

Modelling Fiber Network Materials: Micromechanics, Constitutive Behaviour and AI

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Academic Dissertation which, with due permission of the KTH Royal Institute of Technology, is submitted for public defense for the Degree of Doctor of Philosophy on Friday the 20th of October 2023, at 09.00 A.M. in Kollegiesalen, Brinellvägen 8, Stockholm.

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ISBN: 978-91-8040-724-3
TRITA-SCI-FOU 2023:53
Printed by: Universitetsservice US-AB, Sweden, 2023

بكل حب وامتنان أهدي رسالة الدكتوراة هذه
إلى أبي العزيز سليمان ذو الروح الطيبة ومصدر الحكمة أطال الله عمره وأمده بالصحة والعافية
إلى من وضع المولى الجنة تحت قدميها وقرّها في كتابه العزيز أُمّي الغالية بيان
إلى أجمل هدية من الله تعالى في حياتي، إلى شريكتي و نصفي الآخر روان
إلى عزوتي وسندي في الحياة إخوتي معتصم و عمر و علي و أخواتي جميعا
إلى عائلة زوجتي الكرام عيسى و أمل

*Dedicated to my lovely parents Suleiman & Bayan and
to my soulmate Rawan*

ABSTRACT

This thesis focuses on understanding the mechanical behavior of fiber-based materials by utilizing various modeling approaches. Particular emphasis is placed on their structural variability, anisotropic properties, and damage behavior. Furthermore, the study explores moisture diffusion phenomena within these materials, leveraging machine learning techniques. The research employs a blend of multiscale modeling, experimental investigation, machine learning, and continuum modeling to enhance the predictive capabilities for modelling fiber-based materials.

In **Paper I**, the work investigates the impact of stochastic variations in the structural properties of thin fiber networks on their mechanical performance. A multiscale approach that includes modeling, numerical simulation, and experimental measurements is proposed to assess this relationship. The research also considers the influence of drying conditions during production on fiber properties. The study finds that spatial variability in density has a significant impact on local strain fields, while fiber orientation angle with respect to drying restraints is a key influencer of the mechanical response. In **Paper II**, the research delves into the investigation of anisotropic properties and pressure sensitivity of fiber network materials. It draws a comparison between the Hoffman yield criterion and the Xia model, which are widely utilized for simulating the mechanical response in fiber-based materials. The study performs a detailed analysis of these models under bi-axial loading conditions, assessing their numerical stability and calibration flexibility. Further supporting the research community, the paper provides open-source access to the user material implementations of both models and introduces a calibration tool specifically for the Xia model, thereby promoting ease of usage and facilitating further research in this domain. In **Paper III** a novel thermodynamically consistent continuum damage model for fiber-based materials is introduced. Through the integration of elastoplasticity and damage mechanisms, the model employs non-quadratic surfaces comprised of multi sub-surfaces, augmented with an enhanced gradient damage approach. The model's capability is demonstrated by predicting the nonlinear mechanical behavior under in-plane loading. This study provides valuable insights into the damage behavior of fiber-based materials, showcasing a range of failure modes from brittle-like to ductile. In **Paper IV**, the study examines moisture penetration in fiber-based materials and the resultant out-of-plane deformation, known as curl deformation, using a combination of traditional experiments, machine learning techniques, and continuum modeling. The paper compares the effectiveness of two machine learning models, a Feedforward Neural Network (FNN) and a Recurrent Neural

Network (RNN), in predicting the gradient of the moisture profile history. The study finds that the RNN model, which accounts for temporal dependencies, provides superior accuracy. The predicted gradient moisture profile enables simulating the curl response, offering a deeper understanding of the relationship between moisture penetration and paper curling.

SAMMANFATTNING

Denna avhandling fokuserar på att förstå det mekaniska beteendet hos fiberbaserade material genom att använda olika modelleringsmetoder. Särskild vikt läggs på deras strukturella variationer, anisotropa egenskaper och skadebeteende. Dessutom utforskar denna studie fuktdiffusionsfenomen inom dessa material, med hjälp av maskininlärningstekniker. Forskningen använder en blandning av flerskalemodellering, experimentell undersökning, maskininlärning och kontinuummodellering för att förbättra den prediktiva förmågan för fiberbaserade material.

Artikel I undersöker effekten av stokastiska variationer i strukturella egenskaper hos tunna fibernätverk på mekaniska prestanda. Ett flerskaligt tillvägagångssätt som inkluderar modellering, numerisk simulering och experimentella mätningar föreslås för att studera detta samband. Denna metodik tar också hänsyn till inverkan av torkningsförhållanden under produktionen på fiberegenskaper. Studien visar att spatiala variationer i densitet har en betydande inverkan på lokala töjningsfält, medan fiberorienteringsvinkeln med avseende på hur arket är inspänt under torkningsförloppet är en viktig faktor för den mekaniska responsen.

I **Artikel II** utförs en fördjupad undersökningen av anisotropa egenskaper och tryckkänslighet hos fibernätverk. En jämförelse utförs mellan Hoffmans flytkriterium och Xia-modellen, som används i stor utsträckning för att simulera den mekaniska responsen i fiberbaserade material. Studien innehåller en detaljerad analys av dessa modeller under biaxiala belastningsförhållanden, och bedömer deras numeriska stabilitet och kalibreringsflexibilitet. För att stödja forskarsamhället ytterligare, ges åtkomst till öppen källkod till implementeringen av båda materialmodellerna samt introducerar ett kalibreringsverktyg specifikt för Xia-modellen, vilket främjar användarvänligheten och underlättar ytterligare forskning inom denna domän. I **Artikel III** introduceras en ny termodynamiskt konsekvent kontinuumskademodell för fiberbaserade material. Genom integreringen av elasto-plasticitet och skademekanismer, använder modellen icke-kvadratiska ytor som består av flera underytor, utökad med en förbättrad gradientskademodell. Modellens förmåga demonstreras genom att förutsäga det olinjära mekaniska beteendet under belastning i planet. Den här studien ger värdefulla insikter i skadebeteendet hos fiberbaserade material, och visar en rad brottmoder som sträcker sig från spröda till sega brott. I **Artikel IV** studeras fuktrinträngning i fiberbaserade material och den resulterande deformationen ut ur planet, känd som curldeformation, med hjälp av en kombination av traditionella experiment, maskininlärningstekniker och kontinuummodellering. Studien jämför effektiviteten hos två maskininlärningsmodeller, ett

Feedforward Neural Network (FNN) och ett Recurrent Neural Network (RNN), för att förutsäga fuktprofilhistoriken. Studien finner att RNN-modellen, som tar hänsyn till tidsberoenden, ger en bättre noggrannhet. De predikterade fuktprofilerna används för att simulera curlresponsen, vilket ger en djupare förståelse för sambandet mellan fuktinträngning och curldeformation i papper.

PREFACE

This research was funded by the European Union's Horizon 2020 program under the Marie Skłodowska-Curie Grant No. 764713–FibreNet, a generous support for which I am grateful.

My utmost appreciation goes to Professor Artem Kulachenko, my main supervisor. His invaluable scientific guidance, combined with his open-minded attitude and flexibility, truly made a difference. His distinctive approach to mixing scientific instruction with life lessons greatly assisted me in overcoming many challenges of this research journey.

A special thanks must be made to Assistant Professor Rami Mansour for continuously inspiring and driving my ambition. His valuable guidance and perspectives have largely enhanced the quality of this research.

I am greatly thankful to Professor Johan Tryding (Lund University), my mentor in the EU project. His support and hosting me at Tetra Pak while working on Paper III, have been greatly appreciated. His expertise and guidance were pivotal in shaping this project.

I wish to extend my appreciation to all Professors and fellow Colleagues at the Department of Solid Mechanics for the great environment. The discussions I had with Vedad Tojaga during tea breaks were particularly enlightening and enjoyable. Also, teaching in the department, especially the FEM course, was an enriching experience that helped refine my communication skills.

Also, I would like to thank my friends, whom I met in different countries, for all our good times, to name a few: Ali Hameed, Abdelrahman Azzuni, and Ahmed Al Jamil.

On a personal note, my heartfelt thanks go to my wonderful wife, Rawan. Her understanding, patience, and unwavering support have been my strength throughout this journey. Her belief in me has been a constant source of motivation.

Finally, my deepest gratitude is reserved for my family. Their unconditional love, blessings, and constant encouragement have shaped the person I am today. To my Parents, Brothers and Sisters, no words can describe my gratitude and love. I am forever indebted to you.

Stockholm, September 2023

Mossab Alzweighi

List of appended papers

This thesis is a summary of the following four appended papers.

