sample, a mean coarseness can be calculated as the ratio of sample dry weight to total length. The trend for coarseness was found to be linear (2.2) for the range of values in the study with a coefficient of determination \( R^2 = 0.986 \). This is in agreement with the findings of Karenlampi and Suur-Hamari [12]. The reason of the behavior is unknown, yet it must be related to the tree biology, genetics, and climate. Another source for the correlation, may be due to the fact that coarser fibres are stronger and have a greater resistance to fibre cutting in the pulping process.

![Figure 2.6: Relation between fibre coarseness and length. Coarseness was obtained from the total measured length and the dry weight of each distribution sample. Thus, it is a mean value since there is a length distribution. A linear fit provided the highest coefficient of determination \( (R^2 = 0.986) \). The standard errors, shown as bars in the plot, were obtained from standard deviation among FQA measurements.](image)

\[
\omega = 0.036 \frac{mg}{mm} L_f + 0.12 \frac{mg}{m} \tag{2.2}
\]
At a 95% confidence level, the coefficients of the linear fit (equation 2.2) are $0.036 \pm 0.006$ and $0.12 \pm 0.01$.

Figure 2.5 shows that for all fractions there is a wide range of width for a given length. However, there is a higher concentration of fibres of a certain width. The width value with higher concentration is increasing as the fibres get longer. Following the procedure used by Madani [15], the raw data of all fractions (Figure 2.5) was separated into 0.2 mm length bins. An average width for each bin was calculated. This calculation was done for all BMC fractions, generating curves of length against width for each. The curves are shown in Figure 2.7a. Regardless of the fraction, the generated curves are statistically the same. Thus, this correlation is independent of the fractionation process. Furthermore, the same observation proves that the BMC does not fractionate according to width which is consistent with the findings of Gooding and Olson [5]. In an attempt to reproduce the results of Madani [15], a fit of the form of equation 2.1 was proposed. Nevertheless, for the range of values in our studies and the pulp used, a linear fit (equation 2.3) better predicted the behavior as shown by the coefficients of determination.

![Figure 2.7: Relation between fibre length and width ($D$). Constructed from raw data shown in Figure 2.5. The scatter points represent arithmetic averages of width among fibres in 0.2 mm bins. Left figure (a) shows width values for each BMC fraction. Right figure (b) shows the combined data of all BMC fractions. Mean fibre widths reported by FQA for all fractions have also been included. Fit 1 (equation 2.1 proposed by Madani [15]). Fit 2 (linear fit). The best fit was found to be linear (equation 2.2).]
At a 95% confidence level, the coefficients of the linear fit (equation 2.3) are $2.2 \pm 0.3$ and $24 \pm 1$.

As is the case of the determined relationship for fibre coarseness, it is difficult to establish the cause of correlation between length and width without involving tree genetics and biology. A study of this type is beyond the scope of this research, but a review of genetic and geographical studies on the fibre correlations is provided by Via et al. [24].

### 2.5 Multi-variable Regression

From the different BMC fractions and cuts, handsheets were tested for bulk and strength. The results are shown in Tables A.1 to A.4 of the Appendix.

The most simple models for the tensile index and bulk, in terms of the fibre geometry and press-drying pressure, are the following:

\[
Bulk = C_B L_f^{\beta} D^{\alpha} \omega^{\gamma} P^{\rho} \tag{2.4}
\]

\[
TI = C_T L_f^{\beta} D^{\alpha} \omega^{\gamma} P^{\rho} \tag{2.5}
\]

Applying logarithm to both sides of the previous expressions, the values of the unknown coefficients are obtained through a simple multi-variate linear regression. The regression yields the values shown in Table 2.2. The values of $C_B$ and $C_T$ depend on the units used for the other variables of the models (length, width, coarseness and pressure). They are a function of the elasticity of the fibers and possibly other variables like curl, kappa number and fibre fibrillation. Table 2.2 shows considerable error in the determined coefficients. In the case of bulk, $\gamma_L$ is negligible. Thus, the model shown in equation 2.4 can be improved by removing length as a variable. In the case of tensile index, the data shown in Appendix (Tables A.3 and A.1), reflects great difference in results for Mesh 28 and the feed pulp. Both pulps have similar LWL, yet the strength values are very different. The observed differences are due to the difference in the shape of the distribution. It is known that fines affect the strength of the sheet yet have negligible effect on LWL (Seth [22]). Thus, LWL is not a sufficient measure of length distribution. This means that the model shown in equation 2.5 can be improved by adding the distribution standard deviation ($\sigma$) shown in Table 2.3. The coefficients eliminating length as a variable for bulk and adding $\sigma$ as a variable for $TI$, 

\[
D = 2.2 \frac{\mu m}{mm} L_f + 24.0 \mu m \tag{2.3}
\]
Table 2.2: Coefficients for proposed bulk and tensile index models (equations 2.4 and 2.5) determined through linear regression.

<table>
<thead>
<tr>
<th>Unknown</th>
<th>Value (95% confidence level)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_B$</td>
<td>0.1 ± 0.7</td>
</tr>
<tr>
<td>$\gamma_L$</td>
<td>0.03 ± 0.09</td>
</tr>
<tr>
<td>$\gamma_D$</td>
<td>2 ± 2</td>
</tr>
<tr>
<td>$\gamma_W$</td>
<td>0.1 ± 0.8</td>
</tr>
<tr>
<td>$\gamma_p$</td>
<td>-0.20 ± 0.03</td>
</tr>
<tr>
<td>$C_T$</td>
<td>8e10 ± 4e13</td>
</tr>
<tr>
<td>$\beta_L$</td>
<td>0.70 ± 0.09</td>
</tr>
<tr>
<td>$\beta_D$</td>
<td>-7 ± 2</td>
</tr>
<tr>
<td>$\beta_W$</td>
<td>0.4 ± 0.8</td>
</tr>
<tr>
<td>$\beta_p$</td>
<td>0.31 ± 0.02</td>
</tr>
</tbody>
</table>

Table 2.3: Standard deviation of length-weighted pulp distributions. Obtained using equation 1.8 and the length-weighted distribution shown in equation 1.9

<table>
<thead>
<tr>
<th>Pulp</th>
<th>Sigma(σ) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed Pulp</td>
<td>1.30</td>
</tr>
<tr>
<td>Feed Pulp Coarse Cut</td>
<td>0.95</td>
</tr>
<tr>
<td>Feed Pulp Fine Cut</td>
<td>0.74</td>
</tr>
<tr>
<td>14 Mesh</td>
<td>1.03</td>
</tr>
<tr>
<td>14 Mesh Coarse Cut</td>
<td>1.12</td>
</tr>
<tr>
<td>14 Mesh Fine Cut</td>
<td>0.75</td>
</tr>
<tr>
<td>28 Mesh</td>
<td>0.84</td>
</tr>
<tr>
<td>28 Mesh Coarse Cut</td>
<td>0.90</td>
</tr>
<tr>
<td>28 Mesh Fine Cut</td>
<td>0.67</td>
</tr>
<tr>
<td>48 Mesh</td>
<td>0.56</td>
</tr>
<tr>
<td>48 Mesh Coarse Cut</td>
<td>0.72</td>
</tr>
<tr>
<td>48 Mesh Fine Cut</td>
<td>0.61</td>
</tr>
</tbody>
</table>
Table 2.4: Improved coefficients for bulk and tensile index models (2.4 and 2.5) as obtained from regression.

<table>
<thead>
<tr>
<th>Unknown</th>
<th>Value (95% confidence level)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_B$</td>
<td>0.08 ± 0.4</td>
</tr>
<tr>
<td>$\gamma_D$</td>
<td>1.3 ± 0.6</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>0.1 ± 0.3</td>
</tr>
<tr>
<td>$\gamma_p$</td>
<td>−0.20 ± 0.01</td>
</tr>
<tr>
<td>$C_T$</td>
<td>5e7 ± 8e9</td>
</tr>
<tr>
<td>$\beta_L$</td>
<td>0.4 ± 0.1</td>
</tr>
<tr>
<td>$\beta_\sigma$</td>
<td>0.6 ± 0.1</td>
</tr>
<tr>
<td>$\beta_D$</td>
<td>−5 ± 2</td>
</tr>
<tr>
<td>$\beta_\omega$</td>
<td>−0.6 ± 0.7</td>
</tr>
<tr>
<td>$\beta_p$</td>
<td>0.31 ± 0.02</td>
</tr>
</tbody>
</table>

are those shown in Table 2.4. By comparison of the errors in the coefficients shown in Table 2.2 and 2.4, a clear improvement of the model can be identified. To assess the improvement quality of the fit of the models to the data, the predicted values of the dependent variables with the measured values are plotted. Figure 2.8 shows the quality of the bulk model fit, considering length and $\sigma$ and without considering length at all. Clearly, length has negligible effect on bulk. Figure 2.9 shows the quality of the tensile index model fit under the same mentioned conditions. In this case, the tensile index model is improved by adding length and $\sigma$ as variables. Comparing the figures, not only is there an improvement in the deviation of the tensile index fit, but now the data from feed pulp distributes evenly around the diagonal line.
Figure 2.8: Effect of reducing the number of variables in the bulk model. The measured values of bulk were obtained from calliper and grammage measurements. Left figure (a) considers length and $\sigma$, right figure (b) shows the improved model by eliminating length.

