3D Fiber Models to Simulate and Optimize Tissue Materials

Flávia P. Morais,[a,*] Ana M. M. S. Carta,[b] Maria E. Amaral,[a] and Joana M. R. Curto [a,c]

Tissue materials development using 3D computational tools to predict the influence of the combination of different fibers can be employed in the design of innovative tissue products and furnish optimization. Fibrous materials can be designed using different 3D fiber models for each type of fibers, detailed to the point where the wall fiber thickness, fiber lumen, and collapse degree are considered and presented in this work. *Eucalyptus*, *Pinus*, and *Picea* kraft cellulose pulp fibers were selected because they are representative of differentiated fiber types. The fiber morphological measurements were obtained using two methods: one uses the fibers in suspension, without restraints, and the other uses a capillary fiber alignment. The results indicate good repeatability for both methods but differences of 14% for fiber length weighted in length, 2% for fiber width, 11% for coarseness, 35% for curl, and 88% for fines content. Scanning electron microscopy images were used to identify the fiber dimensions inside the tissue structure. Four different types of fiber models for eucalyptus fibers, with different fiber wall thickness and lumen dimensions, were presented and used to predict 3D computational fibrous structures.

Keywords: 3D Fiber model; Cellulose; Fibrous materials simulation; Tissue materials

*Contact information: a: Fiber Materials and Environmental Technologies Research Unit (FibEnTech-UBI), University of Beira Interior, Rua Marquês d'Ávila e Bolama, 6201-001, Covilhã, Portugal; b: Forest and Paper Research Institute (RAIZ), R. José Estevão, 3800-783, Eixo, Aveiro, Portugal; c: Chemical Process Engineering and Forest Products Research Centre (CIEPQPF), University of Coimbra, R. Sílvio Lima, Polo II, 3004-531, Coimbra, Portugal; *Corresponding author: flavia.morais@ubi.pt*

INTRODUCTION

Natural cellulosic fibers are structural elements with high relevance to produce paper materials, such as tissue products. The three-dimensional (3D) tissue paper structure is directly influenced by the fiber type in its composition, and consequently, this structure affects the performance of tissue products. Pulp fibers can have different origins, namely hardwood and softwood species, and different dimensions and characteristics, depending on the pulping process to which they are subjected (Paavilainen 2002). In this way, the tissue paper properties required by the consumer can be obtained or improved by fibers selection (de Assis *et al*. 2018). Therefore, it is necessary to know the fibers morphological properties suitable for tissue paper production to optimize the furnish management. Consequently, 3D fiber modeling is essential to simulate tissue papers, predicting their 3D structural properties that influence the final end-use properties.

According to Heikkurinen *et al.* (1991), the fiber properties can be classified according to their size distribution, including fibers length, width, wall thickness and coarseness, their shape, including curl and kink deformations, and their cell wall structure, including the flexibility and collapsibility properties. These concepts suggest that fiber characterization with precision can be difficult (Heikkurinen *et al*. 1991). There are several

automatic optical analyzers for fiber properties analysis available on the market, including FS-200, FQA (Fiber Quality Analyzer), FiberLab, MorFi, FiberMaster, Galai CIS-100, and FiberTester (Carvalho *et al.* 1997; Tourtollet *et al.* 2003; Guay *et al.* 2005; Meyers and Nanko 2005; Turunen *et al*. 2005; Hirn and Bauer 2006; Li *et al.* 2011). The measurement differences between these instruments are due to the different hardware and software designs (Li *et al.* 2011). Comparative results with the L&W FiberTester analyzer are scarce in the literature, as well as there are no studies available comparing the results between L&W FiberTester and MorFi analyzers.

All analyzers can measure fiber length, but the same is not true for fiber width measurements. However, the analyzers that can determine this property are correlated reasonably well, although differences in the absolute width levels are observed (Guay *et al.* 2005; Turunen *et al.* 2005). The fiber length influences the tissue paper strength properties; higher fiber length can individually establish more contacts between fibers in the 3D paper structure (Trepanier 2017). Almost all fiber analyzers are unable to measure the fiber wall thickness. Therefore, this property is often determined using other image analysis techniques (Kibblewhite and Bailey 1988; Chinga *et al.* 2007) such as confocal laser scanning microscopy (CLSM) (Jang *et al.* 1996) or scanning electron microscopy (SEM) (Reme *et al.* 2002). SEM also allows measuring the fiber effective thickness (fiber wall plus lumen) in the Z direction of the 3D paper structure (Morais *et al.* 2020a). The effective fiber thickness morphology measured in the paper structure is the main fiber parameter that influences the 3D paper structure, thickness, bulk, porosity, and end-use properties. The fiber coarseness is related to the width and fiber wall thickness (Nordström and Hermansson 2018). The fiber coarseness and fiber length are inversely proportional to the fiber population. These three fiber properties have an important impact on apparent paper density. Measuring this property accurately in fiber analyzers is difficult because only a small amount of dry fiber mass is analyzed, and there is a lot of debris, such as fibrils and fines, in industrial pulps (Paavilainen 1993a). Fibers with equivalent coarseness can have very different fiber effective thickness dimensions. Therefore, the fiber properties are affected not only by the coarseness, but also by the relationship between fiber width, wall thickness, and lumen (Paavilainen 1993a; Curto *et al.* 2009). In addition, fiber collapse in the 3D paper structure has a major impact on tissue paper structure-related properties. In order to describe the relationship between the fiber cross-sectional dimensions and the paper structural properties, different parameters, such as the Runkel coefficient and the flexibility coefficient, were established (Dutt and Tyagi 2011). These factors are associated with stiffness or flexibility properties and fiber collapsibility (Paavilainen 1993b). Fiber flexibility is also directly related to the fiber relative bonding area (RBA) in the 3D paper structure. RBA is the parameter that best defines the paper structure and the fiber bonding degree. Consequently, this parameter can be calculated from the fiber flexibility coefficient, estimating the fiber bonding, and predicting the tissue paper strength properties (Tao and Liu 2011). Therefore, a combined analysis of coarseness and these parameters may result in a much more accurate interpretation of the results.