Paper I

The influence of structural variations on the constitutive response and strain variations in thin fibrous materials

Mossab Alzweighi, Rami Mansour, Jussi Lahti, Ulrich Hirn, Artem Kulachenko

Acta Materialia, 203, 116460. <https://doi.org/10.1016/J.ACTAMAT.2020.11.003>

Paper II

Evaluation of Hoffman and Xia plasticity models against bi-axial tension experiments of planar fiber network materials

Mossab Alzweighi, Rami Mansour, Johan Tryding, Artem Kulachenko

International Journal of Solids and Structures.238, 111358.

<https://doi.org/10.1016/j.ijsolstr.2021.111358>

Paper III

Anisotropic damage behavior in fiber-based materials: modeling and experimental validation

Mossab Alzweighi, Johan Tryding, Rami Mansour, Eric Borgqvist, Artem Kulachenko

Journal of the Mechanics and Physics of Solids. 105430.

<https://doi.org/10.1016/J.JMPS.2023.105430>

Paper IV

Predicting moisture penetration dynamics in paper with machine learning approach

Mossab Alzweighi, Rami Mansour, Alexander Maass, Ulrich Hirn, Artem Kulachenko

Report TRITA-SCI-RAP 2023:006, Department of Engineering Mechanics, KTH.

Contributions to the papers

The author's contributions to the appended papers are as follows:

Paper I. Conceptualization, methodology, software, validation, formal analysis, investigation, data curation, writing – original draft, writing – review & editing, visualization, project administration.

Paper II. Conceptualization, methodology, software, validation, formal analysis, investigation, data curation, writing – original draft, writing – review & editing, visualization, project administration.

Paper III. Conceptualization, methodology, software, validation, formal analysis, investigation, data curation, writing – original draft, writing – review & editing, visualization, project administration.

Paper IV. Conceptualization, methodology, software, validation, formal analysis, investigation, data curation, writing – original draft, writing – review & editing, visualization, project administration.

In addition to the appended papers, the work has resulted in the following manuscript and joint conference contributions:

Uncertainty quantification and damage modelling in multiscale simulation of fiber-based materials

Rami Mansour, Mossab Alzweighi, Artem Kulachenko

(Manuscript in preparation)

Modeling of elastoplastic damage response of fiber-based materials

Mossab Alzweighi, Johan Tryding, Rami Mansour, Eric Borgqvist, Artem Kulachenko

Euromech Colloquium 634, Eindhoven 2023

Uncertainty quantification and propagation in non-woven fibrous materials

Rami Mansour, Mossab Alzweighi, Artem Kulachenko

Euromech Colloquium 634, Eindhoven 2023

On predicting moisture penetration history and curl response of bio-based materials based on machine learning approach

Mossab Alzweighi, Rami Mansour, Alexander Maaß, Ulrich Hirn, Artem Kulachenko

International Paper Physics Conference, Guangzhou 2023

The influence of structural variation on the constitutive response of fibrous Materials

Mossab Alzweighi, Rami Mansour, Jussi Lahti, Ulrich Hirn, Artem Kulachenko

WCCM-ECCOMAS CONGRESS, Paris, 2021.

Decoupling the effect of fiber orientation and drying conditions on the anisotropy of the mechanical properties of paper

Mossab Alzweighi, Rami Mansour, Jussi Lahti, Ulrich Hirn, Artem Kulachenko

Progress in Paper Physics Seminar, Jyväskylä, 2020.

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1. Introduction

In the pursuit of sustainable and innovative solutions across diverse everyday usage and industries, fiber-based materials have increasingly garnered attention. Deriving predominantly from natural origins, these materials distinguish themselves not only due to their economic viability but also for their ecological advantages. Coupled with their multifunctional adaptability, they showcase qualities such as durability, cost-effectiveness, and lightweight properties (Wang et al., 2020). This unique blend of characteristics has driven their incorporation into a diverse range of applications. These span from packaging and composites to more specialized industrial functions, including their role in electrical products (Coelho et al., 2009).

While these materials present pronounced advantages, harnessing their potential effectively presents certain challenges. These challenges primarily stem from their inherent mechanical behavior complexities. To fully capitalize on these materials and optimize their performance, it is pivotal to delve into the intricacies of their anisotropic mechanical behavior, structural variations, and damage, as well as deformation influenced by moisture. The necessity of understanding their mechanical response to utilize them effectively and foster the development of robust, reliable applications becomes evident.

Fiber-based materials are characterized by their intrinsic anisotropic properties, manifesting in marked mechanical differences when examined across various orientations (Harrysson and Ristinmaa, 2008; Tjahjanto et al., 2015). Such variations are particularly observable in terms of stiffness and strength along the Machine Direction (MD), a direction in which the majority of fibers are oriented. In comparison to the Cross-Machine Direction (CD), materials oriented in the MD exhibit superior mechanical properties. They are 2-3 times stiffer under tensile forces and exhibit double the stiffness under shear forces (Mrówczyński et al., 2022). Furthermore, these materials demonstrate asymmetry between tension and compression responses. Specifically, their response is 2-4 times stiffer in tension than in compression. Relying on models that solely account for anisotropy, while neglecting the pressure sensitivity inherent in these materials, may result in inaccurate performance predictions. Consequently, the combined effect of mechanical anisotropy and pressure sensitivity makes the prediction and modeling of their behavior particularly intricate. This complexity underscores the need for the use of more advanced models (Alzweighi et al., 2022).

Beyond anisotropy, fiber-based materials also exhibit a complex structure marked by elements of disorder, heterogeneity, and variations in thickness, density, fiber orientation, and anisotropy (Andreasson et al., 2014; Hristopulos and Uesaka, 2004). Such structural intricacies introduce a level of unpredictability to their behavior, resulting in stochastic failures and variations in mechanical properties (Brandberg and Kulachenko, 2020). In order to accurately model and predict the mechanical performance of these materials, a comprehensive understanding and characterization of their structural variations becomes indispensable (Alzweighi et al., 2021).

Additionally, fiber-based materials are also vulnerable to damage under a variety of loading conditions, which can significantly influence their overall mechanical response (Alzweighi et al., 2023). A profound understanding of the evolution of damage is essential for the dependable design and optimization of fiber-based material applications (Brandberg et al., 2022; Tojaga et al., 2023).

Moreover, the challenge posed by moisture-induced deformation becomes particularly pronounced in the context of fiber-based materials. Owing to their heightened sensitivity to moisture fluctuations, these materials often undergo dimensional alterations, exemplified by phenomena such as curling. As a result, an in-depth exploration of moisture transport dynamics, and its subsequent influence on mechanical attributes is essential for effectively managing and counteracting these moisture-induced transformations (Defrenne et al., 2019; Marin Zapata et al., 2013; Tryding et al., 2022).

In conclusion, fiber-based materials, while holding substantial promise across a spectrum of industries due to their distinct characteristics and merits, bring forth several challenges. Precision in modeling and a comprehensive understanding of these materials, especially under varying loading and environmental scenarios, are paramount to crafting and fine-tuning applications that rely on fiber-based materials. Employing a combination of experimental, computational, and machine learning methodologies, this study endeavors to enhance our comprehension and provide perspectives for the proficient deployment of fiber-based materials.

2. Objective of the thesis

The primary objective of this thesis is to gain a comprehensive understanding of the complexities inherent in fiber-based materials and various modeling approaches. This includes the micromechanical fiber network simulation, continuum modeling and moisture induced deformation.

Specifically, the thesis presents:

1. Fiber network simulation

The research investigates the local structural variations to address the impact of local variations in fiber orientation and anisotropy on the constitutive response of the material. The study further explores the effect of drying conditions during the production process on fiber properties. This was achieved by combining modeling at different scales and experimental measurements.

2. Continuum model evaluation

The work compares the performance of continuum models, specifically investigating models based on the extended conventional von Mises criterion and non-quadratic yield surfaces constructed of multi-sub-surfaces. These advanced models, in addition to accounting for anisotropy, also include pressure sensitivity.

3. Modelling damage behavior

Studying the damage behavior on the sheet level through the development of a novel anisotropic continuum damage model. Derived with specific attention to the behavior of these materials, the model ensures thermodynamic consistency. The model is developed based on a comprehensive experimental study that encompasses measurements across 15 orientation angles, cyclic loading assessments, and evaluations using different sample lengths.

4. Prediction of moisture gradient history

The work investigates the gradient of moisture penetration through the thickness of the material using a combination of experimental measurements, continuum modeling, and a machine learning approach.

By addressing these specific objectives, the thesis aims to contribute towards a robust understanding of fiber-based materials and their responses to varying conditions, thereby facilitating their effective utilization in a multitude of applications.