Figure 2.9: Effect of incorporating the standard deviation ($\sigma$) to the tensile index model. The measured values of tensile index were obtained from a tensile tester. Left figure (a) does not consider $\sigma$ as variable, right figure (b) shows the improved model by adding $\sigma$. 
Thus, bulk and tensile index models (equations 2.4 and 2.5) can be rewritten as equations 2.6 and 2.7.

\[
\text{Bulk} = 0.1 \ D^{1.3} \ \omega^{0.1} \ P^{-0.2} \tag{2.6}
\]

\[
\text{T.I.} = 5e7 \ L_f^{0.4} \ \sigma^{0.6} \ D^{-5} \ \omega^{-0.6} \ P^{0.3} \tag{2.7}
\]

These correlations predicted the bulk and tensile index within 20% and 25% respectively of the actual values.

From the determined relations, one of the findings is that the bulk and T.I are not intrinsically related. Even for the same furnish, the pressure coefficient of the bulk is not the inverse of the pressure coefficient for tensile index. It is true that generally a reduction of one of the two leads to an increase of the other, since the power coefficients of equations 2.6 and 2.7 have opposite signs. Nevertheless, this is not always the case. A change in length may considerably affect strength and have little effect on bulk of the sheet. Furthermore, equations 2.6 and 2.7 show that bulk is much less sensitive than tensile index to being affected by fibre properties.

2.6 Zero Span Tensile Index

Zero span tensile index (ZI) was measured for each sample. This property is dependent on the clamping pressure of the tester. ZI was measured at two clamping pressures (60 psi and 70 psi). The recorded value was the maximum of the two. The values are shown in Tables A.1 to A.4 of the Appendix. A regression performed on the zero span tensile index data yields a very poor correlation as shown in Figure 2.10. Due to the large randomness in recorded values, little is to be said about how the fiber geometry affects the zero span strength. The zero span tensile index is more sensitive to the clamping pressure and grammage than to fibre geometry \(L_f, D\) or \(\omega\). In regards of the press-drying pressure, for most of the pulps, it was found that increasing pressure beyond a certain value (60-100 psi) caused a reduction of ZI (data shown in the Appendix). This was not the case for the tensile index. It is believed that increasing press-drying pressure, while it reduces the voids and increases the degree of bonding, still damages the fibres when it is excessive.
2.7 Combining the Natural Links with the Regression

Given the relations found in the regression analysis (equations 2.6 and 2.7) and the relation of coarseness and width to length (equations 2.2 and 2.3) for the studied pulp, both bulk and $TI$ can be related to two (2) single variables ($L_f$ and $P$):

$$Bulk = 0.1 (2.2L_f + 24.0)^{1.3} (0.036L_f + 0.12)^{0.1} P^{-0.2}$$  \hspace{1cm} (2.8)

$$TI = 5e7 L_f^{0.4} \sigma^{0.6} (2.2L_f + 24.0)^{-5} (0.036L_f + 0.12)^{-0.6} P^{0.3}$$  \hspace{1cm} (2.9)

This can be done provided there is no mechanical modification of fibers (e.g. cutting or refining) since modified fibres will not follow correlations given in equations 2.2 and 2.3.

Equations 2.8 and 2.9 can be represented as surface plots. Figure 2.11 shows the behavior of bulk (equation 2.8 ), while Figure 2.12 corresponds to tensile index (equation 2.9) for two (2) different $\sigma$ values.

From the surface plots, in the case of bulk, we see monotonic behavior with respect to length and pressure. It increases with length and decreases with pressure. In the case of tensile index, it
increases with pressure but shows an optimal length. The optimal value for studied pulp furnish depends on the standard deviation. It is around 2.6 mm for a $\sigma$ of 10%. The two values of $\sigma$ are presented to show that the location of the optimal fraction will also depend on the shape of the distribution (or the fines content). The linear regression shows no optimal value when the variables are considered to be independent. The regression predicts a stronger paper, the longer the fibre. However, longer fibres are coarser and have a larger width. This acts against the strength. The result of the opposing effects is the existence of an optimal length value.

**Figure 2.11:** Surface plot showing bulk for studied pulp in terms of pressure and length. Obtained by combining the model from regression (equation 2.6) and determined correlations between fibre properties (equations 2.2 and 2.3).
Figure 2.12: Surface plot showing tensile index for studied pulp in terms of pressure and length at two $\sigma$ values ((a) 0.1 mm and (b) 10%). Obtained by combining the model from regression (equation 2.6) and determined correlations between fibre properties (equations 2.2 and 2.3).
Chapter 3

Computer Simulations

In this chapter, two-dimensional (2D) and three-dimensional (3D) simulations performed using Matlab are shown. The developed codes are shown in the Appendix B.

3.1 Paper as a 2D Random Network

In this section, the paper structure is modeled as a 2D constant size (length and width) random fibre network. The random networks were created using Matlab imaging toolbox. Each fiber is placed as a 2.25 Megapixel (1500p X 1500p) binary image. Resolution of the image was set to a 5 mm square. Thus, the fibre dimensions were converted to pixels accordingly. An average fibre width of 30 µm is represented as a rectangle of 9 pixels in width. A pixel value of 1 represents fibre area and 0 represents a void. By adding the images we can form the random 2D structure. To avoid edge effects, once the network is constructed, the image was cropped to 80%. The resulting image will not be binary. Thus, there is a pixel value distribution along the plane of the sheet which will be referred as \( P(x,y) \). Figure 3.1 shows random networks created using this method for two different coverage values. The colors of the pixels are assigned according to \( P(x,y) \). Thus, we are not only looking at the structure of the simulated paper, but also the \( P(x,y) \) distribution.

\( P(x,y) \) gives the total number of fibres stacked on top of each other at a given location. This means that information on the number of fibre-to-fibre crossings and the resulting bonded area can be obtained for that location. This is shown in Table 3.1.
Figure 3.1: Simulated fibre networks at different coverage values. Left figure (a) $c = 0.24$ and right figure (b) $c = 12$. For both cases $L_f = 1 \text{ mm}$, $D = 30 \mu \text{m}$ and the sample area is a $5 \text{ mm} \times 5 \text{ mm}$ square.

Table 3.1: Description of the pixel value distribution $P(x, y)$. The bonding area factor is multiplied by the pixel area ($A_p$) to calculate the bonded area at the $(x, y)$ location.

<table>
<thead>
<tr>
<th>Pixel Value ($P(x, y)$)</th>
<th>Region Description</th>
<th>Bonding Area Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Void Regions</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>Fibres</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>Single Fibre-Fibre Crossing Region</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>Double Fibre-Fibre Crossing Region</td>
<td>4</td>
</tr>
<tr>
<td>N</td>
<td>(N-1) Fibre-Fibre Crossing Region</td>
<td>$2(N-1)$</td>
</tr>
</tbody>
</table>

3.1.1 Assumptions and Limitations of the 2D Model

Usually, fibres are horizontally aligned within a thickness scale of 2-3 fibre thickness (M.Deng and Dodson [16]). Consequently, it is reasonable to analyze the paper structure as a 2D formation.

In fibre deposition on the paper machine, fibre centers distribution and fibre orientation are influenced by several phenomena. These include; flocculation of the suspension before the wire, local basis weight unevenness caused by the flow through the forming fabric and preferred orientation caused by the headbox jet. There are simulation studies that take these effects into account. An example is the work done by N.Provatas et al. [18]. The study predicts the statistics of disordered networks and devises a simulation parameter to characterize flocculation. For standard handsheet making there is no preferred orientation, thus the distributions tend to be more random. The simu-
lations shown here focus on standard handsheets, thus each fibre center position and orientation is assumed to be random.

As fibres are stacked, a problem arises when more than two fibres are overlapping. If we consider fibres to be rigid, then as the fibres are stacked, they cannot be in contact with fibres in different layers other than the immediately adjacent layer. However, flexible fibres can bend so that they come into contact with fibres in different layers. Figure 3.2 shows the differences between the two cases. This can lead to issues when counting the fibre crossings within a randomly generated 2D network. For this study, the counting of the crossings is done in the following manner; If there is a double fibre crossing, it counts as two crossings, a triple crossing as three crossings and so on. This is equivalent to considering fibres as infinitely flexible. Thus, in this analysis, fibres are considered to be infinitely flexible and stacked in such, that there are no internal voids. The voids can only be on one of the sides of the sheet and not between the fibres of different layers. In reality fibres are not infinitely flexible. The fibres ability to bend will depend on the loads (induced by pressing and drying) and on the second moment of area of the fibres cross-section calculated from the horizontal axis. However, the model described here is the limiting case. Thus, we expect to overestimate the number of fibre-to-fibre crossings ($N_c$) and relative bonded area ($RBA$) and to obtain a lower paper thickness than that of the real paper.

![Figure 3.2: Difference in fibre contact between rigid and flexible fibres. a) Flexible fibre. b) Rigid Fibre.](image)

Finally, this initial study, only considers constant fibre property distribution. In order to obtain a representative statistical value, five simulations were conducted in the same conditions and the values were averaged. The error bars were obtained from standard deviation among simulations.
3.1.2 Paper Thickness and the Pixel Value distribution

The pixel value \( P(x,y) \) represents how many fibres are stacked on top of the other at that location. Thus it is also the local coverage at that location. M. Deng and Dodson [16] have shown that local coverage behaves as a Poisson distribution. Consequently, the pixel value distribution is also a Poisson distribution as shown in Figure 3.3.

