

# INTERNATIONAL PAPER PHYSICS CONFERENCE 2024

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## Book of Abstracts

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## Sessions

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- S13 Paper chemistry and chemical engineering of lignocellulosics

## Plenary Lectures

### **A multi-scale modelling-experimental approach to predict the degradation of (historical) paper**

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The degradation of historical paper artefacts is a major concern for cultural heritage conservators. It has been estimated that up to 80% of paper documents in western heritage institutions and librarian collections is susceptible to acid-catalyzed hydrolysis reactions, which lead to rapid chemical and mechanical degradation. This contribution presents a multi-scale modelling-experimental framework for predicting the chemo-mechanical degradation of paper [1]. Paper is modelled as a two-dimensional periodic repetition of a fibrous network unit cell, where the fibres are characterized by a moisture-dependent chemo-hygro-elastic constitutive behaviour. Paper degradation occurs primarily due to the hydrolysis of cellulose, which causes a reduction of the degree of polymerization and a consequent decrease of the effective mechanical properties. This may ultimately lead to embrittlement and loss of material integrity. The proposed model accounts for the interplay between the acidity of the paper, the ambient environmental conditions, and degradation behaviour by first determining the coupled time evolution of the degree of polymerization, acidity, and moisture content. A time-dependent evolution law for the tensile strength of the paper depending on these parameters is proposed and calibrated from dedicated micro-tensile experiments [2,3]. A change in moisture content induces internal stresses in the fibrous network, potentially leading to brittle damage once the fibre tensile strength is reached. The effective hygro-mechanical properties of the degrading fibrous network are calculated as a function of time using asymptotic homogenization. Numerical simulations highlight the impact of the time-evolving moisture content, acidity of the paper, and microstructural features on the degradation process. The results of this work may be valuable for conservators of cultural heritage institutions to determine optimal environmental conditions to limit the time-dependent degradation of historical paper artefacts.

[1] Parsa Sadr, A., Maraghechi, S., Suiker, A. S. J., Bosco, E. (2024). A multi-scale approach for chemo-mechanical degradation of paper: insights into the governing factors. *Cellulose*. <https://doi.org/10.1007/s10570-024-06005-5>

[2] Maraghechi, S., Bosco, E., Suiker, A. S. J., Hoefnagels, J. P. M. (2023). Experimental characterisation of the local mechanical behaviour of cellulose fibres: an in-situ micro-profilometry approach. *Cellulose*, 30(7), 4225-4245.

[3] Maraghechi, S., Dupont, AL, Cardinaels, R., Suiker, A. S. J., Hoefnagels, J. P. M., S., Bosco, E. Maraghechi (2023). Assessing rheometry for measuring the viscosity-average degree of polymerisation of cellulose in paper degradation studies. *Heritage Science* 11(15):1–9

## **4evergreen - Perfecting circularity for fibre-based packaging**

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Packaging is a key enabler of the circular economy.

Fibre-based packaging, in particular, is an appropriate solution in a variety of industries to protect goods on route to their final destination and it can be made of 100% renewable material. In Europe, today fibre-based packaging has a recycling rate of 82,5%. 4evergreen was established in 2019 to further improve its circularity and raise this rate to 90% by 2030.

4evergreen is a cross-industry alliance driven by the desire to meet some of the most pressing issues of our time. The global population is rising, resulting in increased food consumption and a greater need for packaging. To reduce pressure on natural resources, we need to focus on circularity. That's why we bring together over 110 companies and organisations from across the value chain, adopting a holistic approach. Our members include consumer goods companies, packaging producers and converters, waste management companies, non-fibre-material suppliers, technology providers, leading research institutes and start-ups. This breadth allows us to reach consensus and implement change.

Our work is structured in four technical workstreams that look at the entire life cycle of fibre-based packaging, and one information workstream. They are all composed of industry experts who share best practices, prepare test programs to address unknowns, and create evidence-based deliverables. All of our guidelines and protocols are developed by members with subject matter expertise, reviewed by peers, and built on a consensus involving approximately 400 delegates.