3. Fiber network simulation

Upon a simple visual inspection of a sample of bio-based materials against a light source, one can readily observe the irregularities in their structural properties. These irregularities can arise from several factors such as variations in thickness, density, fiber alignment, and anisotropy. When these materials are subjected to a load, the unevenness of these structural properties causes the strain distribution to be inhomogeneous. Certain vulnerable areas may show greater strain concentration, which can potentially serve as a locus for damage initiation in the material. Though this issue exists and is acknowledged, singling out the impact of each of those variations and quantifying their individual impact using solely an experimental approach on the local strain field as well as the constitutive response is difficult to achieve. This is primarily due to the difficulties in producing material with controlled structural properties and changing one property at a time. To address such cases, the need to account for their micro properties including modeling of fiber geometries and fiber-fiber interaction using fiber network simulation tools emerges.

One of the earliest fiber network models was presented by Cox, 1952, which delved into the impact of fibers orientation on the elasticity and strength by employing a simplified 2D elastic network. This work has paved the way for numerous subsequent 2D fiber network models (Åström and Niskanen, 1993; Hägglund and Isaksson, 2008; Rigdahl et al., 1984). In the quest for accuracy and closer replication of real fiber networks, 3D fiber network models were developed (Brandberg and Kulachenko, 2020; Heyden, 2000; Kulachenko and Uesaka, 2012).

However, simulating fiber networks presents significant challenges. These challenges primarily arise from the complexities in obtaining data related to fiber geometries, the mechanical properties of fibers, fiber-fiber interactions, and the overall structure of the fiber network, including fiber orientation. The fiber properties have a significant impact on the response of the numerically generated networks (Bosco et al., 2015; Larsson et al., 2018; Lin et al., 2021)

To extract the geometries of fibers, (Hirn and Bauer, 2006) employed an automatic fiber morphology analysis on fibers in their wet state. These measurements were further enhanced with the aid of X-ray tomography scans of the dry sheets, as demonstrated by (Wernersson et al., 2014). For the construction of numerical fiber networks based on these geometries, micro-CT was utilized (Wernersson et al., 2014). However, this technique faced challenges such as low contrast and strong artifacts. These issues were primarily due to high porosity, elevated

carbon content, and the presence of additive materials, which complicated the image processing required for the reconstruction of the fiber structure (Schneider et al., 2016). To overcome these limitations, more advanced techniques, such as 3D synchrotron X-ray microtomography, were introduced (Charfeddine et al., 2019), along with the use of binarized voxel images (Schneider et al., 2016).

Additionally, another approach for constructing the fiber network involves random generation, wherein fibers are positioned randomly within the network (Kulachenko and Uesaka, 2012).

In **Paper I**, random generation is adopted, and Fiber Network (FN) simulation is employed to study the impact of the anisotropy arising from fibers orientation and its subsequent influence on the constitutive behavior of the material. The methodology adopted for generating the network involves the following steps:

- Network generation: fibers are randomly deposited onto a planar surface. Notably, these fibers possess a constant curvature, which runs parallel to the deposition plane.
- Intersection management: during this deposition process, any intersections between fibers are promptly identified. At these intersection points, fibers are elevated to prevent overlapping or penetration, as shown in Figure 1(a).
- Geometry smoothing: post-deposition, the fiber geometry undergoes a smoothing process to eliminate any potential kinks.
- Density considerations: the literature suggests that the density of softwood pulp can vary, ranging from 1200 kg/m^3 (Neagu et al., 2006) to 1500 kg/m^3 (Pintiaux et al., 2015). This variance is often attributed to differences in lignin content. For the purposes of this study, a mean value of 1400 kg/m^3 was adopted during the deposition process.
- Grammage specification: utilizing the density of the fibers, this random deposition continues until the desired grammage is attained, and the fiber network can be visualized in Figure 1(b).

Supplementary materials, including the code for generating this network and its accompanying documentation, are available in (Mansour et al., 2019). In the simulation, fibers are represented using 3-node 3D Timoshenko beam elements with either solid or hollow circular cross-sections. In modeling the bond between fibers, a pointwise contact mechanism involving beam-

to-beam connections is employed. No debonding was considered in the work as it has minimal impact on the hardening response of the material before its failure.

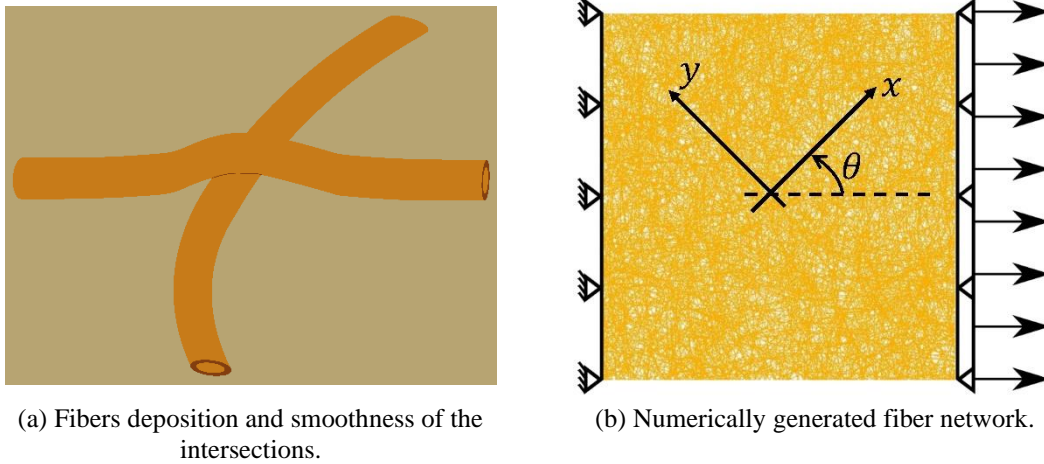


Figure 1: Random fiber network generation using random deposition.

Though the generation of the fiber network is random, the orientation of the fibers can still be controlled during this phase. By adjusting the fiber orientation distribution, depicted in Figure 2(a), the degree of anisotropy λ can be calculated as

$$\lambda = 1 - \frac{b}{a}. \quad (1)$$

In this formula, a and b stand for the major and minor axes of the local fiber orientation distribution ellipse, respectively, as depicted in Figure 2(a). The ability to control the degree of anisotropy provides the capacity to generate several fiber networks with different levels of anisotropy through controlling the orientation of the fibers during the deposition technique. Figure 2(b) shows the mechanical response for different degrees of anisotropy of the FN.

To achieve realistic outcomes in fiber network simulations, it is imperative to define the mechanical properties of the fibers that constitute the numerical network based on the characterization of actual fibers. However, the experimental characterization of these properties is still in its early stages. The primary challenges in characterizing fiber properties stem from the intricacies involved in maintaining complete control during tests, given the small dimensions of the fibers. In a notable effort to understand the response of individual fibers, (Czibula et al., 2021) undertook a study where they measured both the transverse and longitudinal elastic properties using a nanoindentation procedure where the Poisson's ratio was

assumed. In another contribution, Zizek et al., 2022 explored the viscous response of fibers in the longitudinal direction.

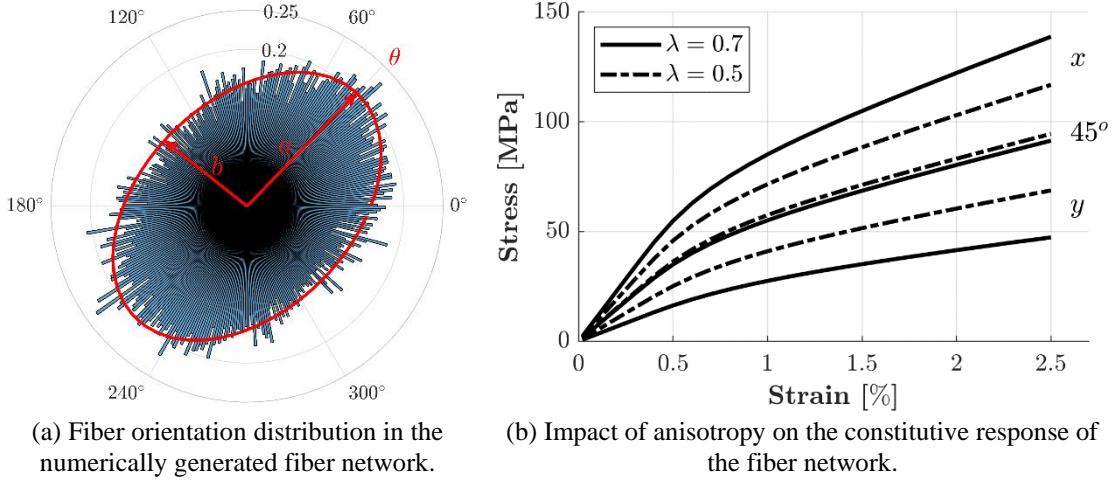


Figure 2: Impact of fiber orientation on the constitutive response of fiber network.