![Figure 3.3: The Poisson distribution of the pixel value \((P(x,y))\) obtained from simulations for two different coverage values. \( L_f = 1 \text{ mm}, D = 25 \text{ \mu m}, N_f = 3000 \) (a) and 10000 (b).](image)

Coverage \((c)\) can be calculated from the pixel value distribution to show that is exactly equal to the mean pixel value \( \overline{P(x,y)} \):

\[
c = \frac{\sum_{i=1}^{N} P_i A_p}{\text{SampleArea}} = \frac{\sum_{i=1}^{N} P_i}{N} = \overline{P(x,y)}
\]  

(3.1)

Furthermore, if \( P(x,y) \) is multiplied by fibre thickness \((\tau_f)\), the result is the network thickness distribution \( \tau_N(x,y) \). The mean network thickness \( \overline{\tau_N} \) can be obtained by integrating over the sample area in the following way:

\[
\overline{\tau_N} = \frac{\int \int \tau_N(x,y) dx dy}{\text{SampleArea}}
\]  

(3.2)

in a discrete form:

\[
\overline{\tau_N} = \frac{\sum_{i=1}^{N} \tau_{Ni} A_p}{\text{SampleArea}}
\]  

(3.3)
where \( N \) is the number of pixels and \( A_p \) is the pixel area.

Equation 3.3 can be rewritten as follows:

\[
\tau_N = \tau_f \frac{\sum_{i=1}^{N} P_i A_p}{\text{SampleArea}} = \tau_f \ c
\]  

(3.4)

Thus, \( \tau_N \) is simply the product of fibre thickness \( \tau_f \) and coverage \( c \). Finally using equation 1.22, \( \tau_N \) can be expressed as:

\[
\tau_N = \frac{BW}{(1-f) \ \rho_f}
\]  

(3.5)

where \( BW \) is the basis weight, \( f \) is the voids fraction in the dried state and \( \rho_f \) is the fibre density.

If our assumptions are valid, this means that bulk for the network is equal to fibre bulk in the dried state \( \frac{1}{(1-f) \ \rho_f} \). Thus, in order to make a bulkier paper, uncollapsible bulkier fibres must be used. It should also be noted that the voids fraction in the dried state is a function of the fibre collapsibility (\( \phi \)) and the cross-section geometry (\( \omega \) and \( D_o \)) in the wet state. Consequently, when the mean thickness is used to calculate the bulk of the network, the bulk only depends on the fibre cross-section (\( \omega \) and \( D_o \)) and not its length.

When measuring paper thickness experimentally, the measuring cylinder that drops down to the paper has a large diameter compared to the dimensions of the fibres. Thus, a more representative paper thickness comparable to that measured experimentally would be the maximum network thickness, \( \tau_{N, \text{MAX}} \). There is no analytical expression for the maximum pixel value \( P_{\text{MAX}} = \frac{\tau_{N, \text{MAX}}}{\tau_f} \). However, the behavior obtained from simulations is shown in Figure 3.4. Since the sample area is a 5 mm square, this would be the thickness measured by a device with an indenter of the same size. Figure 3.4 shows that similar to \( P(x,y) \), \( P_{\text{MAX}} \) depends only on coverage and not the fibre dimensions (\( L_f \) and \( D \)).

By performing a linear regression, \( P_{\text{MAX}} \) was shown to behave as:

\[
P_{\text{MAX}} \approx 10 \ c^{0.6}
\]  

(3.6)

Similar to the way equation 3.5 was obtained, expression 3.6 can be rewritten to show the following:

\[
\text{Bulk} \approx \frac{10}{\ c^{0.4} (1-f) \ \rho_f}
\]  

(3.7)
Figure 3.4: The effect of coverage (c) on the maximum pixel value ($P_{\text{MAX}}$) for different lengths ($L_f$) and widths ($D$). Values obtained from 2D simulations. $P_{\text{MAX}}$ changes only with $c$ and not with $L_f$ or $D$.

\[ \text{or:} \]

\[ \text{Bulk} \approx \frac{10 \cdot \tau_f^{0.4}}{BW^{0.4} (1-f)^{0.6} \cdot \rho_f^{0.6}} \]  

(3.8)

This shows, that when $\tau_{N,\text{MAX}}$ is used, bulk decreases as $BW$ increases. Furthermore, $f$ and $\tau_f$ are functions of the fibre cross-section ($\omega$ and $D_o$) in the wet state. Thus, regardless of the thickness used to calculate bulk (mean or maximum), the network bulk only depends on the fibre cross-section ($\omega$ and $D_o$) and not length.

3.1.3 The Degree of Bonding

The strength of the network can be related to the number of fibre-to-fibre crossings and the relative bonded area.
**Number of Crossings**

When a paper strip is loaded, the tension is distributed through the fibres and the bonds between the fibres. Usually prior to fracture, if each fibre is isolated, the transmitted load is considerably smaller than that required for fibre breakage. Therefore, bonds are usually the first to break. Consequently, it is important to maximize the number of fibre crossings \( N_c \) so that the load distributes through more bonds even if the total bonded area is the same. By increasing \( N_c \), the probability of finding a crossing (along a fracture line) in which the fibres and the load are aligned is higher.

Figure 3.5 shows the effect on \( N_c \) by the addition of fibres to the structure for different lengths and widths. The figure shows that \( N_c \) is only a function of width \( (D) \) and coverage \((c)\). \( N_c \) increases with increasing \( c \) and decreases with increasing \( D \). Thus, paper made from fibres of smaller widths have more fibre crossings at a given basis weight. Length \((L_f)\) has no effect on \( N_c \). From the figure, it can be seen that even for high coverage values, the number of crossings is only a function of coverage and fibre width. The dependence on fibre length is weak because fibres, regardless of length, have high aspect ratios.

![Figure 3.5: The response of coverage(c) on total number of fibre-to-fibre crossings \((N_c)\). \( N_c \) increases as fibre width \((D)\) is reduced and coverage \((c)\) is increased.](image-url)
At a constant coverage, the number of fibres \( N_f \) decreases as length increases. Since \( N_c \) is independent of length, at a constant coverage, increasing length will increase the number of crossings per fibre \( \left( \frac{N_c}{N_f} \right) \). Thus, networks made from longer fibres will be stronger because of the better alignment of the loads in the direction of the fibres and the fact that if a particular bond breaks, the fibre is still held by other bonds that can activate. Furthermore, reducing fibre coarseness will result in a higher coverage. Thus, the total number of crossings will increase. By increasing the total number of crossings, the load is transmitted through more bearing points, and the strength of the paper network increases. The effect of width, at first, is to decrease the number of crossings. However, reducing width (at the same coarseness) may increase or decrease the coverage depending on the flexibility of fibres. Thus we cannot precisely determine the effect of width without considering the network flexibility.

Deng and Dodson (1.24) give an expression (1.24) for the density of the number of crossings for small coverage values. This formula shows that \( N_c \) is independent of \( L_f \). Figure 3.6 shows a comparison of the formula with values from simulation. As shown, the formula is a better prediction as fibre width increases. Furthermore, the formula underpredicts \( N_c \) as \( c \) increases.

![Figure 3.6: Comparison of number of fibre crossings obtained from simulations with statistical formula (1.24) by M.Deng and Dodson [16]. The scattered values were obtained from simulations and the solid lines represent equation 1.24 at different widths.](image)

40
The Relative Bonded Area (RBA)

The relative bonded area (RBA) can be obtained by the pixel values. The total fibre area within the sample can be calculated through the following:

\[ \text{Total Fibre Area} = \sum_{i=1}^{N} 2 \times \text{PixelValue}_i \times \text{PixelArea} \]  (3.9)

Equation 3.10 is used to calculate the total unbonded area.

\[ \text{Total Unbonded Area} = 2 \times \text{Number of pixels (PixelValue > 0)} \times \text{PixelArea} \]  (3.10)

Therefore, RBA can be obtained by expression 3.11.

\[ \text{RBA} = \frac{\text{Total Fibre Area} - \text{Total Unbonded Area}}{\text{Total Fibre Area}} \]

\[ \text{RBA} = 1 - \frac{\text{Total Unbonded Area}}{\text{Total Fibre Area}} \]

\[ \text{RBA} = 1 - \frac{\text{Number of pixels (PixelValue > 0)}}{\sum_{i=1}^{N} \text{PixelValue}_i} \]  (3.11)

Figure 3.7 shows the RBA vs. fibre coverage. From the figure, it is observed that RBA is not a function of length or width of the dried state, but only a function of basis weight or coverage. The blue line in Figure 3.7 represents the theoretical value shown in Chapter 1, in equation 1.23. This shows that length does not affect the total degree of bonding, it only changes the efficiency in the way that load is transmitted (by affecting \( \frac{N_c}{N} \)). On the other hand, decreasing coarseness not only increases the total number of crossings, but also increases the amount of bonded area. This is because decreasing coarseness will increase coverage as shown in equation 1.22. Thus, reducing the coarseness should increase the strength of the paper network.