## **Spreading vs. Penetration – The fate of an ink drop on a paper surface**

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In inkjet printing, spreading and absorption processes determine the final area of a printed dot, which is decisive for print quality in terms of coverage and resolution. In this work, the printed dot area of overall 140 paper-liquid pairings representative for the operational window of an inkjet printer is evaluated. The results are explained by a model including spreading, absorption, and evaporation. The surface tension and viscosity of the liquids, as well as the pore size and polarity of the substrates were varied systematically to represent the range of uncoated paper-liquid pairings applicable for inkjet printing. We propose a novel modeling approach for liquid wetting and liquid penetration from surface energies of substrate and liquid.



For this purpose, the contact angle and liquid penetration is modeled by polar and dispersive surface energies, utilizing the theories of Owens-Wendt-Rabel-Kaelble (OWRK), Wu, or van Oss, Good, Chaudhury (vOGC). Frequently used saturated pore models for liquid penetration in paper are discussed (Lucas Washburn, Darcy), particularly under the perspective that the actual flow regime in paper is unsaturated pore flow. Why are the common models working then?

## **New chemistries - New properties: Novel approaches to tailor-made papers**

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In order to control the properties of paper, several different routes of chemical modification have been used to tailor the properties of paper to specific needs. Such paper modification additives can, for example, make paper hydrophobic, control protein adsorption or improve its mechanical properties. Most paper modification processes use physically adsorbed polymers in which the polymeric additive is simply deposited on the surface of the paper fibrils. Such physically deposited molecules are inherently at risk of being replaced by competing adsorbents and may eventually be released into the environment. An alternative and important route is based on chemical modification reactions and makes use of the abundant number of hydroxyl groups in cellulose, for example through the formation of ethers or esters. However, removing a significant number of hydroxyl groups from the cellulose greatly alters the properties of the paper. In addition, many of the substances used to modify paper are not environmentally friendly. Examples include wet strength agents based on epichlorohydrin or formaldehyde resins. They also make it rather difficult to recycle the paper, a problem well known for wet-strengthened paper.

We describe a novel approach to paper modification using C,H insertion reactions. The paper is coated with a thin layer of a prepolymer containing dormant crosslinking units. These crosslinkers can be activated by heat or light, leading to crosslinking of the polymer and simultaneously to insertion reactions with the cellulose molecules, thus covalently immobilizing the forming network. The crosslinker moieties comprise benzophenone, anthraquinone or diazoester chemistries. By tuning the details of the chemical composition of the crosslinker units we can reduce the energy input for the chemical reactions very strongly. We describe the preparation and characterization of papers with very unusual properties and give some initial results on how the use of dynamic linkages can make such papers easier to recycle.

## 3D structure characterization of filled paper based on X-ray CT analysis

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Based on the powerful non-destructive 3D microscopic imaging capability of X-ray CT scanning technology, and combined with the digital image processing method, this study developed the three-dimensional structural model of filled paper, visualized the distribution of filler, and conducted the permeability simulation of filled paper.

Initially, short cotton fiber and precipitated calcium carbonate (PCC) filler were used as raw materials, two types of fillers of PCC1 (4.15  $\mu\text{m}$ ) and PCC2 (5.45  $\mu\text{m}$ , preflocculated PCC1) were applied respectively, and two kinds of hand-made paper sheets with the same basis weight ( $105\pm 1$  g/m<sup>2</sup>) were manufactured accordingly. After the scanning of X-ray CT equipment, the obtained CT images were pre-processed by Otsu algorithm to separate the parts of fiber, pore and filler in the images. Next, the three-dimensional structural models of the filled paper sheets were developed by the software of Avizo. The sizes of Representative Elementary Volume (REV) were determined preliminarily for decreasing computation load. Subsequently, the pore network models were established, and the parameters of porosity, tortuosity, filler particle size and the spatial distribution of pore space were extracted. Finally, based on the developed structural model, liquid permeation simulations were carried out on the horizontal and thickness directions of the filled paper, to study the effects of the particle size and spatial distribution of fillers on the three-dimensional pore structure and permeability of filled paper.