Fibers present deformations throughout the pulp production process (Page *et al.* 1985). The fiber wall morphological properties affect the development of these fiber deformations. In tissue paper production, the use of curly fibers decreases the tensile index properties and, consequently, increases the softness properties (Morais *et al.* 2020b). Therefore, deformations increase contributes to a more open 3D paper structure, with less inter-fiber bonding, and consequently, an increase in bulk, porosity, and absorption properties (Trepanier 2017). In addition to the fiber deformations, the fine elements present

in cellulose pulps also have an impact on the tissue paper properties. In the 3D paper structure, the fines fill the voids between fibers, creating a more organized and closed structure, which contributes to the inter-fiber bonding increase and bulk decrease (Odabas *et al.* 2016).

Due to strong competition, the tissue industry is looking for innovative methods to analyze the behavior of the tissue paper properties. The influence of fibers morphological properties reveals the need for 3D fiber modeling. Several 3D computational simulation studies of the fibers impacts on the paper properties have been developed over the years (Kallmes and Corte 1960; Niskanen and Alava 1994; Bloch and Roscoat 2009; Curto *et al.* 2011; Lavrykov *et al.* 2012; Marulier *et al.* 2015). However, this study is the first to use different 3D fiber models to simulate tissue materials.

The main goal of the present work is to identify the 3D fiber model for each type of fiber and to use it in 3D fiber based computational simulations for the tissue materials. For this purpose, the measurements from two different fiber analyzers were compared on different pulp mills suitable for tissue paper materials.

EXPERIMENTAL

Materials

Industrial hardwood and softwood virgin fiber pulp mills were selected for this study (Table 1). The selected pulps presented the morphological and final end-use properties suitable for their use in tissue paper production, as shown previously (Morais *et al.* 2019).

Table 1. Description of the Pulp Samples, Fiber Reference, the Type of Cooking, and the Bleaching Sequences Applied

Pulp Denomination	Fiber reference	Cooking	Bleaching Sequences*
EUC_1	*Eucalyptus* (Brazil)	Kraft	ECF (OECF)
EUC_2	*Eucalyptus* (Portugal)	Kraft	TCF (OOZPP)
EUC_3	*Eucalyptus* (Portugal)	Kraft	ECF (DEpDD)
Pinus_4	*Pinus* (Finland)	Kraft	ECF
Pinus_5	*Pinus* (Finland)	Kraft	TCF (OOQPo)
Pinus_Abies_6	*Pinus* and *Abies* (Sweden)	Kraft	ECF

* ECF: Elemental Chlorine Free; TCF: Total Chlorine Free. The description of the different bleaching sequences can be found in Morais *et al.* 2019

Methods

Before testing, pulp samples were disintegrated according to ISO 5263 (1995). The morphological properties of the six pulp samples were automatically analyzed by two fiber analyzers for comparison: MorFi LB01 Fiber Size Analyzer (TECHPAP, Grenoble, France) and Lorentzen & Wettre Fiber Tester (Kista, Sweden). Both instruments were calibrated and used according to the manufacturers' specifications. More detailed information about MorFi and FiberTester can be found in Tourtollet *et al.* (2003) and Li *et al.* (2011), respectively. Table 2 summarizes the major features of these analyzers. The MorFi equipment presents a high-resolution camera (4 μm/pixel) with non-polarized light, and the fiber suspensions are analyzed through a channel (Hirn and Bauer 2006). The Fiber

Tester equipment uses a 10 µm/pixel resolution camera with non-polarized light, and the fiber suspension is measured by a space between glass plates, which ensures good alignment of the fibers (Li *et al.* 2011). Because some air bubbles can be detected as fine elements when non-polarized light is applied, the two analyzers use a vacuum to remove the air before measurements.

Table 2. Features Characteristics of MorFi and Fiber Tester Analyzers

Analyzer	Camera resolution (µm/pixel)	Light	Measurement Cell Shape	Sample (mg)	Fiber population (million/g)	Fine elements
MorFi	4	Non-polarized	Channel	600	5-30000	Length < 200 µm and/or width < 5 µm
Fiber Tester	10	Non-polarized	Capillary	100	5-30000	Length < 200 µm

Diluted suspensions of 20 mg/L (for hardwoods samples) and 30 mg/L (for softwoods samples) were analyzed in the MorFi, while 10 mg/L (for both hardwoods and softwoods samples) were analyzed in the Fiber Tester. The pulp fiber properties, such as fiber length weighted in length, width, coarseness, curl, and fine elements, were determined by the two analyzers. The ratio between fiber length and fiber width was also determined (Dutt *et al.* 2011). The repeatability of the analyzers was determined with a total of five replicates of *Eucalyptus* kraft bleached pulp (sample EUC_3). For the other samples, triplicate assays were performed, and the properties average was reported.

In addition, the fiber wall and lumen dimensions were analyzed in 100 fibers of the pulps in suspension, using an optical microscope (Leitz Wetzlar, Wetzlar, Germany) with use of an integrated image analysis system (Leica Microsystems, IM500, Heerbrugg, Switzerland). From these measurements, the Runkel and flexibility coefficient were calculated (Dutt *et al.* 2011).

Using these pulp samples, a complementary study by SEM analysis was carried out in handsheets with basis weight of 20 g/m^2 produced according to an adaptation of the ISO 5269-1 (1998). This modification consisted of the suppression of the handsheet pressing process and the basis weight modification, to mimic tissue papers (Morais *et al.* 2020b). Therefore, the handsheets were cut and the cross-sections were covered with gold using a Sputter Quorum Q 15 OR ES (Laughton, East Sussex, UK) and analyzed by Hitachi S2700 SEM (Tokyo, Japan), with a Bruker detector (Karlsruhe, Germany) operating at +20 kV and at different magnifications.