Size Distributions

Since width affects the number of crossings \( N_c \), the effect of the width distribution was studied. This was done by creating random networks made from fibres with a normal width distribution. The simulated structure of a normal width distribution is shown in Figure 3.8. Several simulations
Figure 3.7: The relative bonded area (RBA) against coverage (c) of simulated 2D networks for different lengths ($L_f$) and widths ($D$). RBA is only a function of $c$ and unaffected by $L_f$ or $D$. The area along the thickness of the fibre ($2 \cdot \tau_f \cdot L_f$) was not considered for RBA calculation. The solid line represents the statistical approximation provided by M.Deng and Dodson [16] as equation 1.23 at different width standard deviation ($\sigma_D$) and mean width ($\bar{D}$) were performed. The number of crossings was recorded at different coverage values. The results of these simulations are shown in Figure 3.9. The figure shows that only the mean width ($\bar{D}$) affects the number of fibre crossings. The width standard deviation ($\sigma_D$) has no effect on the number of crossings.

3.2 Two-Dimensional (2D) Deposition

From the 2D analysis, under the validity of assumptions (low coverage or high press-drying pressure), it is observed the length has no considerable effect on; the bulk, the number of Crossings ($N_c$) or RBA. Fibre width ($D$), shows an effect on $N_c$, increasing as $D$ reduces. However, experimental
evidence shows length effects on both bulk and tensile strength. In the initial assumptions, the packing density changes due to geometry, were not considered. Thus length and width may have effects on the packing density, specially at low press-drying pressures, such as to change thickness and number of crossings. A 2D random deposition brings light into the answer of the previous question.

In the previous sections of this chapter, random network simulations were performed to study the plane of the sheet (x,y). In this section, the focus is the vertical plane (x,z) along the thickness of the sheet. Matlab was used to develop a code to simulate the fibre deposition in this vertical plane. The deposition model considers fibres to be rigid beams of large friction factor and bonding force being deposited by the action of gravity. Figure 3.10 shows a deposition generated using

\[ c = 0.969, \bar{D} = 45 \mu m \text{ and } \sigma_D = 40 \mu m. \]
**Figure 3.9:** Effect of width standard deviation (σ_D) of a normal distribution on the number of crossings N_c. The values of σ_D are in μm. σ_D shows no effect on N_c. Filled data points are for an average width (D̄) of 30 μm and data points with no fill are for D̄ = 45 μm.

This code. The total fibre area is 74 \times 10^3 \mu m^2 or around 100 fibres, the fibre length is 1 mm and thickness is 15 μm.

**Figure 3.10:** Simulated two-dimensional (2D) deposition. Fibres are considered to be rigid beams with high friction factor and high bonding force. Total fibre area is 74 \times 10^3 \mu m^2, L_f = 1 mm and τ_f = 15 μm. Resolution is 25 μm^2 per pixel.

Each simulated beam was deposited vertically from a random x position and at a horizontal orientation. Once the beam encountered the formed mat, if equilibrium was not reached, it rotated until finding another contact point. At this point another fibre is deposited a so on. It must be said
that in the deposition model, the fibres are considered rigid with a large friction factor and bonding strength.

By performing several simulations, a statistical average can be obtained to measure the effect of length on the mean and maximum height of the deposition. This is shown in Figures 3.11 and 3.12. The figures show that for both heights (mean and maximum), there is a slight increase with length. This is an indication that packing density reduces as fibre length is increased. In the next section, this question will be answered by performing a 3D simulation.

**Figure 3.11:** Mean height of a rigid fibre 2D deposition against total area of deposited fibres. Data obtained from simulations. Each point represents an average of three simulations repeated under the same conditions. The fibre thickness $\tau_f$ is 15 $\mu m$. 

![Figure 3.11](image-url)
3.3 The Three-Dimensional (3D) Structure of Paper

In the previous sections we have studied the in plane and vertical statistics of randomly deposited fibres by 2D simulations. In this section the focus is on the statistics of the 3D random network. The developed 3D Matlab code is an extension of the 2D codes. A 3D network can be simulated as a 3D image. In this case, a pixel value of unity in the 3D array represents fibre material, whereas a pixel value of zero is empty space. In contrast with the 2D random network code, each fibre is a 3D array representing a volume. The network is created by translation and rotation of the volume. As the fibre is being deposited, intersection is detected when pixel values greater than unity appear. Once the intersection is detected, the fibre will rotate until coming into contact with another point of the mat. Both of these operations can be broken down into translations and rotations of 2D images. Figure 3.13 show a 3D deposition of 300 fibres in a 5 mm square using the developed code ($L_f = 1 \text{ mm}$ and $GSM \approx 10$). Figure 3.14 shows a top view of the simulated network, where the height (in pixels) of the network is represented by a color scale.

3.3.1 Assumptions and Limitations

The starting point for deposition is picked randomly at a random orientation within the horizontal plane. The intersection, as the fibre is being deposited, is obtained by adding the pixel value and
Figure 3.13: Simulated random fibre network generated in Matlab. The model used considers fibres as rigid beams of high friction factor and bonding force. The fibre dimensions are $L_f = 1 \, mm$, $D = 25 \, \mu m$ and $\tau_f = 15 \, \mu m$. The figure shows 300 fibres deposited in a $5 \, mm$ square (10 GSM).

Figure 3.14: Top view image of the simulated random fibre network shown in Figure 3.13. Color has been added to show the height distribution in pixels. Resolution is $5.8 \times 10^{-7} \, mm^3$ per voxel.

detecting a value greater than unity. Once the intersecting height is determined, the fibre is rotated up to point where it will come into contact with another point of the existing network. The sign of the rotation angle is chosen by comparing the free lengths on each side of the contact pivot point. After that, the fibre becomes permanently attached to the network. Thus, our assumptions are the following:
• Fibres are considered to be rigid beams of a known width, fibre thickness and length.
• The size and shape for all fibres are the same. Property distributions are not considered.
• The friction factor of the fibres is large enough so that there is no sliding.
• The bond force is large enough such that there is no sudden restructuring due to the fibres own weight. That is, the deposition of each fibre does not change the previously formed mat.
• The deposition of each fibre is done at a random location and orientation. Thus flocculation or other forming effects are not considered.

3.3.2 The Three-Dimensional (3D) Algorithm
• A fibre center position and orientation angle is selected randomly.
• The fibre is deposited vertically until there is contact with the network (Initially it is a flat surface).
• After contact, a 2D height map similar to Figure 3.14, is cropped to the size of the fibre. The cropped image is used to predict the possible fibre rotation.
• The free lengths of the fibre are compared and side of rotation is determined.
• The rotation angle is calculated from the 2D height map and the pivot point.
• The fibre is rotated and the first step is repeated until a certain number of fibres is reached.

For every iteration, the total volume of the fibre network is obtained by summing the total pixels. The height is calculated by creating a 2D array of the maximum height of the 3D structure. From the 2D array, the maximum and mean height are estimated. The developed code, differs from those explained in the introduction (Conceio et al. [3]). In the code used here, rotation has been incorporated and fibres are considered rigid. It is believed, that this is a more realistic simulation for high rigidity and low pressure cases. The other code would overpredict the bulk by preventing rotation.
3.3.3 Length Effect

By adding fibres to the mat, it is obvious that the mean height increases. This is because adding fibres is equivalent to increasing the basis weight of the mat. If the mean height of the mat is plotted against the fibre total volume, the effect of length at a constant fibre total volume can be observed. Figure 3.15 shows the effect of length at a given fibre total volume. It can be inferred from the figure, that length has the effect of increasing the mean height of the mat after 1 mm$^3$ of fibre volume. This volume is equivalent to a basis weight of approximately 50 GSM.

3.3.4 Degree of Bonding of a Three-Dimensional (3D) Network

Unfortunately, obtaining the number of crossings is a difficult task in 3D. Nevertheless, some information can be inferred. The 3D simulations (voids are considered), show the mean height increasing with length. In contrast, 2D simulations (voids are not considered), show a constant mean height. Thus, the amount of voids, or in other words packing density, is dependent on length and pressure. At low pressure, length has the effect of producing a higher bulk. However, at higher pressure, length has no effect.

![Figure 3.15: Mean height of a simulated 3D random network ($\hat{c}_N$) against fibre volume ($N_f \cdot L_f \cdot D \cdot \tau_f$). Fibre thickness and width are $\tau_f = 15 \, \mu m$ and $D = 15 \, \mu m$. Each point represents the average of three simulations and error bars are from standard deviation. The figure shows an increase in $\hat{c}_N$ with $L_f$ and fibre volume.](image)

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Figure 3.16: Maximum height of simulated 3D random network ($\tau_{N,MAX}$) against fibre volume ($N_f \cdot L_f \cdot D \cdot \tau_f$). $\tau_f = 15 \mu m$ and $D = 15 \mu m$. Each point represents the average of three simulations and error bars are from standard deviation. Comparing with Figure 3.15, as more fibres are added the difference between $\tau_{N,MAX}$ and $\bar{\tau}_N$ is reduced, yet for low fibre volumes, $\tau_{N,MAX}$ is in some cases ten folds $\bar{\tau}_N$. 
Chapter 4

Conclusions and Final Remarks

The combination of fibre fractionation and guillotine cutting, proved to be a successful method for the study of the paper structure and the effects of fibre geometric properties. Furthermore, the 2D imaging method used here to simulate fibres, shows to be relatively fast and successful. It has the benefit compared to other methods, that fibre-to-fibre contacts can be easily computed. Both simulation and experiments, show that some of the effects can be attributed to the statistics while others are due to mechanical responsive properties.