Key findings from the simulation study include: (1) The parameters of porosity, tortuosity and fractal dimension of filled paper tend to be stable with the increase of REV side length. The REV dimensions were determined as  $600\times 600\times 630$  pixels (unfilled paper),  $600\times 600\times 470$  pixels (PCC1 filled paper) and  $600\times 600\times 560$  pixels (PCC2 filled paper).

(2) The filler distribution in the horizontal direction of paper is more uniform than that in the thickness direction (Z direction). Whereas the filler in the Z direction is concentrated in the middle and lower areas of the paper sheets, and the distribution of filler with small particle size (PCC1) is more uniform in the Z direction.

(3) The filler with small particle size (PCC1) is prone to be flocculated during filling process, which reduces the paper porosity, improves the tortuosity and fractal dimension of the pores, making the pore structure becomes complicated.

(4) A filler with smaller particle size has a greater impact on the paper permeability. In comparison to the horizontal direction, filling operation exhibits a more pronounced alteration in the paper permeability in the Z direction.

## S01 | Measuring the mechanical response of fibers, paper, and board

### High strain-rate tensile testing of planar cellulose fibre networks

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During the processing and manufacturing, paper and pulp products can be exposed to high load rates. However, there is a scarcity of data on the mechanical behaviour of these products at higher strain-rates, exceeding  $1 \text{ s}^{-1}$ . This work deals with the tensile characterization of planar cellulosic networks up to high strain-rates involving a specially designed Split Hopkinson bar for the dynamic strain-rates. Quasi-static reference tests were performed on a Universal testing machine. In order to find a suitable dynamic test setup a digital twin of the whole test bench was created using explicit Finite element simulation. Experimental tests were conducted in a strain-rate range from  $0.0083 \text{ s}^{-1}$  to  $212 \text{ s}^{-1}$  or testing velocities between  $0.0003 \text{ m/s}$  ( $20 \text{ mm/min}$ ) and  $13.6 \text{ m/s}$ . For the dynamic tests, high-speed images were taken in order to determine the sample elongation via target tracking and digital image correlation (DIC). The tests revealed a mean increase in tensile strength between the lowest and the highest strain rate of roughly 58 %. The initial stiffness between the lowest and the highest rate even increased by 115 %. It has been demonstrated that both the increase in tensile strength and in initial stiffness can be well described with a Cowper-Symonds model. On the other hand, the failure strain, which was about 6 % at quasi-static strain-rates decreased to about 3 % in the dynamic strain-rate range.

[1] Andersson O., Sjöberg L., Tensile studies of paper at different rates of elongation, Svensk Papperstidning, 16, 615-624, 1953.

[2] Kouko J., Retulainen E., The influence of strain rate and pulp properties on the stress-strain curve and relaxation rate of wet paper, Tappi J, 14, 8, 515-524, 2015

### Effects of in-plane loading on out-of-plane delamination of paperboard

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The present study aims at increasing our understanding of how in-plane straining affects the delamination strength of paperboard. During the shaping of a box, paperboard is first creased to form a precisely damaged zone around which the paperboard is folded [1]. In the damaged zone the paperboard is delaminated to form plies. During folding, the plies buckle and forms a

permanent edge of a box. Good folds are characterized by precise shape and intact containments properties of the box. During creasing, the paperboard is usually constrained from in-plane motion. The large deformations during creasing give large in-plane strains in the paperboard. Currently, the delamination properties of paperboard are assumed to be independent of in-plane straining. In the present study, we evaluate experimentally effects of pre-straining paperboard on its delamination strength. Paperboard is first pre-strained in MD to fracture and then tested in ZD. Comparisons of the strength to the same paperboard in its virgin state to its properties in a pre-strained state shows that pre-straining gives between 8 and 13% decrease in the delamination strength. The standard deviation in the strength is shown not to be influenced by pre-straining. The effect is of a similar in magnitude as the influence of decreasing the deformation rate to a tenth of the nominal 10 mm/min. The present study indicates a noticeable effect of in-plane straining. It is noted that the standardized ZD-test provides reasonable values of the delamination strength in comparison to DCB-tests that provides the complete cohesive law for delamination of paperboard [2]. However, the delamination strength is just one parameter that characterizes the delamination properties. A more complete characterization is given by a complete cohesive law for delamination [2]. For example, a complete cohesive law also gives the fracture energy of delamination. Future studies will influences of pre-straining on the cohesive law.