Owing to the limited literature available on the elasto-plastic properties of fibers, a numerical fiber network was created with an average anisotropy of $\lambda = 0.34$. This network was then calibrated against stress-strain curves obtained from the same material, and tested in three distinct directions: MD, 45-degree direction, and CD. This calibration or fitting approach was deemed necessary as the methods to comprehensively characterize fiber properties remain in their developmental phase. During the fitting process, the effects of restrained drying in MD and free shrinkage in CD were incorporated. This was achieved by modeling the fiber's properties based on its orientation angle θ_f relative to MD. The relationship can be presented as

$$E_f(\theta_f) = E_f^{MD} \cos^4 \theta_f + E_f^{CD} (1 - \cos^4 \theta_f) \quad (2)$$

in this equation, E_f represents the fiber's elastic modulus, while E_f^{MD} , and E_f^{CD} are fitting parameters denoting the elastic modulus of fibers oriented in MD and CD respectively. The function $E_f(\theta_f)$ describes how the elastic modulus varies between the MD and CD orientations based on the orientation angle θ_f . The selection of this function, although being empirical, is motivated by the analytical transformations presented in (Cox, 1952). The analysis of the results depicted in Figure 3(a) reveals that solely considering the measured anisotropy was insufficient to attain a close match with experimental findings across all orientations.

Nevertheless, when the drying influence was integrated into the model, a much-improved alignment with experimental data was observed, as shown in Figure 3(b).

Once the fiber properties were established, a series of fiber networks were generated, each with a distinct degree of anisotropy. The simulations of these FNs rendered the constitutive responses.

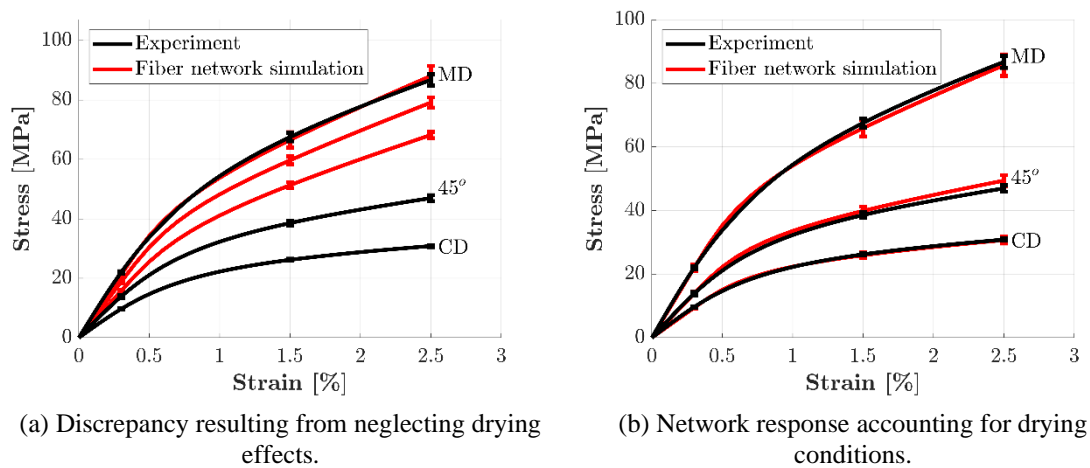


Figure 3: Matching fiber properties using simulations and experimental data. Error bars indicate standard deviations across different tests.

As can be observed in Figure 4, the elasto-plastic material properties are defined as a function of anisotropy. This approach allows to isolate the material behavior that is directly influenced by anisotropy, thereby effectively eliminating any potential interference from other structural fluctuations.

As stated earlier, the fiber network simulation tool provides detailed micromechanical insights, allowing for considering local micro-variations within the material. However, this tool has a significant drawback as the high computational cost restricts its application to much smaller sample sizes, such as $4 \times 4 \text{ mm}^2$, compared to the actual product dimensions.

In **Paper I**, this limitation is effectively eliminated through the integration of the robust computational efficiency afforded by the continuum model with the detailed results from the micromechanical simulation tool. Consequently, it becomes feasible to model larger specimens effectively. This is achieved by defining the material properties in accordance with local structural measurements. As illustrated in Figure 4, the material properties are defined as a function of the degree of anisotropy and fiber orientation. A similar approach is adopted for both thickness and density. Specifically, the thickness of elements in the FE model is matched

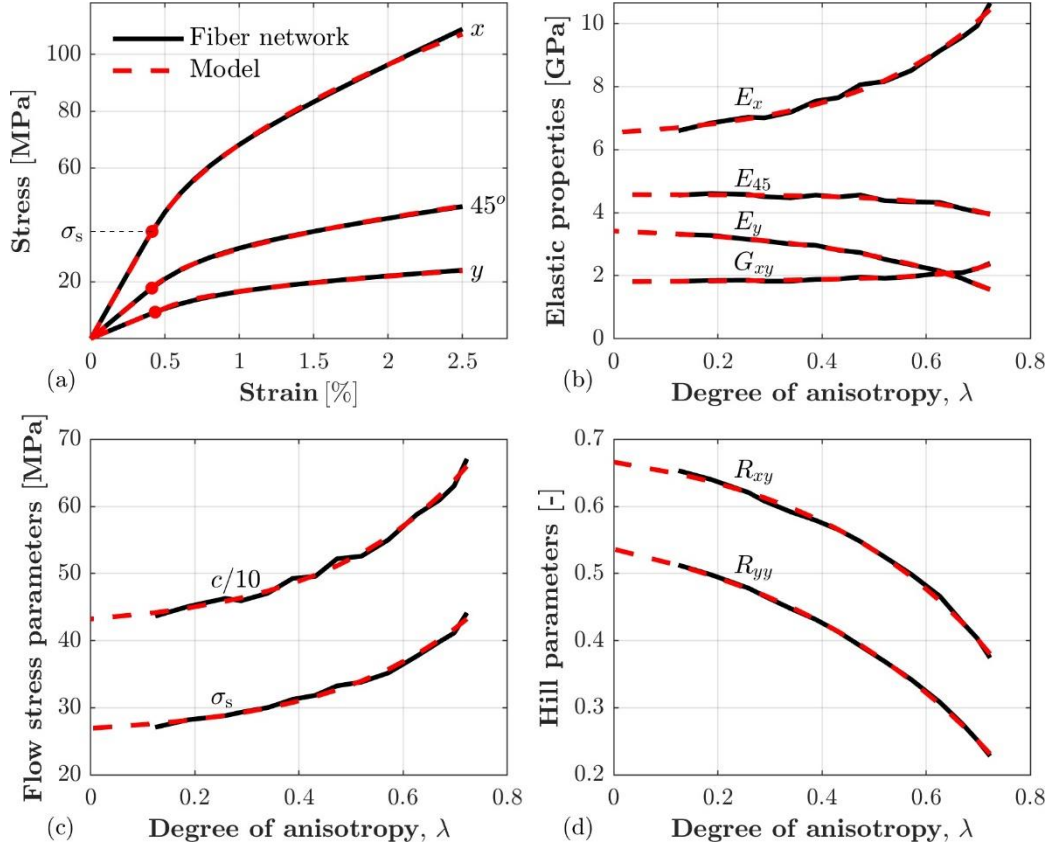


Figure 4: Anisotropy impact on fiber network properties. (a) Stress-strain curves for $\lambda = 0.6$. (b) elastic properties. (c) flow plastic stress parameters. (d) Hill's anisotropy plastic parameters.

with the local thickness measurement taken from the sample. For density variations, the material properties are scaled linearly using the following equation

$$k_\rho = \frac{\rho - \rho_{per}}{\rho_{ave} - \rho_{per}} \quad (3)$$

where ρ is the local density. ρ_{ave} stands for the average density of the sheet. ρ_{per} is estimated to be approximately 200 kg/m^3 (Niskanen, 2011) and represents the percolation point for density. A density lower than this value indicates an insufficient number of fibers to maintain connectivity throughout the network. Figure 5 visually represents the spatial distribution of these structural properties in the continuum model, featuring elements of a $4 \times 4 \text{ mm}^2$ size, similar to the dimensions used in the fiber network simulation tool.