By relating the fibre properties for the studied pulp, fibre coarseness ($\omega$) and width ($D$) were found to increase linearly with fibre length ($L_f$). Regardless of the fraction, the correlations were the same. This shows that the Bauer McNett Classifier (BMC), separates the fibres according to their length ($L_f$) independent of their width ($D$) or coarseness ($\omega$).

The results from the performed linear regression, are consistent with the findings in the literature (Clark [2]). It was found that length, when considered as an independent property, has no significant effect on the bulk of the sheet. However, the same is not true for the strength. Length and the standard deviation of the length distribution ($\sigma_f$), were found to considerably increase tensile index ($TI \propto L_f^{0.4} \sigma_f^{0.6}$). Width and coarseness were found to increase bulk ($Bulk \propto \omega^{0.1} D^{1.3}$) and to decrease strength ($TI \propto \omega^{-0.6} D^{-5}$). It should be said that the proposed equation models (equations 2.4 and 2.5) are a first approach for studying the bulk and tensile index behavior. This type of empirical model allows a comparison with the work developed by Clark [2] and O’neil et al. [19]. This type of fit implies that the effect of one of the variables is independent of the other and forces monotonic behavior. Thus, the model needs to be improved. An approach to improve the model is mentioned in the recommendations for future work.

When the correlations between fibre geometric properties ($L_f$, $D$ and $\omega$) are combined with
the empirical relations determined by linear regression, the result is an optimal length fraction for a stronger paper. The linear regression shows no optimal value when the variables are considered to be independent. The regression predicts a stronger paper, the longer the fibre. However, longer fibres are coarser and have larger widths. This acts against the strength. The result of the opposing effects is the existence of an optimal length. This explains why the original feed, being shorter than the longest mesh (M14) yet longer than the shortest mesh (M48), made the strongest paper. Thus, the tensile index can be increased through the use of fibre fractionation. However, the determined fibre property correlations are not universal among all fibre species and types of pulp furnish. The existence of an optimal value on other types of pulps will depend on how the fibre geometric properties are correlated.

The performed two-dimensional (2D) simulations provide insight into the observed strength behavior. Increasing fibre length, by increasing the number of fibre crossings per fibre \( \frac{N_c}{N_f} \), increases strength. This is because by increasing the number of crossings per fibre, since the fibre is mostly straight, will increase load alignment. Furthermore, during elongation if a bond between fibres breaks, each fibre has other bonds that can activate to support the load. Increasing coarseness, reduces the network coverage (equation 1.22). This in turn, decreases the degree of bonding (RBA and \( N_c \)), making a weaker paper. The effect of width is difficult to obtain from 2D simulations without involving the fibres ability to collapse and bend. Width in the wet state (cylindrical fibre) is different than width in the dried state (rectangular fibre). Increasing width in the wet state (at the same coarseness) will increase or decrease coverage at the dried state depending on collapsibility. Furthermore, 2D simulations provide an overestimate of \( N_c \) and RBA. The initial assumptions of the 2D model is that fibres are infinitely flexible. In reality this is not the case. Reducing width will reduce the area moment of inertia allowing the fibres to bend and better approximate the 2D structure. The effect of fines is also difficult to relate with 2D simulations. Fine coarseness is very low, thus the coverage is increased. However, they are also very short. So, why is it that fines enhance strength? We believe that this can be explained by the filling effect of fines rather than by the change in average length or coarseness. We have said that in reality the fibres are not infinitely flexible. Thus, at a particular fibre crossing the fibre does not bend at a 90\(^\circ\) angle to come into contact with fibres of another level (see Figure 3.2). Since fines are small they fill in these voids such as bring the structure closer to the 2D approximation. This means that adding fines after a certain threshold has little benefit in terms of enhancing strength. In fact, if fibres were infinitely flexible it is predicted that adding fines would have little to no effect. However, it is recognized that this explanation is simplistic and requires further studying to prove.

Simulations also explain the bulk behavior. We studied the two limiting cases of infinitely
flexible and infinitely rigid fibre. Two-dimensional simulations show that when fibres are very flexible, length had no effect on bulk. On the other hand, three-dimensional (3D) simulations show that when fibres are very rigid, increasing length increases bulk. This attributes to the notion that paper is for the most part, a 2D structure since the 2D model better predicts the behavior. The stresses induced by drying and fibre flexibility, are sufficient to cause the fibres to assemble into a dense 2D structure. However, the 2D model is still a limiting case and the approximation of paper as a 2D structure is itself dependent on the fibre geometry.

4.1 Recommendations for Future Work

The experimental work to follow is to study the application of the determined empirical relations to other types of furnish and to account for the effect of fibre flexibility. This can be done by examining data from other researchers or by repeating the experimental methodology described here. Flexibility can be changed by beating or by chemical treatments. However, fibre cutting with guillotine proved to be a tedious task. Thus for future work, perhaps it is necessary to develop an apparatus to cut the fibres in a controlled manner.

Furthermore, the simple empirical models (equations 2.4 and 2.5) can be improved by replacing them with equations that can predict bulk and strength on a broader range of values. The form of equations 2.4 and 2.5 allow a comparison with the work done by other researchers. However, we know that in order to be consistent with the physics, the form of equations 2.4 and 2.5 should be different. These equations assume that the effect of each variable is independent and monotonic. In reality, we know for example that changing the coarseness at a given width changes the fibre collapsibility. A change in coarseness will have a smaller effect on wall thickness the larger the width. Furthermore, it is expected that as pressure is increased the effect of the rest of the variables should be smaller. Thus, a better approach is to preform an analysis of variance and use a non-linear model that accounts for interaction between variables. We predict strong interactions between pressure \((P)\) and the rest of the variables \((L_f, \omega\) and \(D)\) as well as between \(D\) and \(\omega\). However, this will also require increasing the data points and varying the properties in ranges that may not be possible.

Finally, it has been seen that statistics of random networks explain qualitatively the effects of fibre geometry to bulk and tensile index. However, there is a need to link them directly in a quantitative way. This will allow the development of a wholesome theory to predict the behavior of any pulp. Nevertheless, it will require an analysis of the mechanical response of fibres to; the flow field during deposition, the applied pressure, the forces induced by the drying process, and the
tensile force during elongation. Even in a two-dimensional random network predicting breakage is difficult. The stress at a particular bond is not constant but a distribution that depends on the tension of the bonded fibres, the fibre dimensions, and the orientation between fibres. All of which are changing from bond to bond. Thus, computer solving through FEA (Finite Element Analysis) may be useful relating network statistics \((N_c, RBA, \tau_N)\) to the strength.
Bibliography


Appendix A

Experimental Data
Table A.1: Experimental handsheet data: bulk, $T I$ and $Z I$ for the feed pulp and different cuts

<table>
<thead>
<tr>
<th>Mesh Size</th>
<th>Length ($mm$)</th>
<th>Width ($\mu m$)</th>
<th>Curl Index</th>
<th>Coarseness ($\text{mg}^3/m$)</th>
<th>Pressure (psi)</th>
<th>Bulk ($\text{cm}^3/g$)</th>
<th>T.I. ($N\cdot m/g$)</th>
<th>Zero Span ($N\cdot m/g$)</th>
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</thead>
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<tr>
<td>Feed Pulp</td>
<td>2.4 ± 0.2</td>
<td>28 ± 1</td>
<td>0.17 ± 0.01</td>
<td>0.20 ± 0.01</td>
<td>Airdried ($\geq 5$)</td>
<td>3.6 ± 0.1</td>
<td>11.9 ± 0.5</td>
<td>16 ± 6</td>
</tr>
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<td>-</td>
<td>-</td>
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<td>-</td>
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<td>2.62 ± 0.05</td>
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<td>2.3 ± 0.1</td>
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Table A.2: Experimental handsheet data: bulk, TI and ZI for the M14 fraction and different cuts

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<th>Bulk (cm³/g)</th>
<th>T.I. (Nm/g)</th>
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<td>3.3 ± 0.2</td>
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Table A.3: Experimental handsheet data: bulk, TI and ZI for the M28 fraction and different cuts

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<td>40</td>
<td>2.6 ± 0.1</td>
<td>7.6 ± 0.8</td>
<td>20 ± 1</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>60</td>
<td>2.5 ± 0.1</td>
<td>8.0 ± 0.6</td>
<td>15 ± 2</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>80</td>
<td>2.4 ± 0.2</td>
<td>8.8 ± 0.6</td>
<td>16 ± 3</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>100</td>
<td>2.25 ± 0.02</td>
<td>10.1 ± 0.4</td>
<td>13 ± 3</td>
</tr>
</tbody>
</table>
### Table A.4: Experimental handsheet data: bulk, TI and ZI for the M48 fraction and different cuts