[1] Coffin, D.W., Nygård, M., Creasing and folding. In *Advances in Pulp and Paper Research*, Oxford 2017, Trans. of the XVIth Fund. Res. Symp. Oxford, 2017, (W. Batchelor and D. Söderberg, eds), 69-136, FRC, Manchester, 2018.

[2] Biel, A., Tryding, J., Ristinmaa, M., Johansson-Näslund, M., Tuveesson, O., Stigh, U., Experimental evaluation of normal and shear delamination in cellulose-based materials using a cohesive zone model. *Int. J. Solids Struct.* Vol. 252, 111755, 2022

## **Enhancing practicality in evaluating out-of-plane shear behavior of paperboards using a refined split double cantilever beam**

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This research introduces a refined configuration for the split double cantilever beam (SDCB) specimen, addressing practical challenges in assessing the out-of-plane shear behavior of paperboards. The original SDCB design by Biel et al. [1], though effective, posed difficulties in handling due to its length (1 m) and weight (1.4 kg). Through systematic experimental design and finite element analysis, this study explores modifications to the SDCB specimen, resulting in a smaller and more practical geometry. A new design that balances measurement quality with ease of handling has been identified. The revised design reduces the specimen's length and weight to 0.6 m and 0.84 kg, respectively, making it more manageable for a single person. Additionally, the length of the paper strip in the specimens was reduced from 0.7 m to 0.3 m,

significantly easing provision and storage. This work offers a pragmatic solution for studying paperboard behavior that aligns with experimental accuracy and practical usability.

[1] A. Biel, J. Tryding, M. Ristinmaa, M. Johansson-Näslund, O. Tuveesson, and U. Stigh, Experimental evaluation of normal and shear delamination in cellulose-based materials using a cohesive zone model, *International Journal of Solids and Structures*, Vol. 252, p. 111755, 2022.

## **On the design of corrugated boards: a new FEM modeling and experimental validation**

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A recent corrugated board-related review has identified certain gaps, in particular related to Finite Element Method (FEM) modeling. There is evidence of significant evolution in terms of simulation power, techniques, and reported results on the homogenization of corrugated boards [1], from which simulations of corrugated boards may benefit in order to be more accurate, as referred to in the literature [2]. By integrating the latest homogenization studies, our research aims to refine existing FEM models of corrugated boards, which were developed before such advancements. Our approach includes a preliminary FEM model that predicts the mechanical behavior of corrugated boards with enhanced accuracy, incorporating contact mechanics simulation. The robustness of the model is validated through experiments using a Zwick machine, establishing a correlation between theoretical predictions and practical observations. Furthermore, we employ standard tests such as ECT, SCT, CMT, and FCT for comparative analysis, ensuring that our model aligns with industry benchmarks. The discussion deals with issues related to the numerical analysis, highlighting the simplifications made from a physical perspective. These simplifications are necessary for computational feasibility while maintaining model accuracy. The paper critically examines the balance between model complexity and practical applicability, offering insights into the potential and limitations of FEM in the context of corrugated board mechanics. This study not only advances the understanding of corrugated board behavior under various conditions but also sets a precedent for future research in packaging materials and optimization of the design of corrugated boards. The way is paved for more efficient and reliable design practices in packaging engineering.