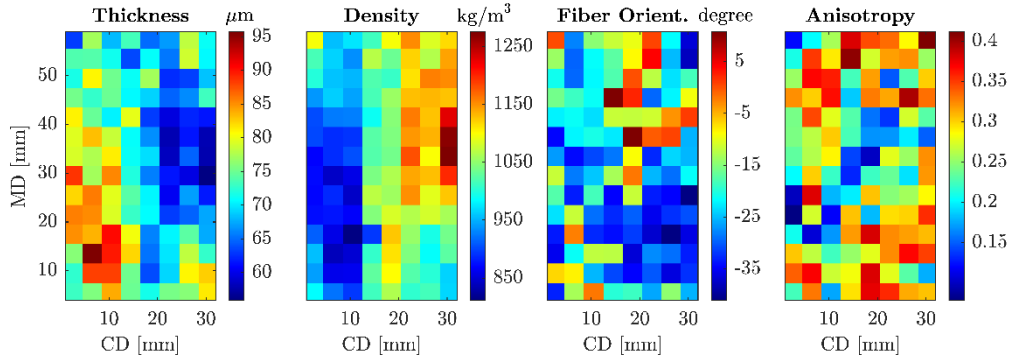


Figure 5: The spatial fields serve as input parameters for the micromechanical finite element model.

4. Continuum modeling of fiber based materials

Continuum modeling of paper-based materials stands as a pivotal tool in product development, particularly when exploring behaviors on a larger scale, such as entire products. A unique feature of these materials is the uncoupled behavior between in-plane and out-of-plane directions. Numerous studies, including those by (Garbowski et al., 2012; Li et al., 2017, 2016; Stenberg, 2003) observed that the in-plane response becomes virtually negligible when subjected to out-of-plane deformation. Such uncoupled behaviors between these planes have become a common practice in modeling paper-based materials. This decoupling is largely attributed to the inherent anisotropy in these materials. The manufacturing process predominantly aligns fibers in the in-plane direction (Huang et al., 2014), contributing to this distinct behavior unique to paper-based products. Therefore, the impact of out-of-plane deformation is typically considered inconsequential (Boes et al., 2023), especially under in-plane loadings. Depending on the model application, adjustments are usually made to primarily focus either on in-plane or out-of-plane behaviors.

In **Paper II**, a comprehensive comparison of two continuum models, widely applied in modeling fiber-based materials, is presented. The overarching advantage of these models lies in their capacity to reproduce the materials anisotropy and distinct tension-compression characteristics.

The first model is based on the Hoffman criterion (Hoffman, 1967). This criterion serves as an advancement of the Hill yield criterion (Hill, 1948). Its primary advantage is its enhanced capability to include both the anisotropic nature of the material and the difference between

tension and compression responses. The representation of the Hoffman yield criterion can be illustrated as follows

$$f = \frac{1}{2} \boldsymbol{\sigma}^T \mathbf{P} \boldsymbol{\sigma} + \mathbf{q}^T \boldsymbol{\sigma} - (\sigma_0 + K(\kappa))^2 \quad (4)$$

where \mathbf{P} is the anisotropic matrix, \mathbf{q} is a vector that features the difference in the yield stress between tension and compression. Also, σ_0 is the initial yield stress, and $K(\kappa)$ is the hardening function.

The second criterion is based on Xia criterion (Xia et al., 2002) which is a non- quadratic yield surface that differs from the anisotropic yield criterion derived based on von Mises as

$$f = \sum_{v=1}^6 \chi^{(v)} \left(\frac{\boldsymbol{\sigma} : \mathbf{N}^{(v)}}{K^{(v)}} \right)^{2k^p} - 1 \quad (5)$$

where χ is a switch control as

$$\chi^{(v)} = \begin{cases} 1 & \boldsymbol{\sigma} : \mathbf{N}^{(v)} > 0 \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

the shape parameter k^p controls the shape of the yield surface. Tensors $\mathbf{N}^{(v)}$ characterize the gradient of the sub-yield surfaces v . The components of these tensors represent a unit vector orthogonal to the sub-yield surface v . Specifically, the relationship $\mathbf{N}^{(v)} : \mathbf{N}^{(v)} = 1$ ($v = 1, 2, 3$; no summation) holds. $K^{(v)}$ is the hardening function.

To assess the flow stability and compare the two models, the convexity of the yield criterion is examined through the Hessian, represented as $\mathbf{H}_{hes} = \frac{\partial^2 f}{\partial \boldsymbol{\sigma}^2} \geq 0$ (Ottosen and Ristinmaa, 2005).

The Xia criterion maintains unconditioned convexity, consistently fulfilling the condition

$\mathbf{H}_{hes} = \frac{\partial^2 f}{\partial \boldsymbol{\sigma}^2} \geq 0$. In contrast, the Hoffman criterion's convexity is contingent, adhering to

$\mathbf{H}_{hes} = \frac{\partial^2 f}{\partial \boldsymbol{\sigma}^2} = \mathbf{P} \geq 0$. This is only met if all eigenvalues of the matrix \mathbf{P} are positive or semi-definite (Holzapfel, 2002).

Additionally, in terms of required input, the Hoffman model requires fewer material properties in comparison to the Xia model. Nevertheless, the comprehensive parameters of the Xia model facilitate superior material characterization. For each loading direction, the Xia model has discrete parameters for yield stress, hardening modulus, and hardening exponent. Meanwhile in the Hoffman model, these plastic parameters are only established for a single loading direction. By utilizing the components of the orthotropic plastic matrix \mathbf{P} , these parameters aim

to align with the experimental response, though they might not consistently provide an optimal fit. Furthermore, the research emphasizes the significance of using a biaxial test to calibrate the shape parameter k^p . Specifically for paper materials, a shape parameter of $k^p = 2$ offers a good match with experimental results.

Both the Hoffman and Xia models have been integrated into User Material routines (UMAT) that are compatible with Ansys and Abaqus simulation software. Alongside these UMAT routines, interested readers can also access an input file and a MATLAB calibration tool for the Xia model. All these resources can be obtained from the provided link: <https://doi.org/10.5281/zenodo.5777175>. The purpose of sharing these materials is to support open research. By making these tools freely accessible, we aim to promote collaboration, transparency, and replication in scientific endeavors.

The findings of Paper II served as the foundation for the advancements detailed in Paper III. **Paper III** is dedicated to the formulation of a thermodynamically consistent continuum damage model, which is carefully derived to replicate the behavior of the fiber-based materials. This model effectively integrates elasto-plasticity with damage mechanisms, rendering an accurate representation of the nonlinear mechanical behavior experienced under in-plane loading. The model incorporates the Xia plastic criterion for plasticity, as elucidated in Paper II. Building on this framework, a damage criterion has been introduced. This criterion comprises three sub-surfaces, each distinctively representing tensile behaviors in the MD, the 45° direction, and CD as follows

$$f^d = \sum_{v=1}^3 \left(\frac{Y^{(v)}}{R_0^{(v)} + \eta^{(v)} T_n^{(v)} g(r^{(v)}, c)} \right)^{2k^d} - 1 \quad (7)$$

where $Y^{(v)} = \sigma^{(v)} \varepsilon^{e(v)} / 2$ represents the thermodynamic damage driving force, commonly referred to as the damage energy release rate. k^d is the shape parameter for the damage surface similar to k^p . Here, $R_0^{(v)}$ denotes the initial damage parameter. The term $\eta^{(v)}$ is a dimensionless parameter, and $T_n^{(v)}$ designates the tensile strength. The function $g(r^{(v)}, c)$ describes the normalized fracture energy and defined as

$$g(r^{(v)}, c) = r^{(v)} \left[1 - \frac{c}{c+1} \cdot \sqrt[c]{\frac{r^{(v)}}{x_c}} \cdot {}_2F_1 \left(c+1; 1; c+2; -\sqrt[c]{\frac{r^{(v)}}{x_c}} \right) \right] \quad (8)$$

the dimensionless parameter c represents the shape of the damaged stress curve, and r is the normalized widening in the localized region.

Figure 6 presents a comparison between the experimental data and the simulation outputs for damaged samples. These samples measure 25 mm in length and 15 mm in width, featuring central holes of 5 mm and 8 mm in diameter. The alignment between the experimental observations and the numerical results demonstrates the model's capability to replicate the hardening response as well as the softening behavior.

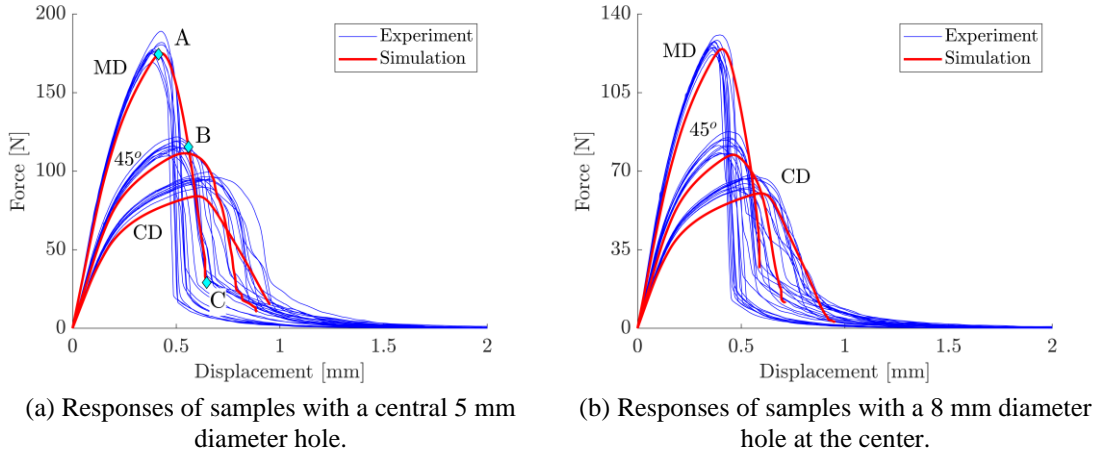


Figure 6: Comparison between experimental measurements and simulation results for damaged samples, each measuring 25×15 mm and featuring a hole in the center.