<table>
<thead>
<tr>
<th>Mesh Size</th>
<th>Length (mm)</th>
<th>Width (µm)</th>
<th>Curl Index</th>
<th>Coarseness (mg/m)</th>
<th>Pressure (psi)</th>
<th>Bulk (cm³/g)</th>
<th>T.I. (Nm/g)</th>
<th>Zero Span (Nm/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>48 Mesh</td>
<td>1.65 ± 0.03</td>
<td>26.7 ± 0.8</td>
<td>0.139 ± 0.009</td>
<td>0.184 ± 0.004</td>
<td>Airdried (≈5)</td>
<td>4.4 ± 0.1</td>
<td>7.0 ± 0.4</td>
<td>9 ± 2</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>20</td>
<td>2.79 ± 0.05</td>
<td>13.5 ± 0.6</td>
<td>9 ± 3</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>40</td>
<td>2.5 ± 0.1</td>
<td>15.1 ± 0.6</td>
<td>10 ± 4</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>60</td>
<td>2.4 ± 0.1</td>
<td>16.0 ± 0.7</td>
<td>12 ± 5</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>80</td>
<td>2.2 ± 0.1</td>
<td>19.4 ± 0.4</td>
<td>20 ± 4</td>
</tr>
<tr>
<td>(coarse cut)</td>
<td>1.4 ± 0.1</td>
<td>-</td>
<td>0.14 ± 0.07</td>
<td>-</td>
<td>Airdried (≈5)</td>
<td>3.8 ± 0.1</td>
<td>4.8 ± 0.5</td>
<td>16 ± 1</td>
</tr>
<tr>
<td>-</td>
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<td>-</td>
<td>20</td>
<td>2.71 ± 0.06</td>
<td>8.3 ± 0.5</td>
<td>14 ± 8</td>
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<tr>
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<td>-</td>
<td>40</td>
<td>2.43 ± 0.04</td>
<td>10.1 ± 0.4</td>
<td>13 ± 2</td>
</tr>
<tr>
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<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>60</td>
<td>2.31 ± 0.05</td>
<td>10.9 ± 0.8</td>
<td>12 ± 2</td>
</tr>
<tr>
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<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>80</td>
<td>2.17 ± 0.03</td>
<td>12 ± 1</td>
<td>13 ± 1</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>100</td>
<td>2.15 ± 0.01</td>
<td>12.2 ± 0.3</td>
<td>17 ± 4</td>
</tr>
<tr>
<td>(Fine cut)</td>
<td>1.2 ± 0.3</td>
<td>-</td>
<td>0.12 ± 0.06</td>
<td>-</td>
<td>Airdried (≈5)</td>
<td>3.83 ± 0.08</td>
<td>7.4 ± 0.6</td>
<td>13 ± 2</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>20</td>
<td>2.66 ± 0.05</td>
<td>12 ± 1</td>
<td>18.0 ± 0.7</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>40</td>
<td>2.3 ± 0.1</td>
<td>14 ± 1</td>
<td>18 ± 1</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>60</td>
<td>2.26 ± 0.07</td>
<td>14.6 ± 0.7</td>
<td>19 ± 2</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>80</td>
<td>2.15 ± 0.06</td>
<td>16 ± 1</td>
<td>17.8 ± 0.5</td>
</tr>
<tr>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>100</td>
<td>2.04 ± 0.01</td>
<td>16.5 ± 0.4</td>
<td>19 ± 4</td>
</tr>
</tbody>
</table>
Appendix B

Matlab Codes
function [TotalCrossings,RBA,MPixel,M,BasisWeight]=cgrnc2(Lf,w,t,No)
%Returns the Total Number of Fibre Crossings, The RBA, The Maximum
%Pixel
%Value, The Mean Pixel Value and the Basis Weight assuming a constant
%voids fraction and a fibre density. The Inputs are the Fibre
%Length, The
%fibre Width, Fibre Thickness and the Total Number of Fibres
fdensity=1200*(10^3);%Fiber density in kg/m3
%

-------------------------------------------------------------

---------

$$$$$$$$$$$$$$$$$$$$$$$$Creating the area the
sheet$$$$$$$$$$$$$$$$$$$$$$$$
%
-------------------------------------------------------------

---

Lmm=5;%Edge of Network Length in mm
Lpixel=1500;%Edge of Network in Pixels
CANVAS=zeros(Lpixel,Lpixel);
pixelArea=((Lmm/Lpixel)^2)*(10^-6);
%Fiber dimensions Conversion for mmXmm canvas:
%w in micrometers
%Lf in mm
wp=w*(10^-3)*Lpixel/Lmm;
Lfp=Lf*Lpixel/Lmm;
%

-------------------------------------------------------------

---------

$$$$$$$$$$$$$$$$$$$$$$$$Creating a Mask to avoid edge
effects$$$$$$$$$$$$$$$$$$$$$$$$
%
-------------------------------------------------------------

---

MaskSize=0.9;%Mask dimension factor (fraction of full length)
%Vector of x coordinates delimiting the mask:
x=[(1-MaskSize)*Lpixel MaskSize*Lpixel MaskSize*Lpixel (1-MaskSize) ]
% Vector of y coordinates delimiting the mask:
y = [(1 - MaskSize) * Lpixel (1 - MaskSize) * Lpixel MaskSize * Lpixel
     MaskSize * Lpixel];
Mask = poly2mask(x, y, Lpixel, Lpixel);
MaskArea = (MaskSize * Lmm^2 * (10^-3))^2;

%%% Random deposition of fibres to create Network

Network = zeros(Lpixel, Lpixel);
p = 0;
while p < No
    Xp = rand(1) * Lpixel;
    Yp = rand(1) * Lpixel;
    Alpha = rand(1) * pi;
    Xf1 = Xp + (-Lfp/2) * cos(Alpha) + (wp/2) * (-sin(Alpha));
    Yf1 = Yp + (-Lfp/2) * sin(Alpha) + (wp/2) * cos(Alpha);
    Xf2 = Xp + (-Lfp/2) * cos(Alpha) + (wp/2) * (-sin(Alpha));
    Yf2 = Yp + (-Lfp/2) * sin(Alpha) + (wp/2) * cos(Alpha);
    Xf3 = Xp + (Lfp/2) * cos(Alpha) + (wp/2) * (-sin(Alpha));
    Yf3 = Yp + (Lfp/2) * sin(Alpha) + (wp/2) * cos(Alpha);
    Xf4 = Xp + (Lfp/2) * cos(Alpha) + (wp/2) * (-sin(Alpha));
    Yf4 = Yp + (Lfp/2) * sin(Alpha) + (wp/2) * cos(Alpha);
    temp = roipoly(CANVAS, [Xf1, Xf2, Xf3, Xf4], [Yf1, Yf2, Yf3, Yf4]);
    Network = Network + temp;
end
Network = -Mask;
display('the number of fibres is'); p = p + 1
BasisWeight = ((fdensity*t*(10^-6)*pixelArea)/MaskArea) * sum(sum Network)
(Network))
end
M=max(max(Network));

%Calculating the Number of fibre crossings
for k=1:(M-1)
   BW = Network > k ;
   L = bwlabel(BW);
   s = regionprops(L, Network, {'Area'});
   Crossing(k)=numel(s);
end
TotalCrossings=sum(Crossing);

%Calculating the RBA
BW2 = Network > 0 ;
L2 = bwlabel(BW2);
sRBA = regionprops(L2, Network, {'Area'});
CrossedAreas=numel(sRBA);
for i=1:CrossedAreas
   AreaCrossingsPixel(i)=(sRBA(i).Area(1));
end
TotalUnbondedAreaCrossingsPixel=2*sum(AreaCrossingsPixel);
TotalFiberAreaPixel=2*sum(sum(Network));
%Calculated RBA:
RBA=(1-(TotalUnbondedAreaCrossingsPixel/TotalFiberAreaPixel));
%Mean Pixel Value (related to thickness of the sheet):
MPixel=mean(mean(Network));
function [TotalCrossings CoverageV]=VGrnc(W,No,sigmaxW)
%This Function Returns the Total Number of Fibre Crossings Vector
%and the Coverage Vector.
%The input is the Fibre Width, the total number of fibres and the
%width
%standard deviation. The fibre length can be changed in the code, it
%has
%been set to 2mm.
%Creating the area the sheet----
Lmm=5; %Length of Paper in mm
Lpixel=1500; %Length of Paper in pixels
CANVAS=zeros(Lpixel,Lpixel);
pixelArea=(Lmm*(10^-3)/Lpixel)^2; %Area of a pixel in m2
%$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$ Fibre Properties
$Lf=2;
Lfp=Lf*Lpixel/Lmm; %Length in pixels
%
---
%$$$$$$$$$$$$$$$$$$$$$$$$$$ Width Distribution PDF
%$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
%
---
%PDF:
Prob=@(x) (1/(sigmaxW*sqrt(2*pi)))*exp(-0.5*((x-W).^2)/(sigmaxW^2));
%Bin lengths and Number of fibres in each bin
BinL=1;
Wmax=60;
xbin=[0:BinL:Wmax];
%Discrete distribution:
for i=1:length(xbin)-1
    Nbin(i)= floor( (( Prob(xbin(i+1))+Prob(xbin(i)) )/2 )*BinL*No);
    Wbin(i)= ( xbin(i+1)+xbin(i) )/2;
end
No=sum(Nbin); %Adjusted Number of fibers
Wfp=Wbin.*Lpixel/Lmm;%Width vector in pixels
%Creating Fibre basket
Wtot=[];
for k=1:length(Wbin)
    if Nbin(k)>0
        temp=ones(1,Nbin(k)).*Wbin(k);
    else
temp=[];
    end
Wtot=[Wtot,temp];
end
%shuffle of basket
Wtot2=Wtot;
i=1;
while length(Wtot2)>0
    tempRand=floor(rand(1)*length(Wtot2)+1);
    Wall(i)=Wtot2(tempRand);
    Wtot2(tempRand)=[];
    i=i+1;
end
Wallp=Wall.*Lpixel/(Lmm*(10^-3));%Width in pixels
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% %
%%
%Creating a Mask
MaskSize=0.9;
x=([1-MaskSize]*Lpixel MaskSize*Lpixel MaskSize*Lpixel (1-MaskSize) %
*Lpixel];
y=([1-MaskSize]*Lpixel (1-MaskSize)*Lpixel MaskSize*Lpixel %
MaskSize*Lpixel];
Mask = poly2mask(x,y,Lpixel,Lpixel);
MaskArea=((2*MaskSize-1)*Lmm*(10^-3))^2;
MaskAreaP=((2*MaskSize-1)*Lpixel)^2;
%-------------------------------------------------------------------
%%%%$$$$$$$$$$$$$$ Creating the Random Network$$$$$$$$$$$$$$ %
%-------------------------------------------------------------------
Network=zeros(Lpixel,Lpixel);
N=1; count=1; q=1;
while N<N0
Xp=rand(1)*Lpixel;
Yp=rand(1)*Lpixel;
Alpha=rand(1)*pi;
Xf1=Xp+(-Lfp/2)*cos(Alpha)+(-Wallp(count)/2)*(-sin(Alpha));
Yf1=Yp+(-Lfp/2)*sin(Alpha)+(-Wallp(count)/2)*cos(Alpha);