A 3D simulator of fibrous materials (Conceição *et al.* 2010; Curto *et al.* 2011) was used to simulate the 3D structures with the fiber dimensions obtained experimentally. This simulator, named voxelfiber, is open source software, and the code is available on GitHub (https://github.com/eduardotrincaoconceicao/voxelfiber). Voxelfiber is a morphological simulator for porous materials that can be modeled as planar random networks, as is the case of tissue papers. The fibers are represented by a chain of voxels in a 3D discrete spatial grid, allowing the direct use of methods developed for the 3D image field. The 3D simulator uses the fiber dimensions and properties, such as length/width ratio, fiber wall thickness, lumen thickness, fiber flexibility, and resolution (number of layers in the thickness direction), in order to produce the resulting 3D structure made from these modeled fibers. The key property of fiber flexibility is implemented through the

mechanism originally proposed for the KCL-PAKKA simulator, by Niskanen and Alava (1994). A more detailed description of the 3D simulator can be found in Conceição *et al.* (2010) and Curto *et al.* (2011). An approach of different 3D fiber models, with different dimensions of fiber wall thickness and lumen, was also performed. The 3D computational structures will be processed to obtain important properties, such as apparent thickness, inter and intrafiber porosities. Computational studies were carried out using MATLAB® (R 2020a, 9.8.0.1323502, MathWorks, Natick, MA, USA).

Statistical Analysis

All data analysis was performed using Microsoft Excel Office 365, and statistical analysis was performed using independent samples t-test with a 95% confidence level with IBM SPSS Statistics 25 (Armonk, NY, USA).

RESULTS AND DISCUSSION

Fiber Pulps Morphology

The knowledge of the fibers 2D morphological properties of two different analyzers is an important milestone of pulp characterization. These properties influence the tissue product properties and are important for 3D fiber modeling in a realistic way. The fiber length is an important property because it influences the strength and the formation of the paper sheets, especially softwood fibers (de Assis *et al.* 2019). The fiber length weighted by length is the quotient of the sum of individual fiber lengths squared and the sum of the individual fiber lengths (Guay *et al.* 2005). From Fig. 1a, the MorFi results showed fiber length weighted by length between 0.71 and 1.96 mm, while the Fiber Tester results showed between 0.66 and 2.41 mm. Fiber Tester measurements averaged 14% higher than those of MorFi. The fiber lengths weighted by length showed a relative agreement between both analysis instruments for the hardwood samples, but the same did not happen for the softwood samples. These small differences may be due to the different image analysis systems of both methods, such as camera resolution, for example (Li *et al.* 2011). For both analysis instruments, fibers pulp EUC_3 and Pinus_Abies_6 were the longest of the hardwood and softwood samples, respectively.

The differences of fiber width were smaller compared with those of fiber lengths (Fig. 1b), and the MorFi results were on average 2% higher than the Fiber Tester. Fiber widths between 18 and 30.9 μm were obtained for the MorFi, while fiber widths between 17.6 and 40.0 μm were obtained for the Fiber Tester. Overall, these measurements of both equipment were in good agreement for all samples studied. Pulp EUC_3 was the widest of the hardwood samples for both analysis instruments; however, pulp Pinus_5 and pulp Pinus_Abies_6 were the widest of the softwood samples for MorFi and Fiber Tester, respectively. In the Fiber Tester, the largest fibers were also the longest, for both hardwood and softwood samples. The same did not occur for MorFi, as only the hardwood samples showed this trend. In addition, the slenderness ratio also showed some differences because the length and width measurements were also different in both analyzers. These differences were, again, more pronounced in softwood pulps. On average, the Fiber Tester results were 24% higher than the MorFi. This ratio is related to the handsheet density and strength properties, as the fibers with a good slenderness ratio are readily collapsed, producing good surface contact and inter-fiber bonds (Dutt *et al.* 2011; Joutsimo and Asikainen 2013). However, despite these small differences found, measurements of the length and width

properties on both analyzers did not show significant differences (Table 3). The critical value of student's *t* distribution with 10 degrees of freedom is 1.812, with 95% confidence level.