Figure 7 showcases isometric visualizations of the damage field when the specimen is loaded in MD. Three key displacement levels, labeled as A, B, and C, are highlighted, as referenced in Figure 6(a). Figure 7(a), at point A, which marks the onset of damage, the iso-plot reveals a damage level nearing 0.3 mm. This extends about 0.6 mm past the edge of the hole, oriented perpendicularly to the loading direction, at its peak load. In Figure 7(b), at point B, which corresponds to roughly 70% of the peak load, the iso-plot of the damage displays a level ranging from 0.917 to 1.0. This indicates a crack growth of nearly 2 mm. The damage field extending from the edge of the hole measures around 3.2 mm in width and 2.5 mm in the length of the sample. In Figure 7(c), at point C, equivalent to around 30% of the peak load, the iso-plot of the damage level spans 0.917-1.0. Here, the crack growth continues, stretching about 3.5 mm beyond the hole's edge. The damage spreads approximately 5 mm lengthwise on the sample. As damage progresses towards the boundary, a shear slip occurs, leading to a directional shift of 45° relative to the CD direction of the damage zone. The sequence of events concerning the plastic strain in the MD, denoted by $\varepsilon^{p(1)}$, is detailed in Figure 7(d) through

Figure 7(f). Together, these images portray a systematic accumulation of plastic strain, occurring in parallel with the material's escalating damage.

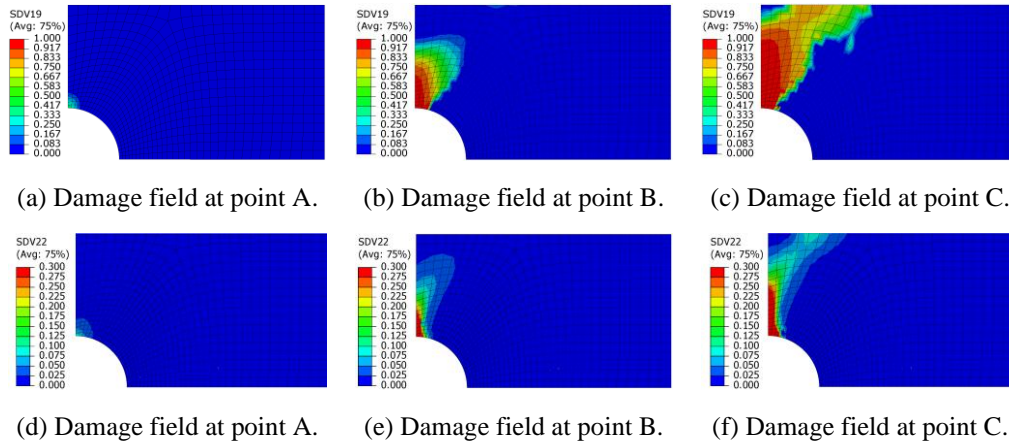
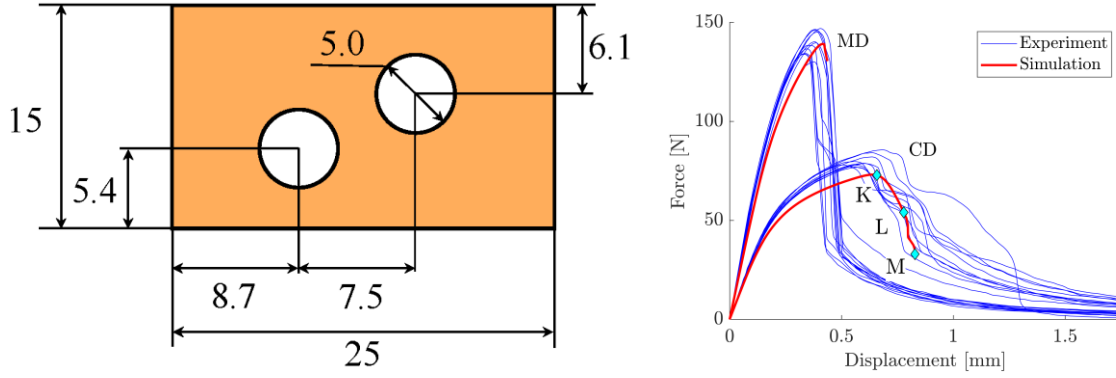


Figure 7: Evolution of damage parameter and the plastic strain for samples measuring 25×15 mm, containing a central hole with a diameter of 5 mm. The samples are loaded in the MD direction, represented as the horizontal direction in the figure.

Additional testing was carried out to evaluate the performance of the proposed model. This involved using samples measuring 25×15 mm², each containing two asymmetrically positioned holes, each 5 mm in diameter, as illustrated in Figure 8(a). In Figure 8(b), tests show a brittle-like failure in the MD direction, which simulations closely capture. Conversely, the CD direction displays a progressive failure, aligning with simulated results.

The continuum model from Paper III designed to replicate the elasto-plastic characteristics of fiber-based materials, carries with it high flexibility stemming from the multi sub-surfaces criteria. This model bridges the limitations of the modeling gap identified in Paper I where the continuum model is limited for elasto-plastic response. Comparisons between experimental and simulated results for samples with pre-punched holes validate the model capability in predicting anisotropic elasto-plasticity and damage in fiber-based materials. This tool aids in optimizing and analyzing these materials under varied load scenarios to ensure their dependability in real-world applications.



(a) Illustration of the sample geometry and dimensions in millimeters.

(b) Comparison between the simulation and experimental response.

Figure 8: Specimen with two holes asymmetrically located.

5. Machine learning in prediction moisture gradient history

One of the primary challenges that limit the broader utilization of fiber based materials is their moisture-sensitive characteristic (Niskanen et al., 1997; Strömbro and Gudmundson, 2008). This sensitivity leads to notable degradation in their mechanical performance (Caulfield, 1990; Lin et al., 2022; Placet et al., 2012; Rhim, 2010; Wang et al., 2014), and also affects their dimensional stability (Samantray et al., 2022). Such alterations may manifest in deformations like cockling (Lipponen et al., 2008), fluting (Kulachenko et al., 2007, 2005), and out of plane deformation known as curl (Dano and Bourque, 2009; Lipponen et al., 2009). Curling is particularly problematic during the printing process, see Figure 9, as it introduces issues related to handling and waste, hence presenting significant economic ramifications (Carlsson, 1981; Yoon et al., 2020).

The structure of paper-based materials consists of an intricate network of fibers and pores (Bandyopadhyay et al., 2002, 2000). When moisture interacts with this structure, it follows a complex process of penetration into the pores, and subsequently, it diffuses into the fibers (Larsson and Wågberg, 2010). As the fibers attempt to equilibrate with their surroundings, they absorb and desorb moisture (Lee and Yoon, 2017). The moisture taken up by the fibers, resulting in their swelling and subsequent hygroexpansion, is termed as Deformation Moisture (DM) (Lindner, 2017). Fibers are found to hygroexpand more in the transverse direction than in the longitudinal one (Uesaka, 1994). As a result, the orientation of fibers in

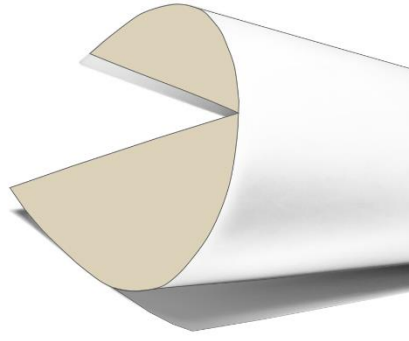


Figure 9: Curl response due to the gradient of the moisture throughout the thickness.

the material and the drying process, especially when the paper is dried under tension in the Machine Direction (MD), significantly influence its response to moisture (Alzweighi et al., 2021; Hansson et al., 1989).