[1] Mrówczyński, Damian, Anna Knitter-Piatkowska, and Tomasz Garbowski. 2022. Non-Local Sensitivity Analysis and Numerical Homogenization in Optimal Design of Single-Wall Corrugated Board Packaging. *Materials* 15, no. 3: 720. <https://doi.org/10.3390/ma15030720>

[2] Fitas, Ricardo, Heinz Joachim Schaffrath, and Samuel Schabel. 2023. A Review of Optimization for Corrugated Boards. *Sustainability* 15, no. 21: 15588. <https://doi.org/10.3390/su152115588>

## Transient deformation & swelling of paper by aqueous co-solvent solutions

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Inkjet printing inks frequently contain polar liquids of low volatility such as glycerol or poly(ethylene glycols) in addition to the main solvent water. The deposition of these liquids on paper sheets induces swelling of the cellulose fibers, which leads to an overall, anisotropic deformation of the sheet. We characterized the corresponding strain components by means of a grid projection method and white light interferometry. For pure water, most of the hydroexpansion strain vanishes again after drying is complete. However, for aqueous solutions of non-volatile co-solvents, a large fraction of the deformation persists after the water has evaporated. Because swelling occurs only after liquid enters the cellulose fibers, monitoring the dynamics of expansion provides insight into the pore-fiber distribution of co-solvents. The corresponding timescales of pore-fiber transport strongly depend on the co-solvent concentration, as a sufficient quantity of water is needed to plasticize the fiber walls.

[1] Wijburg M.G., Wang S. and Darhuber A.A. Transport and evaporation of aqueous co-solvent solutions in thin porous media. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 656, p.130268, 2023.

[2] Wong C.L., Wang S., Karimnejad S., Wijburg M.G., Mansouri H., and Darhuber A.A., Transient deformation and swelling of paper by aqueous co-solvent solutions. *Soft Matter*, 19(6), pp.1202-1211, 2023.

## Fibre distributions as a microscopic probe of pulping phenomena

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We demonstrate how data from optical fibre analysers can be used to study fibre deformation phenomena in pulping unit processes. For this purpose, we compare data measured before and after a process step and then test if the observed changes can be reproduced with a stochastic model for the local deformations that we anticipated. Focusing on particle sizes in the case of industrial LC refining [1] of a thermomechanical pulp (TMP) and chemical pulps (softwood and hardwood), we could identify the dominant mechanisms that in each case explained most of the changes we saw in measured distributions of  $10^5$  particles. In the case of the TMP, the measured changes could be reproduced with lengthwise cutting of



long fibres and radial splitting of short fibre fragments (fine material). The probabilities of these two types of local “fragmentation” events were the only adjustable parameters in the stochastic model. For the LC refining of chemical pulps that we studied, the fragmentation of fibres was less important. Instead, the fibres appeared to elongate and, in the case of the hardwood, swell in the radial direction. Swelling agreed with the accumulation of local swelling “impacts” whose magnitude and probability were the adjustable parameters of the stochastic model. Work is in progress on the apparent elongation of fibres that could arise from the straightening of localized microcompressions [1] or macroscopic deformations (bends or folds), or from instrumental artefacts. In summary, we show how changes in fibre distributions can be used to extract quantitative information about different fibre phenomena that can occur in a fibre processing equipment. In that respect, it complements earlier studies of fibre distributions that also considered refiner conditions such as plate geometry, flow rate and angular velocity (see e.g. [2]).

[1] Page, D., The Beating of Chemical Pulps—The Action and Effects. Trans. of Fundamental Symposium (F. Bolam Ed.) Tech. Sect. BP&BMA Oxford (1989).

[2] Berna, J.E.R., Martinez, D.M. and Olson, J.A., A comminution model parametrization for low consistency refining. Powder Technology, 328 (2018), 288 - 299.

## Mechanics of reverse-side crease cracking of paperboard

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Previous work [1, 2] showed that a creasing operating window can be defined with two metrics of creasing severity: critical shear and critical draw. Shear produced by creasing causes internal delamination and reduces resistance to folding; the critical shear describes the point beyond which the folding resistance is below a target. Creasing draw provides a measure of the tensile deformation of the material into the crease and was shown to be correlated with reverse-side (bead-side of the crease) crease cracking. Beyond a critical point, cracks will be initiated on the surface, which can then be propagated by folding. Critical draw describes the threshold from stable & minimal to unstable & significant cracking. However, draw is in terms of length, not strain, so it isn't obviously transferable to systems with different geometry and constraints. Further, the effects of tensile load and sample dimensions are unclear, as the effect of creasing tooling geometry was studied under a single tensile load and sample dimensions.