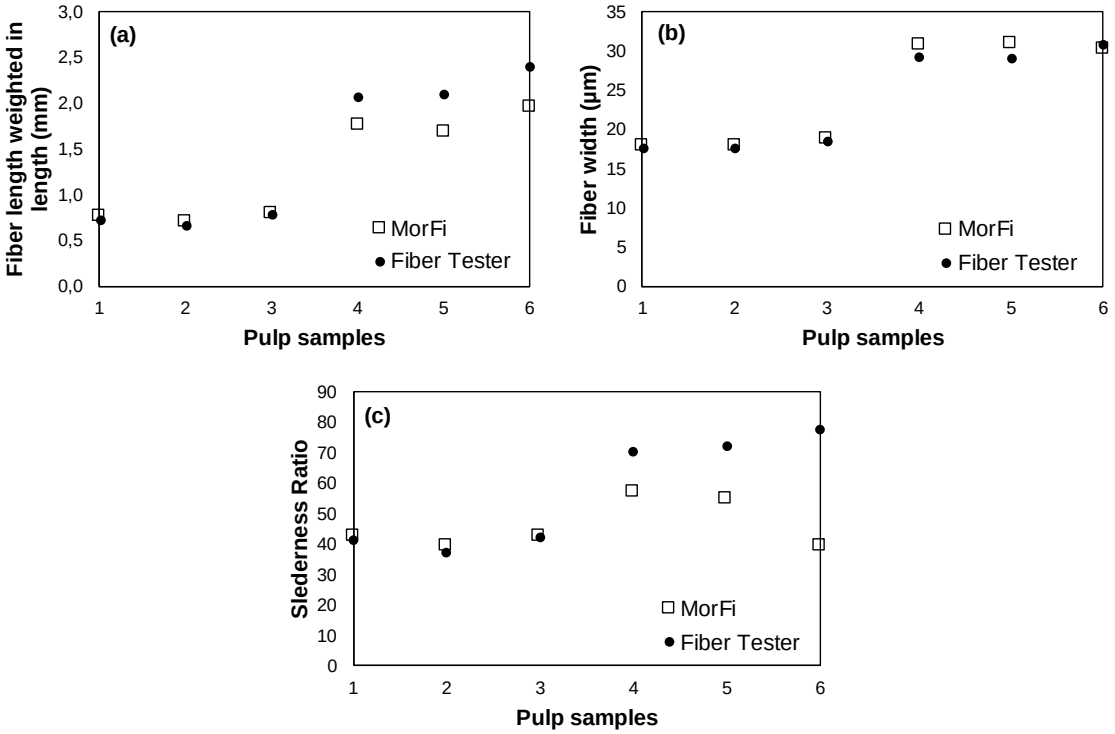

Fig. 1. Comparison of (a) fiber length weighted in length, (b) fiber width, and (c) Slenderness ratio between MorFi and Fiber Tester

Table 3. Statistical Analysis Using Independent Samples T-Test with 95% Confidence Level of the Parameters Analyzed in MorFi and FiberTester

	t*	df*	*p**
Length weighted in length	-0.793	10	0.446
Width	0.150	10	0.884
Coarseness	0.418	10	0.685
Curl	-2.192	10	0.053
Fine elements content	13.107	5.114	0.000
* t: t-values; df: degrees of freedom; *p*: significance level			

For the 3D tissue paper simulation process to be as realistic as possible, it is important to generate a 3D structure with the structural elements, the fibers, according to their distribution in the pulp furnish (Lavrykov *et al.* 2012). Therefore, the distribution of length and width properties studied for the six pulps by MorFi was considered (Fig. 2). In hardwood pulps, fiber lengths between 0.71 and 0.97 mm were further observed for pulp EUC_1 (38%) and pulp EUC_3 (37%), while pulp EUC_2 presented 38% of the fibers with lengths between 0.46 and 0.71 mm. Fibers with lengths larger than 1.74 mm were barely visible in these three samples. In softwood pulps, 49%, 51%, and 48% of the pulp Pinus_4, Pinus_5, and Pinus_Abies_6, respectively, presented lengths between 1.50 and

3.00 mm. Widths between 15 and 20 µm were mostly observed in the hardwood samples (35%, 34% and 30% of the pulp fibers EUC_1, EUC_2, and EUC_3, respectively) and between 30 and 50 µm in the softwood samples (46 %, 44% and 45% of the pulp fibers Pinus_4, Pinus_5, and Pinus_Abies_6, respectively). Overall, the pulps studied showed good distribution of fiber dimensions, concluding that both hardwood and softwood samples did not have only small and large dimensions, respectively, for the fiber lengths and widths.

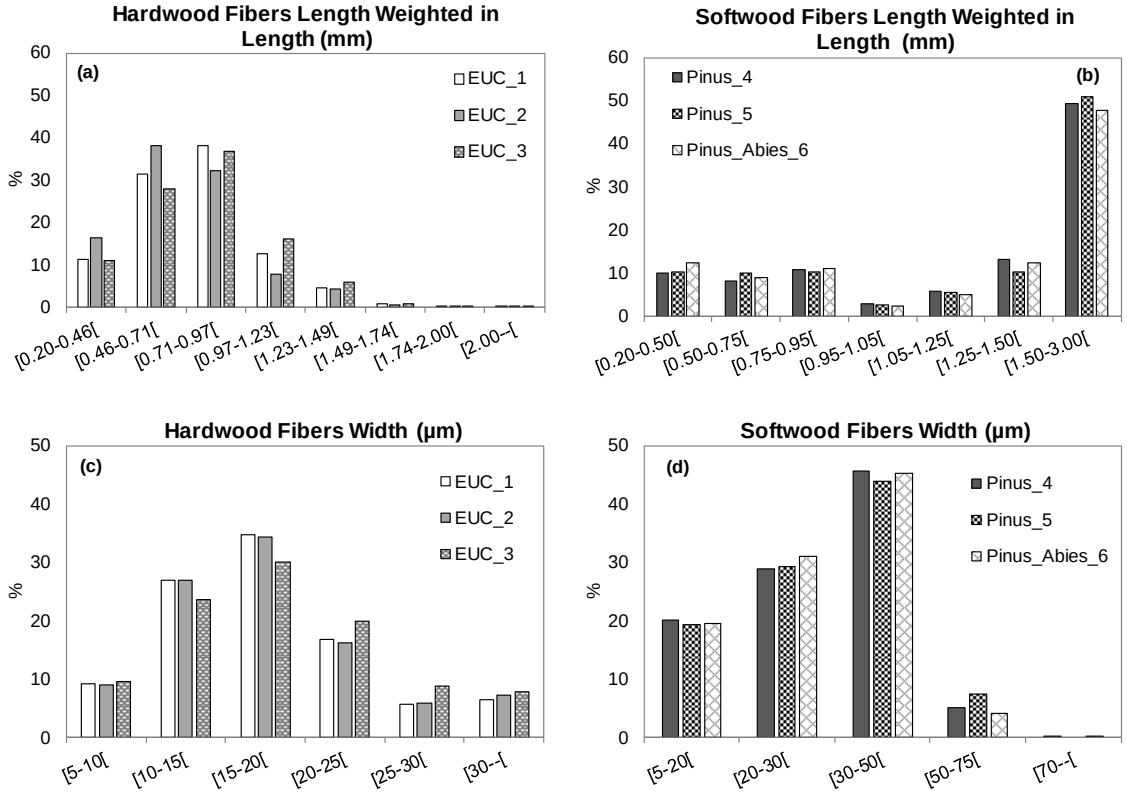

Fig. 2. Distribution of (a) hardwood and (b) softwood fibers length weighted in length, and (c) hardwood and (d) softwood fibers width, measured in MorFi