Xf2=Xp+(-Lfp/2)*cos(Alpha)+(-Wallp(count)/2)*(-sin(Alpha));
Yf2=Yp+(-Lfp/2)*sin(Alpha)+(-Wallp(count)/2)*cos(Alpha);

Xf3=Xp+(Lfp/2)*cos(Alpha)+(-Wallp(count)/2)*(-sin(Alpha));
Yf3=Yp+(Lfp/2)*sin(Alpha)+(-Wallp(count)/2)*cos(Alpha);

Xf4=Xp+(Lfp/2)*cos(Alpha)+(Wallp(count)/2)*(-sin(Alpha));
Yf4=Yp+(Lfp/2)*sin(Alpha)+(Wallp(count)/2)*cos(Alpha);

temp=roipoly(CANVAS, [Xf1,Xf2,Xf3,Xf4], [Yf1,Yf2,Yf3,Yf4]);
Network=Network+temp;
Network(-Mask) = 0;
Coverage=sum(sum(Network))/MaskAreaP;
display('the coverage is'); Coverage
display('the Number of fibres is'); N
count=count+1;

M=max(max(Network));
%Calculating the number of crossings on P intervals
if N/30==floor(N/30)
  for k=1:(M-1)
    BWI = Network > k ;
    L = bwlabel(BWI);
    s = regionprops(L, Network, {'Area'});
    Crossing(k)=numel(s);
    k;
  end
  TotalCrossings(q)=sum(Crossing);
  CoverageV(q)=Coverage;
  q=q+1;
  end
  N=N+1;
  end
end
%picture of Network
%LN=label2rgb(Network);
%Remove comment for visualization of the network
function [Height, MaxHeight, Af] = deposition2D(Lf, t, Nf)
% This function returns the Maximum, Mean Height and Total Fibre Area of a 
% 2D random deposition. The inputs are the Length of the fibres, the fibre 
% thickness and the total number of fibres 
% w = t; % fibre thickness in micrometers 
Lmm = 7; % Network Length in mm 
Lpixel = 1400; % Network length in Pixels 
Tpixel = 250; % Maximum Network Height in pixels 
CANVAS = zeros(Tpixel, Lpixel); 
pixelArea = ((Lmm/Lpixel)^2)*(10^-6); % pixel area in m^2 
pixelAreaum = ((Lmm/(Lpixel)*10^3)^2); % pixel area in micrometers^2 
ho = 10; 
wp = floor(w*(10^-3)*Lpixel/Lmm); 
LfP = Lf*Lpixel/Lmm; 
Initial = [zeros(Tpixel-ho, Lpixel); ones(ho, Lpixel)]; 
Game(:, :, 1) = Initial; 
N = 1; 
mFArea = 0; 
Xmin = Lfp; 
Xmax = Lpixel - Lfp; 
while N <= Nf 
Xp(N) = (Lpixel/Lmm) + rand(1) * (Lpixel - 2*(Lpixel/Lmm)); 
Yp = wp; 
XF1(N) = Xp(N) + (-Lfp/2); 
YF1(N) = Yp + (wp/2); 
XF2(N) = Xp(N) + (-Lfp/2); 
YF2(N) = Yp + (-wp/2); 
XF3(N) = Xp(N) + (Lfp/2); 
YF3(N) = Yp + (-wp/2); 
XF4(N) = Xp(N) + (Lfp/2); 
YF4(N) = Yp + (wp/2); 
Fibre(:, :, N) = roiopoly(CANVAS, [XF1(N), XF2(N), XF3(N), XF4(N)], [YF1(N), ~] 
XF2(N), YF3(N), YF4(N))}; 
% Fibre vertical Deposition 
Intersection(N) = 0; P(N) = 0;
while (Intersection(N)==0)
    MovingFibre(:,:,N)=imtranslate(Fibre(:,:,N),0,P(N)*wp);
    Network1(:,:,N)=Game(:,:,N)+MovingFibre(:,:,N);
    BW = Network1(:,:,N) > 1;
    L = bwblabel(BW);
    s = regionprops(L, Network1(:,:,N), {'Area'});
    Intersection(N)=numel(s);
    P(N)=P(N)+1;
end

%returning the fibre
del(N)=0;
while (Intersection(N)>0)
    dely=((P(N)-1)*wp)-del(N);
    MovingFibre(:,:,N)=imtranslate(Fibre(:,:,N),0,((P(N)-1)*wp)-
    del(N));
    Network1(:,:,N)=Game(:,:,N)+MovingFibre(:,:,N);
    BW = Network1(:,:,N) > 1;
    L = bwblabel(BW);
    s = regionprops(L, Network1(:,:,N), {'Area'});
    Intersection(N)=numel(s);
    del(N)=del(N)+1;
end

NetworkFibre=imtranslate(Fibre(:,:,N),0,((P(N)-1)*wp)-(del(N)-1));
IntFibre(:,:,N)=imtranslate(Fibre(:,:,N),0,((P(N)-1)*wp)-(del(N)-2));
NetInt(:,:,N)=Game(:,:,N)+IntFibre(:,:,N);

%Will the fibre rotate? if yes to which side?
Pivot=find(NetInt(:,:,N)>1);
PivotX1=ceil(Pivot(1)/Tpixel);
PivotX2=ceil(Pivot(length(Pivot))/Tpixel);
PivotY1=Pivot(1)-floor(Pivot(1)/Tpixel)*Tpixel;
PivotY2=Pivot(length(Pivot))-floor(Pivot(length(Pivot))/Tpixel)*Tpixel;
a(N)=Xf1(N)-PivotX1;
b(N)=Xf4(N)-PivotX2;
sign(N)=0;
if (abs(a(N))>0.5*Lfp)
    sign(N)=1;
    PivotPoint=PivotX1;
end
if (abs(b(N))>0.5*Lfp)
    sign(N)=-1;
    PivotPoint=PivotX2;
end

% In case of rotation:
if (sign(N)==1 || sign(N)==-1)
    Rotation=0; k=0;
    while (Rotation<1 && k<90)
        k=k+1
        delta=sign(N)*k;
        RotFibre=imrotatexy(NetworkFibre,delta,PivotPoint,PivotY1);
        Network2=Game(:,:,N)+RotFibre;
        BW2 = Network2 > 1 ;
        L2 = bwrlabel(BW2);
        s2 = regionprops(L2, Network2, {'Area'});
        Rotation=numel(s2)
    end

% Coordinates of final rotated fibre:
    delta=sign(N)*(k-2);
    RotFibre=imrotatexy(NetworkFibre,delta,PivotPoint,PivotY1);
    NetworkFibre=RotFibre;
end

% End of Rotation
N=N+1
    temp=Game(:,:,N-1)+NetworkFibre;
    temp(temp>1)=1;
    Game(:,:,N)=temp;
    mfArea=sum(sum(Game(:,:,N)))
end
D2=Game(:,:,N);
D3=imcrop(D2,[(Lpixel/Lmm) 0 Lpixel-2*(Lpixel/Lmm) Tpixel]);
Mf2=sum(sum(D3)); %sum of fibre area in pixels
%determining the network height (mean and max):
for j = Xmin:Xmax;
    i=0; cond=0;
    while cond==0;
        i=i+1;
        cond=D2(i,j);
    end
    MaxY(j-Xmin+1)=i;
end
Height=(Tpixel-mean(MaxY))*(Lmm/Lpixel)*10^3;
MaxHeight=(Tpixel-min(MaxY))*(Lmm/Lpixel)*10^3;
Af=(Mf2-(Lpixel-2*(Lpixel/Lmm))*ho)*pixelAreaum; %total fibre area in micrometer^2
end
function [Height MaxHeight FibreVolumeMeter Wsim tfsim]=deposition3D(Lf,W,tf,Nof)
%This function returns the mean height, maximum height, total fibre volume
%and corrected values of fibre thickness and width to adjust for the
%resolution of the 3D array.
% the inputs are the fibre length, fibre width, fibre thickness and
%the
% number of deposited fibres. This function uses other defined
%functions
% for volume rotation and image rotation
%
---