Given the material complexity, a thorough understanding of the interaction between moisture and fiber-based materials is challenging. Various models have been suggested to elucidate this interaction, spanning sorption (Parker et al., 2006; Tryding et al., 2022), transport (Alexandersson et al., 2016; Bedane et al., 2016; Bronlund et al., 2014; Marin Zapata et al., 2013), and diffusion (Bandyopadhyay et al., 2002; Defrenne et al., 2019; Gezici-Koç et al., 2017; Mattsson et al., 2021; Nicasy et al., 2021). More specifically, models to understand out-of-plane mechanical deformations due to moisture in fiber-based materials have been introduced, for instance, (Lee and Yoon, 2017; Östlund, 2006; Seidlhofer et al., 2022).

In **Paper IV** an approach is introduced that is capable of predicting the gradient of the deformational moisture across the thickness direction over time. This is achieved by combining experimental measurements, continuum modeling of curl, and a machine learning approach. For the first time this combination showed the ability to predict gradient of the deformational moisture, which has not yet been possible with alternative approaches.

The experimental setup for this approach starts with curl measurements. As depicted in Figure 10(a), the setup consists of an aluminum frame that accommodates a timer relay-controlled spraying system and a Keyence LJ-X8400 2D laser sensor. Once the laser sensor is active, the spraying apparatus is initiated via the timer relay and the amount of water sprayed is controlled through controlling the spraying time. Throughout a span of 530 seconds, the consequent paper curl is observed. The curl response, as a crucial result of this experiment, is delineated as the out-of-plane deformation, UZ , of the paper in the cross direction of the sheet, represented by

the X coordinate. This is captured using the aforementioned laser sensor. For a comprehensive analysis, ten samples were examined, and the curl measurements were recorded. The average curl response from the different samples is presented in Figure 10(b). Illustrated in Figure 10(b) are the various stages of curl deformation over specific time intervals throughout the experimentation. Initially, there is a noticeable increase in the curl response until it reaches its maximum (represented by solid black lines). Subsequently, as the material undergoes the drying process, there is a gradual reduction in curl (denoted by dashed black lines).

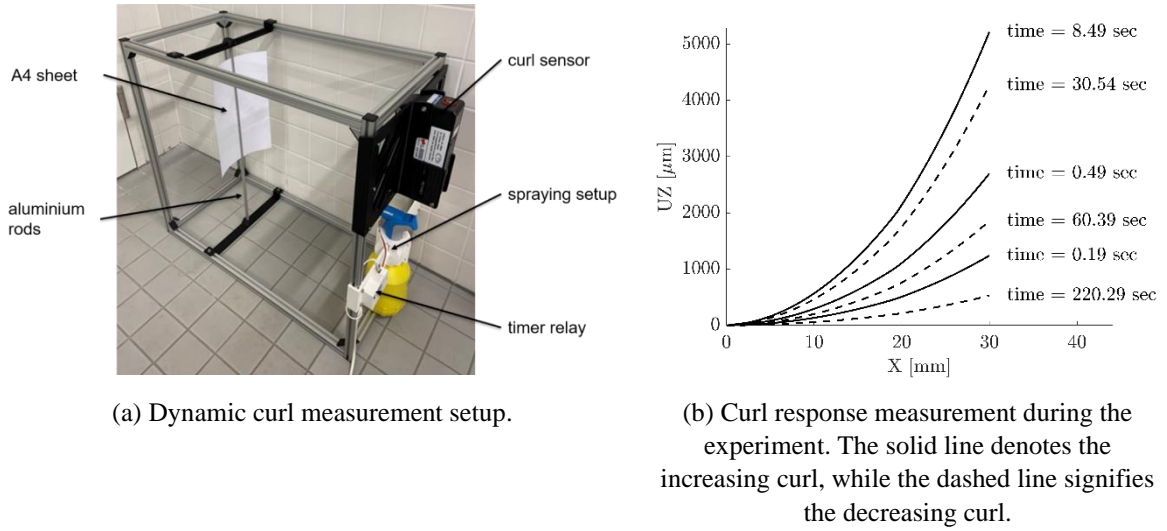


Figure 10: Experimental setup for curl measurement and the measured curl response.

The continuum model incorporates anisotropic plastic behavior with asymmetric tension-compression, which is crucial for accurately representing the behavior of paper materials. The model further integrates both viscoelasticity and creep characteristics. The model is moisture-dependent and attributes the principal cause of the simulated curl as the moisture gradient profile across the thickness, as well as its progression over time. The model is calibrated against experimental measurements at four different levels of moisture content. Figure 11 shows the calibration results of the model in comparison with a subset of the experimental data at a designated moisture level.

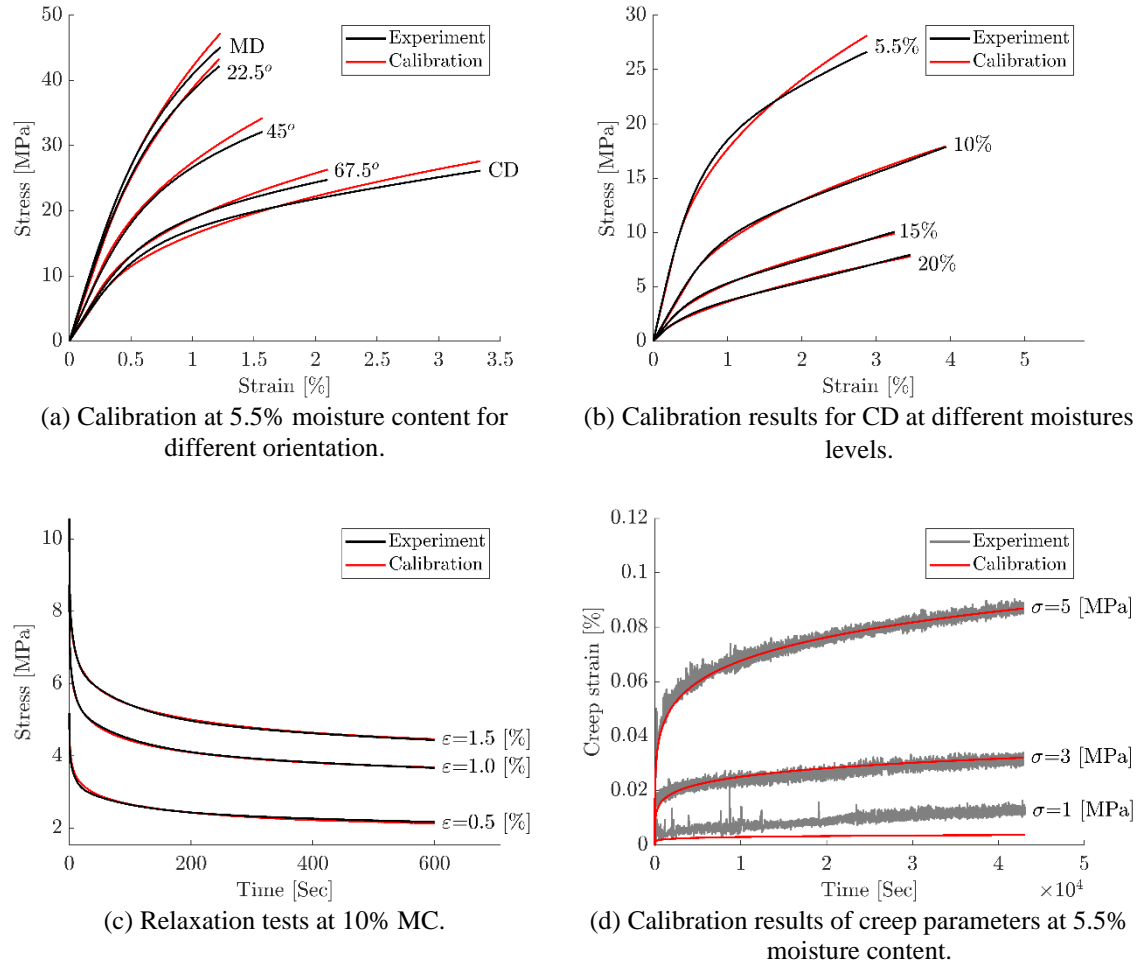


Figure 11: Calibration results of the continuum model at various moisture levels.

Defining the moisture penetration through the material is notably challenging, underpinned by three key factors:

- Initial moisture uncertainty: the starting moisture distribution within the material is unclear.
- Complex drying dynamics: the drying of sheets, like paper, depends on mass transfer between paper and air, a process complicated by boundary layer flow. This introduces numerous variables when trying to deduce a reliable diffusion coefficient for the sheet.
- Variable moisture impact: not all absorbed moisture causes deformation. Some get trapped in pores, termed as ineffective moisture, having no effect on deformation. In contrast, deformational moisture absorbed by fibers causes them to swell.