The fiber coarseness is defined as the oven-dried pulp mass per unit total fiber length, depending on the total number of fibers analyzed (Li *et al.* 2011). Coarseness is influenced by fiber thickness, width, and pulp fiber population (Curto *et al.* 2009). Therefore, it is also important to analyze factors that are related to fiber thickness, such as the Runkel and flexibility coefficients. However, these parameters are obtained with fibers in suspension, so the fiber morphology in water suspension or the paper structure can be different. Consequently, an analysis of the fiber effective thickness in the paper structure is essential to understand its influence on the tissue structural properties, model the third dimension of the fiber, and optimize the tissue structure-related properties (Morais *et al.* 2020a). From Fig. 3a, the results obtained for the coarseness by MorFi (values between 6.71 and 19.66 mg/100m) were on average 11% higher than those of Fiber Tester (values between 6.30 and 19.38 mg/100m). These results were obtained since the fiber length measured by MorFi was systematically smaller than that measured by Fiber Tester. The total number of fibers analyzed by MorFi (21.1 million/g for hardwood and 5.2 million/g for softwood) was even higher than those analyzed by Fiber Tester (19.3 million/g for

hardwood and 3.2 million/g for softwood). The higher Runkel index is related to the lower fiber collapse potential and the higher flexibility coefficient with the lumen diameter and, consequently, with the more flexible fibers. *Eucalyptus* fibers with high coarseness, Runkel coefficient, and low flexibility coefficient are ideal for tissue papers (de Assis *et al.* 2018). However, softwood fibers with low coarseness, Runkel coefficient, and good flexibility coefficient are desired to ensure the tissue strength properties and the paper machine runnability (de Assis *et al.* 2019). The Runkel and flexibility coefficients obtained for the six pulps did not present a linear correlation with the coarseness properties of MorFi or Fiber Tester (Fig. 3b). It is also for this reason that a complementary SEM analysis of the fiber thickness in the paper structure is important to follow the differences found for coarseness in both analyzers in order to identify the most realistic measurement with different hypotheses of 3D fiber modeling. Although the coarseness measurements of both analyzers were not comparable, they did not show significant differences (Table 3).

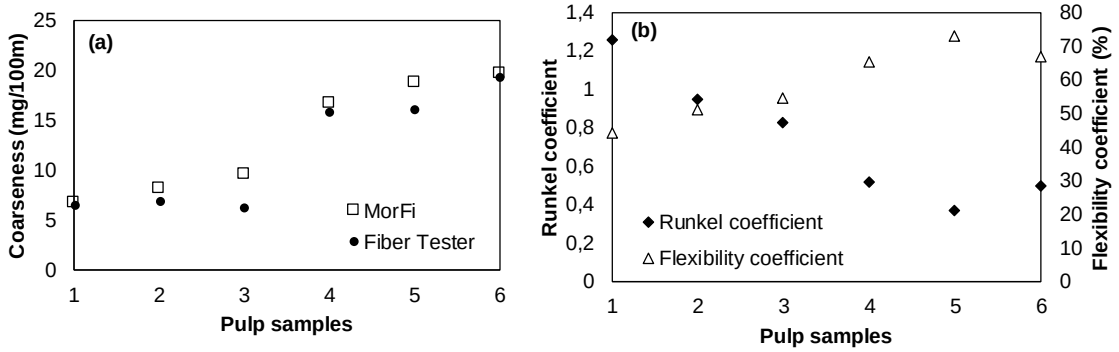

Fig. 3. Comparison of (a) fiber coarseness between MorFi and Fiber Tester, and (b) Runkel and flexibility coefficients of the six pulp samples

The fiber curl is described as the deviation from the fiber axis straightness (Li *et al.* 2011) and is important to achieve higher softness properties in tissue products (de Assis *et al.* 2018). From Fig. 4a, the results obtained for the curl by Fiber Tester (values between 9.2 and 22.6 %) were on average about 35% higher than those of MorFi (values between 8.6 and 14.4 %). These differences may be related to the higher fiber length obtained for the Fiber Tester, because the longer fibers are more likely there are to have a higher fiber curvature (Li *et al.* 2011). Despite these differences, the trend in the curl measurements was similar, and the two analyzers did not show statistically significant differences (Table 3). In addition, the fine elements (% in length) are defined as the quotient between the sum of the fines length and the total fibers and fines length in the samples (Guay *et al.* 2005). Higher fines content will promote better adhesion between the Yankee surface and the paper web (de Assis *et al.* 2018). From Fig. 4b, the MorFi showed fines content between 30.4 and 44.1%, while the Fiber Tester showed fines content between 4.2 and 5.9%. MorFi measurements averaged 88% higher than Fiber Tester. The fines content did not show a good relative agreement between both analyzers for the six samples. The independent t-test showed that, on average, both analyzers presented statistically significant differences for the fines content ($t(5.114) = 13.107$; $p < 0.05$), as presented in Table 3. The critical value of student's *t* distribution with 5 degrees of freedom is 2.015, with 95% confidence level. This may be due to the MorFi considers fine elements with lengths less than 0.2 mm and/or widths smaller than 5 μm, and Fiber Tester considers only lengths smaller than 0.2 mm. In general, the fines present in the pulps may not significantly affect fiber length measurements, but they affect the fiber coarseness measurements.