%Creating the Volume of the sheet

---

Lmm=5; %Edge of Network Length in mm
tmm=Lf; %Height of Network Length in mm
Lpixel=600; % Edge of Network in Pixels
Tpixel=floor(tmm*(Lpixel/Lmm));
pixelArea=((Lmm/Lpixel)^2)*(10^-6);
pixelVolume=((Lmm/Lpixel)^3)*(10^-9);
CANVAS=zeros(Lpixel,Lpixel);
Network=zeros(Lpixel,Lpixel,Tpixel);
Network(:,:,1)=ones(Lpixel,Lpixel);
Network(:,:,2)=ones(Lpixel,Lpixel);
Network(:,:,3)=ones(Lpixel,Lpixel);
Network(:,:,4)=ones(Lpixel,Lpixel);
%Pyramid=pyramid(0.5*Lpixel,0.5*Lpixel,1,Lpixel,0.15*Lpixel,[Lpixel,Lpixel,Tpixel]);
%Network=Pyramid;
%Fiber dimensions Conversion for mmXmm canvas:
w in micrometers
Lf in mm
tf in micrometers

wp=ceil(W*(10^-3)*Lpixel/Lmm);
Wsim=wp*(Lmm/Lpixel)*(10^3);
Lfp=Lf*Lpixel/Lmm;
tfp=ceil(tf*(10^-3)*Lpixel/Lmm);
tfpsim=tfp*(Lmm/Lpixel)*(10^3);
del=ceil(Lfp);

fdensity=1200*(10^3); %Fiber density in kg/m3

%------------------------------------------
---%
% Random deposition of fibres to create Network
%------------------------------------------
---%
Fn=1;
while Fn<=Nof

%creating the random position and angle for deposition:
Xp=rand(1)*Lpixel;

Yp=rand(1)*Lpixel;

Alpha=rand(1)*pi;

%vertices coordinates
Xf1=Xp+(-Lfp/2)*cos(Alpha)+(wp/2)*(-sin(Alpha));
Yf1=Yp+(-Lfp/2)*sin(Alpha)+(wp/2)*cos(Alpha);
Xf2 = Xp + (-Lfp/2) * cos(Alpha) + (-wp/2) * (-sin(Alpha));
Yf2 = Yp + (-Lfp/2) * sin(Alpha) + (-wp/2) * cos(Alpha);

Xf3 = Xp + (-Lfp/2) * cos(Alpha) + (-wp/2) * (sin(Alpha));
Yf3 = Yp + (-Lfp/2) * sin(Alpha) + (-wp/2) * cos(Alpha);

Xf4 = Xp + (Lfp/2) * cos(Alpha) + (wp/2) * (-sin(Alpha));
Yf4 = Yp + (Lfp/2) * sin(Alpha) + (wp/2) * cos(Alpha);

Fibre = roipoly(CANVAS, [Xf1, Xf2, Xf3, Xf4], [Yf1, Yf2, Yf3, Yf4]);

% Vertical fibre deposition:
P = 0; Intersection = 0;
while (Intersection == 0 && P < Tpixel)
    Temp = Network(:, :, Tpixel - P) + Fibre;
    BW = Temp > 1;
    L = bwlabel(BW);
    s = regionprops(L, Temp, {'Area'});
    Intersection = numel(s);
    P = P + 1;
end

IntersectedArea = 0;
for i = 1:numel(s)
    IntersectedArea = (s(i).Area) + IntersectedArea
end

if Intersection > 0
    s2 = regionprops(L, Temp, {'centroid'});
    Vc = s2.Centroid;
    Xc = floor(Vc(1));
    Yc = floor(Vc(2));
end

%--------------------------------------------------------
% Creating the 3D Fibre
%--------------------------------------------------------

75
Fibre3D=zeros(Lpixel,Lpixel,Tpixel);
for k=(Tpixel-P+2):(Tpixel-P+2)+tfp
    Fibre3D(:,:,k)=Fibre3D(:,:,k)+Fibre;
end

%picking the side of rotation;

A=[1 0 -cos(Alpha) 0;1 0 0 -sin(Alpha);0 1 -sin(Alpha) 0;0 1 0 cos(Alpha)];
Result=inv(A)*[Xp Xc Yp Yc]';
Xr=Result(1);
Yr=Result(2);
Lambda=Result(3);
turnright=0;

if ( Lambda<0 && IntersectedArea<(wp*Lfp*0.5) )
    turnright=1;
end

if ( Lambda>0 && IntersectedArea<(wp*Lfp*0.5) )
    turnright=-1;
end

%In case of rotation:
if (turnright == 0)
    %Creating Height Matrix
    for i=1:Lpixel
        for j=1:Lpixel
            k=Tpixel; cond=0;
            while cond==0
                cond=Network(i,j,k);
                k=k-1;
            end
            MaxZ(i,j)=k;
        end
    end
end
if turnright==1
    MaxOZ=imrotatexy2(MaxZ,Alpha*180/pi,Xr,Yr,
Lfp);
end
if turnright==-1
    MaxOZ=imrotatexy2(MaxZ,Alpha*180/pi+180,Xr,
Yr,Lfp);
end
%Crop Matrix

MaxOZ=imcrop(MaxOZ,[Xr Yr-0.5*wp 0.5*Lfp+abs
(Lambda) wp]);

%create MaxZ vector:

maxV=max(MaxOZ);
maxV(maxV==Tpixel-P+2)=0;

%initialization
Lv=1; condv=0; verify=0; beta=0;

%finding the angle of rotation
while (verify==0 & condv<=Lv)
    beta=beta+(pi/180)
    level=sin(beta)*[1:length(maxV)];
    Zrf=Tpixel-P+2-level;
    Intlocation=(Zrf<=maxV);
    verify=sum(Intlocation);
    if verify>0
        v=find(Intlocation==1);
    else v=0;
    end
    Lv=(0.5*Lfp+abs(Lambda))*cos(beta);
    condv=max(v);
end
angle=beta*turnright*(-1)*180/pi
Fibre3D = volrotate3(Fibre3D, Xr, Yr, Tpixel-P+3, 0, \cos(\text{Alpha}) \times \text{angle}, -\sin(\text{Alpha}) \times \text{angle}, \text{del});
end

Network = Network + Fibre3D;
Network(Network>1) = 1;
Fn = Fn + 1
FibreVolumePixel = sum(sum(Network));
FibreVolumeMeter = FibreVolumePixel * pixelVolume;
end

% Toshow = Network(:, :, 5:Tpixel);
% volshow(Toshow)

for i = 1:Lpixel
    for j = 1:Lpixel
        k = Tpixel; cond = 0;
        while cond == 0;
            cond = Network(i, j, k);
            k = k - 1;
        end
        MaxZ(i, j) = k;
    end
end

HeightPixel = sum(sum(MaxZ))/numel(MaxZ);
Height = ((Lmm/Lpixel) * (10^3)) * HeightPixel;
MaxHeightPixel = max(max(MaxZ));
MaxHeight = ((Lmm/Lpixel) * (10^3)) * MaxHeightPixel;
end
function [Final]=volrotate3(Vol,X,Y,Z,degX,degY,degZ,del)
% This function rotates a 3D array cropped to a cube of length del
% A is the original array and X, Y and Z are the location of the center of
% rotation and degX, degY and degZ are the angles of rotations (in the principle axes.
sizeV=size(Vol);
  sizeY=sizeV(1);
  sizeX=sizeV(2);
  sizeZ=sizeV(3);
  Final=zeros(sizeY,sizeX,sizeZ);

% Rotation around Y axis:
  for i=1:sizeY
    imY=Vol(i,:,:);
    imY=reshape(imY,sizeX,sizeZ);
    Final(i,:, :)=imrotatexy2(imY,degY,Z,X,del);
  end

% Rotation around X axis:
  for j=1:sizeX
    imX=Final(:,j,:);
    imX=reshape(imX,sizeY,sizeZ);
    Final(:,j,:) = imrotatexy2(imX,degX,Z,Y,del);
  end

% Rotation around Z axis:
  for k=1:sizeZ
    imZ=Final(:, :,k);
    Final(:, :,k) = imrotatexy2(imZ,degZ,X,Y,del);
  end
end
function Mnew=imrotatexy2(A,alpha,X,Y,del)
%This function rotates an image (2D array) cropped to a square of
%length del
%A is the original array and X and Y are the location of the center
%of
%rotation
sizeV=size(A);
sizex=sizeV(1);
sizexy=sizeV(2);
Xc=sizex/2;
Yc=sizexy/2;
Mnew=zeros(sizexy,sizex);
A=imtranslate(A,(Xc-X),(Yc-Y));
A=imcrop(A,[Xc-0.5*del Yc-0.5*del del del]);
A=imrotate(A,alpha,'nearest','crop');

for i=max(1,floor(0.5*del-Y)+1):min(floor(del),floor(sizexy-Y)+0.5*del)
    for j=max(1,floor(0.5*del-X)+1):min(floor(del),floor(sizex-X)+0.5*del)
        Mnew(i+ceil(Y-0.5*del),j+ceil(X-0.5*del))=A(i,j);
    end
end
end