Adding to the complexity, stated above, is the continuous moisture exchange between fibers and pores, causing constant changes in the deformational moisture and the ineffective moisture. Additionally, the drying of the sheet is mainly driven by mass transfer at the interface between paper and air, which is quite complex as it is heavily influenced by boundary layer flow. In

conclusion, there are simply too many parameters to be determined or estimated to obtain a reliable result for the diffusion coefficient within the sheet.

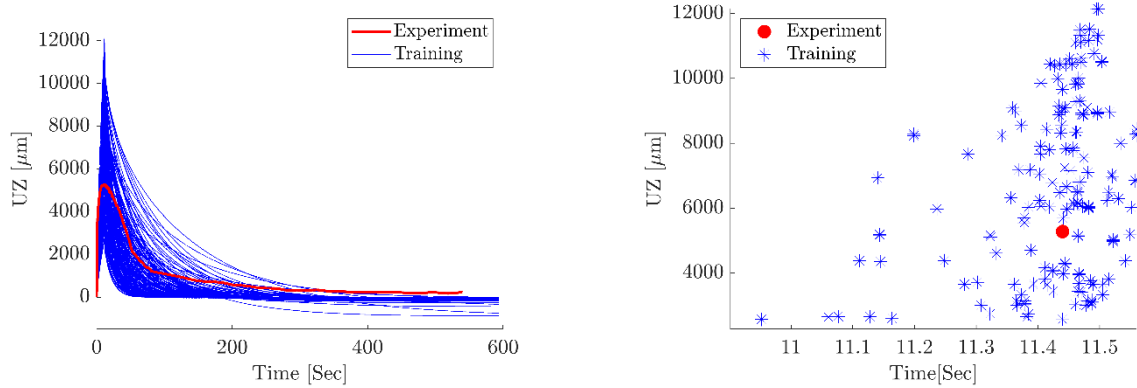
Noteworthy, an alternative to the traditional approach involves defining the diffusion coefficient inversely by directly fitting it to the curl response. This, however, also requires making assumptions such as estimating a moisture distribution from moisture content and making assumptions about the fraction of water that is contributing to fiber swelling. Also, here, it has to be suspected that the final result is totally driven by the many assumptions made. Furthermore, combined with an inverse problem, this approach requires considerable computational resources, as it necessitates a large number of simulations to be done during the fitting approach. The fitting using the inverse solution of the problem by fitting the diffusion coefficient to the curl response can lead to the accumulation of error. The curl response is history-dependent hence the accuracy in fitting of current step depends largely on the fitting accuracy of the previous step.

All the matters discussed above are motivating to estimate the gradient of the deformational moisture profile in the sheet over time by Machine Learning (ML) techniques.

In this study, a Recurrent Neural Network (RNN) was employed. The RNN is favored due to its intrinsic capacity to handle sequential data using its internal loops. These loops facilitate the transmission and retention of information from one phase of the network to the next. This characteristic is valuable for our study where the moisture profiles are not only influenced by their previous states but also by the history of curl data. Additionally, the Bidirectional Long Short-Term Memory (BiLSTM) was integrated into the network. The BiLSTM enhances the standard LSTM by concurrently analyzing data from past and future sequences, providing a holistic view of sequences. This bidirectional methodology empowers the BiLSTM to discern the intricate relationship between moisture profiles and curl history.

For training purposes, reliance was solely placed on numerical data, as collecting experimental data poses challenges. This training dataset comprises numerically derived moisture profiles and the corresponding simulated curl response via the continuum model simulation. Figure 12 displays the extensive variety of the training data in comparison to the experimental curl measurements, showcasing a broad spectrum of training data. During the preprocessing of the training data, noise was reduced, and a gap of 4 points was introduced between dataset points. The data was then randomly partitioned, designating 80% for training and 20% for validation. This randomized data split allows for the monitoring of model performance throughout training

and aids in mitigating overfitting, ensuring the model effectiveness on unfamiliar data. The training utilized the Adam optimization algorithm over 5000 epochs. L2 regularization, with a 0.5 factor, was employed, alongside a mini-batch size of 512, to counteract overfitting. The used RNN network in this study features a layered design, encompassing a sequence input layer, dual BiLSTM layers, a fully connected layer, and a regression output layer.



(a) Curl response UZ from experiment and training data. (b) Peak curl response in the experiments UZ compared to the peak curl response from training data.

Figure 12: Comparison between the peak curl response from the experiment and the simulated peak curl response using the numerically generated moisture profiles.

Following the training of the RNN with numerical data, the curl measured experimentally was fed into the networks. Subsequently, the networks provided an inverse prediction of the moisture profile history associated with the observed curl.

The moisture profile history, as predicted by the RNN, is depicted in Figure 13(a). This profile signifies the deformational moisture responsible for curl deformation. The predicted moisture profile history, from Figure 13(a), shows a reduced extent of moisture gradient. This can be observed with most of the moisture penetration concentrated at a depth approximating 40% of the total thickness, albeit minor variations in DM appear at about 60% of the thickness. The moisture profiles predicted by the RNN exhibited a degree of consistency and stability, reflecting a reliable representation of moisture diffusion across the material. Additionally, the moisture profile histories predicted by the RNN served as inputs for the continuum model, facilitating the simulation of the corresponding curl response. The results of these simulations are illustrated in Figure 13(b) at different time intervals. The RNN's simulated curl results, as seen in Figure 13(b), display a refined performance, aligning closely with the experimental data.

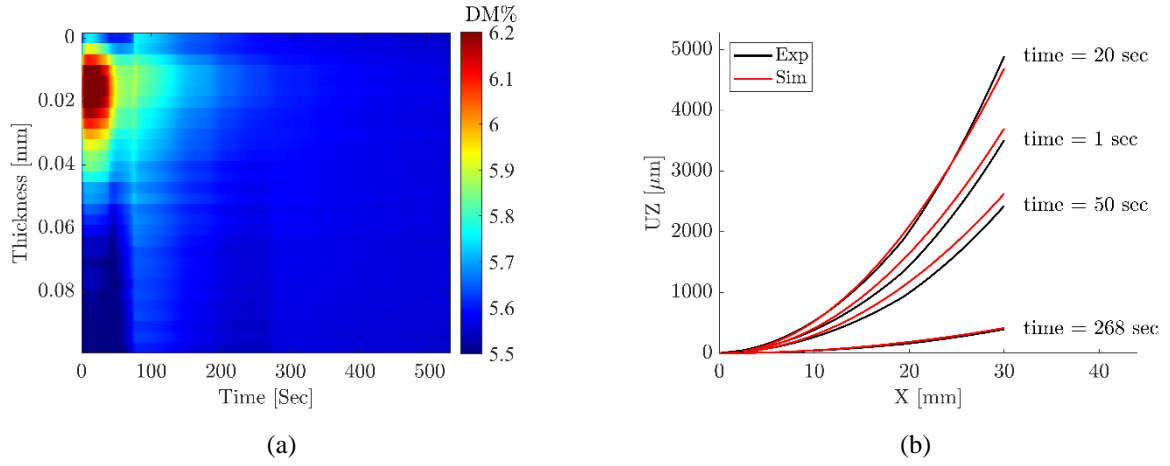


Figure 13: Prediction results of RNN. (a) The predicted deformational moisture profile history. (b) Comparison between simulated curl response using the predicted moisture profile and the measured curl at different time frames.

The curl response results closely align with the experimentally measured curl, which is an indication of the potential of utilizing the machine learning approach for such complex problems.

6. Concluding remarks

This thesis aimed to enhance our comprehension of the complex mechanical behaviors exhibited in fiber-based materials. Modeling these materials poses a prominent challenge due to their intrinsic inhomogeneity and local variations. Such complexities in the local structure can lead to stochastic and unpredictable failures, which cannot be adequately addressed solely by traditional methods. This limitation not only compromises the broader usage of these materials but also has adverse environmental impacts. A prevalent practice during the production process is to over-dimension the product size to mitigate these failures, resulting in increased consumption of raw materials and negative ecological effects.

The research makes strides in connecting micro-mechanical responses to macro-level response by leveraging fiber network simulation tools and multiscale approach. It also introduces a novel anisotropic continuum model that has been carefully developed to replicate the anisotropic elastoplastic response, including ductile damage behavior. Furthermore, the study places particular focus on their hygroexpansive, specifically addressing the out-of-plane deformational responses induced by moisture gradients across their thickness. This work advances the field through the employment of machine learning techniques in combination with modeling and experimental data.

This thesis represents an important step forward in paving the way to achieve the ultimate objective of predicting strength uniformity parameters and understanding the factors that control them. Achieving this will be crucial for predicting the performance of fiber-based materials in their end-use applications and for optimizing material usage through the selection of appropriate safety factors.

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8. Appended papers