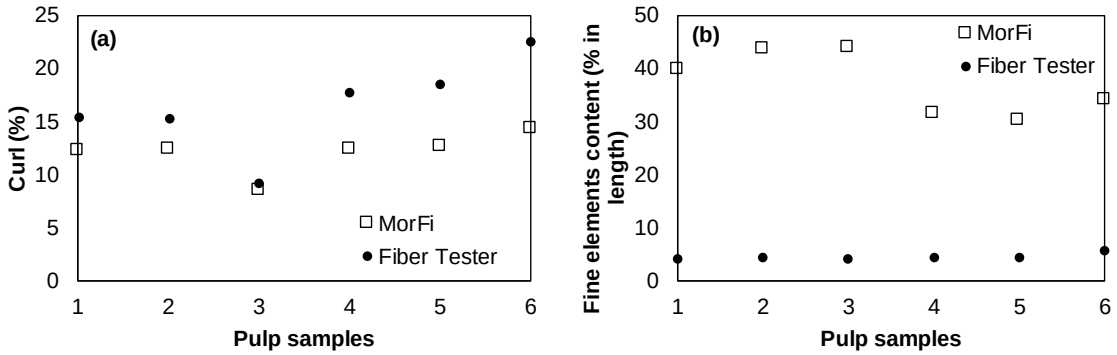

Fig. 4. Comparison of (a) fiber curl, and (b) fine elements content between MorFi and Fiber Tester

The repeatability of the assays was analyzed in five replicates of the pulp EUC_3. Both analyzers showed good repeatability, since low variation coefficient values were obtained for each parameter, as shown in Table 4. The fines content was the property with the highest variability for both analyzers; however, the Fiber Tester also showed some variability of the fiber curl measurements. Despite this good precision, the measurements of the properties analyzed for the six pulps cannot be compared. Both analyzers have different functionalities that must be considered when analyzing the measurements on each equipment.

Table 4. Repeatability of MorFi and Fiber Tester Performed in Five Replicates of the Pulp EUC_3

	Length Weighted in length (mm)	Width (µm)	Coarseness (mg/100m)	Curl (%)	Fine elements content (%)
*SV $_{MorFi}$	0.00	0.00	0.00	0.00	0.90
Mean $_{MorFi}$	0.80	18.80	9.56	8.60	44.10
*VC $_{MorFi}$	0.25	0.00	0.01	0.00	2.04
SV $_{Fiber\ Tester}$	0.00	0.10	0.00	0.10	0.10
Mean $_{Fiber\ Tester}$	0.79	18.60	6.30	9.20	4.20
VC $_{Fiber\ Tester}$	0.00	0.54	0.00	1.09	2.38
* SV: standard deviation; VC: variation coefficient					

Hypothesis for Different 3D Fiber Models

Cellulose fibers are complex structural elements with different properties that influence the structural properties of tissue materials. Designing a realistic 3D fiber model to make use of the fiber properties obtained experimentally is essential. The experimental planning reported in this work can serve as a source for the introduction of fiber dimensions in simulators based on 3D fiber modeling. Table 5 summarizes the fiber dimensions important to be implemented in these models, for example for the pulp EUC_3. The fiber effective thickness reported in this table was obtained through a previous study to analyze a significant number of fibers (322 fiber measurements) in the cross-section paper structure (Morais *et al.* 2020a). This study was carried out by the vector placement method in the SEM images of the handsheet cross-section structure made with pulp EUC_3. Obtaining this third fiber dimension allows investigating different approaches to modeling the fiber thickness realistically. This property, as previously mentioned, is related to the fiber

coarseness and the data from the two fiber analyzers showed differences for it. In order to understand the most correct coarseness value to simulate the 3D tissue paper structures, it is essential to model different hypotheses of the fiber wall and lumen dimensions and to understand which one relates effectively to the fiber coarseness of each analyzer. Our 3D computational simulator uses fiber properties such as fiber length/width ratio, fiber flexibility, fiber wall thickness, and fiber lumen, as input parameters, which is directly related to fiber coarseness. Therefore, through the modeling of 3D structures and different hypotheses, we can understand which fiber properties best reflects the fiber coarseness for the different pulps (in this case, EUC_3). As the coarseness showed differences in the two fiber analyzers, the computational simulator is also capable of predicting which coarseness best reflects the structural properties of the low basis weight structures produced and, consequently, optimizing the 3D modeling of these materials.

Table 5. Fiber Properties of Pulp EUC_3 Important for 3D Fiber Modeling, as Obtained by MorFi and Fiber Tester Analyzers

Analyzers	Length weighted in length (mm)	Width (µm)	Coarseness (mg/100m)	Fiber effective thickness (µm)*
MorFi	0.80	18.80	9.56	4.00
Fiber Tester	0.79	18.60	6.30	
* Third fiber dimension obtained by SEM according to the vector placement method in (Morais *et al.* 2020a)				

The fiber effective thickness of the pulp EUC_3 pulp (4 µm) includes the fiber wall and lumen, obtained from the paper structure, being different from that obtained from the fibers in water suspension. These differences are verified due to the tensions and pressures that the fibers are subjected in the paper formation, causing their collapse and variations in the cross-sectional fiber thickness (Kallmes and Bernier 1963). In SEM images, differentiating the fiber wall thickness and lumen is not always possible. Due to these pressures, the fibers can have different shapes, from tubular to ribbon, as shown in Fig. 5a. The fiber lumen may not be visible due to the fiber collapse (Fig. 5b). In other cases, the fibers can collapse differently and present different fiber wall thickness and lumen dimensions (Fig. 5c, d).

Due to the differences found in the 3D tissue paper structure, different hypotheses for fiber modeling were suggested for the EUC_3 pulp fibers (Fig. 6). According to the proposed collapse models, the fibers can have a fiber thickness without lumen (Fig. 6a) or with a lumen with different dimensions (Fig. 6b-d) according to the fiber collapsibility and conformability. The proposed fiber model in Fig. 6a presents only one thickness dimension. With different dimensions of fiber length, width and thickness, namely length less than 0.2 mm and widths smaller than 5 µm, this model can also describe the fines and fillers present in pulp EUC_3. Fiber deformations, namely fiber curl, were not considered for these fiber models. In these conditions, a 3D tissue paper structure can be simulated with the different proposed fiber models, according to the fiber size distribution in pulps (Fig. 2).

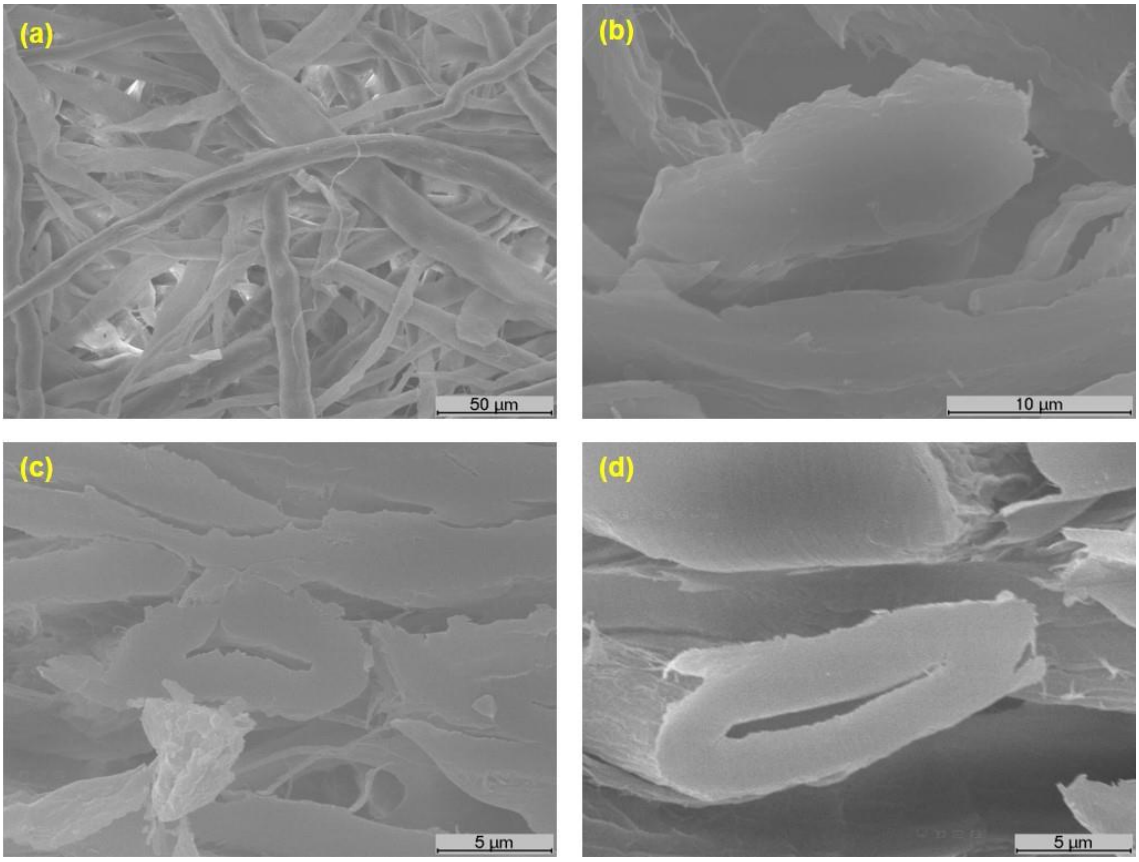

Fig. 5. SEM images of the (a) 3D network structure of handsheets with 20 g/m^2 made with pulp EUC_3 (magnification of 500x). SEM images of the fiber thickness in the cross-section of these handsheets, where a (b) fiber without lumen (magnification of 4000x) and (c, d) fibers with different lumen dimensions and shapes (magnification of 5000x) were visible

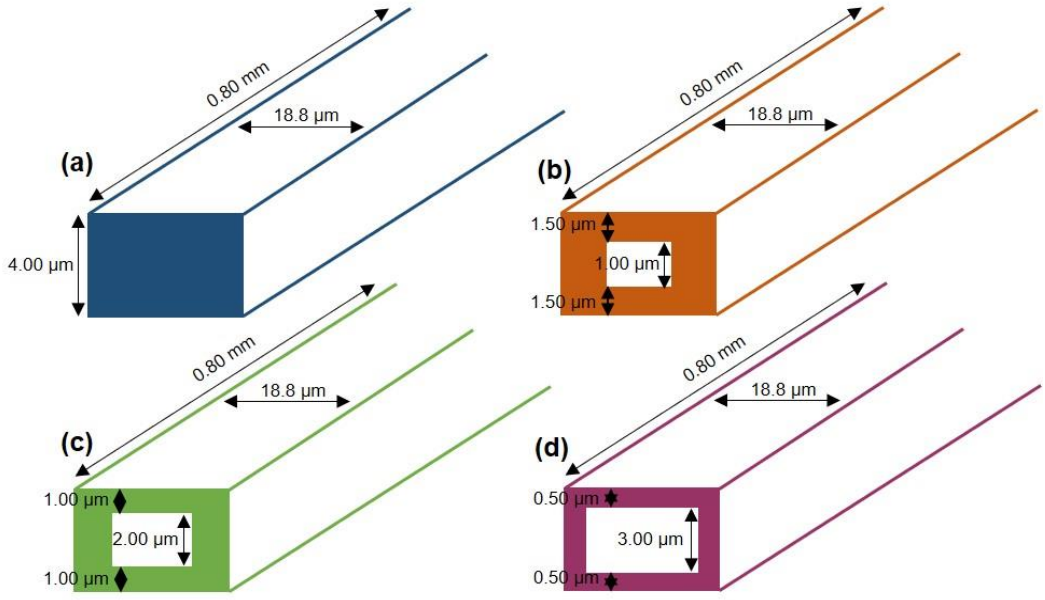

Fig. 6. The four 3D fiber models proposed for the eucalyptus fibers. The proposed models consist of (a) fiber without lumen, with a fiber thickness of 4 µm, or fibers with lumen with different dimensions, namely (b) 1 µm, (c) 2 µm and (d) 3 µm

Using the 3D fiber-based computational simulator, it was possible to model the fibers individually. The 3D structure was formed by the sequential fiber deposition and conformation to the existing structure. The simulation results (Fig. 7) were presented to study the different hypotheses of the fiber models and the variations in structural properties (Table 6). The model included the fiber properties shown in Table 5 and Fig. 6. To simulate the tissue materials, the 3D structures presented a basis weight of 20 g/m^2. The results showed that the different simulated fiber models formed structures with different thickness and inter- and intra-fiber porosities. These differences are due to the presence or absence of the lumen and its dimensions. It was evident that the different fiber collapse degrees had a great influence on the tissue structures' thickness. The thickness of the simulated structures (cross-section images of Fig. 7) increases with the increase of the lumen dimensions in the simulated fibers. As a lumen equal to zero corresponds to a fully collapsed fiber, the structures made with these fibers showed a low thickness. In contrast, the lumen equal to three, corresponding to approximately 75% of the fiber wall thickness, presents a structure with a thickness twice as large as the structure made with fibers without a lumen. On the other hand, the differences in the inter-fiber porosity were not significant according to the different fiber collapse models. The properties of intra-fiber porosity are in accordance with the increase of the fiber lumen. The different 3D fiber models can also be simulated simultaneously in order to form a more realistic 3D structure for tissue materials.

From this stage, a comparison of the computational and experimental structures can be performed in order to validate the predictive character of the structural properties of tissue papers, with the aim of optimizing the production of each type of tissue paper. An approach of combining experimental characterization and computational modeling contributes not only to valuable information for the study of the relationships between fibers and the network structures formed by them, but also to predict the influence of the combination of different fibers on the design of innovative tissue materials and furnish optimization.

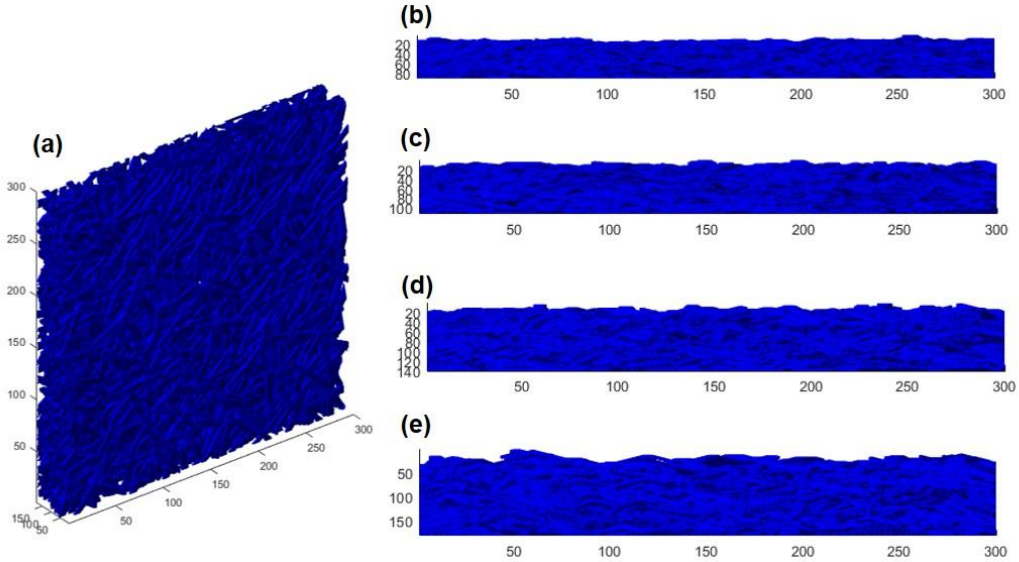

Fig. 7. Modeling results of different 3D structures simulated with fiber dimensions presented in Table 5 and Fig. 6. The computational simulator makes it possible to model a 3D structure that mimics tissue materials of low basis weight (20 g/m^2) (a), with different structural properties. The 3D structure thickness (cross-section image) is changed using different 3D fiber models: modeling of fibers without lumen (b) and with different lumen dimensions (c-e).

Table 6. Inputs and Outputs Parameters of 3D Computational Simulations Used to Produce the 3D Structures with Different Fiber Wall Thickness and Lumen

Input Parameters				Output Parameters		
Basis weight (g/m^2)	**Number of fibers**	**Fiber wall thickness***	**Lumen dimension***	**Apparent thickness***	**Interfiber porosity***	**Intrafiber porosity***
20	2720	2	0	70	0.5777	0.0000
20	2718	2	1	90	0.5909	0.2000
20	2684	2	2	114	0.6085	0.3333
20	2696	2	3	139	0.6268	0.4286
* Units in computational voxel						

CONCLUSIONS

1. In this study, a comparison of the morphological properties of the six pulps suitable for tissue papers in two fiber analyzers was performed in order to propose different 3D fiber models to realistically simulate the 3D structure of these materials, and consequently, optimize the furnish management and the final end-use properties of the tissue papers. The two analysis methods available contributed to a better perception of the differences found in the morphological properties in both analyzers, which are essential for a realistic 3D modeling of the fiber properties, as is the case of the coarseness properties, to simulate tissue paper materials.
2. The results showed that both analyzers presented good repeatability but different fiber properties measurements. Compared to MorFi, FiberTester measurements were, on average, 14% and 35% higher for fiber length and curl, respectively, and 2%, 11%, and 88% lower for fiber width, coarseness and fines content, respectively. Statistically, the two methods are not comparable to the fines' properties.
3. The 3D fiber modeling together with the study of obtaining 3D data of the fibers and the structures formed by them was essential to propose different fiber models and simulate them in the computational simulator. Four different types of fiber models for eucalyptus fibers, with different fiber wall thicknesses and lumen dimensions, were used to simulate the 3D fibrous structure more accurately and, consequently, predict tissue paper properties, in order to optimize the various types of tissue materials.

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