In this work, the mechanics of reverse-side crease cracking was further investigated with physical and numerical experiments on the effect of the sample dimensions and tension. The physical experiments were conducted using a laboratory creasing unit and an coated paperboard. Under the tooling of the same geometry, the critical draw decreases linearly as the strip tension increases. A strip with a width greater than the creasing tooling shows a higher critical draw than a strip with a narrower width. The gage length can cause a decrease in critical draw for

MD oriented creases, but did not cause a decrease for CD oriented creases.

Numerical experiments were completed using the material point method (MPM). MPM is used because of advantages for contact (with loading rods), large deformation, cohesive zone modeling, and damage mechanics. Paperboard deformation is modeled as an anisotropic material with Hill plasticity. Shear damage is modeled with mixed mode (tension and shear) cohesive zones. This is a new approach that is not available in commercially available numerical modeling packages; it also works for 3D deformations (eg deep draw modeling). The simulation results show that there is a higher stress in the creased region corresponding with the conditions with lower critical draw in the previous work.

[1] Coffin, D.W., Panek, J.C., On the nominal transverse shear strain to characterize the severity of creasing, TAPPI J., 17(4):231-240, 2018.

[2] Panek, J.C., Smith, S.D., Coffin, D.W., Creasing severity and reverse-side cracking, TAPPI J., 19(4):219-227, 2020.

## **Point load measurements on carton board packages and bulging**

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In the manufacture of carton board packages, cardboard is creased and folded before the package is erected, filled and used. The creasing is a folding instruction, or push-in, of the material that is carried out to reduce the bending resistance during the folding. The material is intentionally damaged or deformed during creasing to facilitate folding. The goal is to diminish the bending resistance to facilitate the folding, that is to get the cardboard to work more like a hinge. [1]

Depending on the residual momentum at bending, the panels of the package may after erection bulge more or less. This study demonstrates how the bulging of the carton board package may be picked up by point load measurements. Results of the point load measurements are discussed.

[1] Coffin D. and Nygårds M., Creasing and folding, Advances in Pulp and Paper Research, Oxford 2017, Trans. of the XVIth Fund. Res. Symp. Oxford, 2017, (W. Batchelor and D. Söderberg, eds), pp 69–136, FRC, Manchester, 2018. DOI: 10.15376/frc.2017.1.69

## **L-Crush test - A method for assessing the creasing and failure behavior of paper folding core structures**

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Folding cores made of paper represent an innovative and sustainable sandwich core structure with high lightweight potential. Paper offers great potential for growing markets such as packaging, furniture construction and lightweight applications. Previous research work has

investigated the correlation between paper properties and the mechanical properties of folding cores as well as methods for assessing creasing. Creasing is necessary in the manufacturing of folding cores in order to bring the folding pattern into the paper and thus define the fold lines for folding. The L-crush test is a test in which a folded, L-shaped clamped sample is crushed. This test method is intended to simulate a single fold and the failure behavior within folding cores and based on the Ring Crush Test (RCT). For the test, the sample is first creased and then clamped in a fixture at a  $90^\circ$  angle for compression. When carrying out the test, the load-displacement curve and so the L-crush resistance and the stiffness are determined. The results to show that the failure modes of the L-shaped samples and the folding cores are comparable. It can also be seen that at very high creasing forces the samples tend to fail by tearing along the fold, whereas at lower creasing forces the failure occurs by buckling along the fold edge. The course of the load-displacement curve of the L-shaped sample can be qualitatively compared with the course of the stress-strain curve of folding cores. The results so far indicate that the L-Crush Test offers great potential for assessing the creasing quality and for estimating the mechanical properties of folding cores. However, it is still unclear what correlations there are between the paper properties and the results of the LCT. The experimental design method is used to find out what influences the height and length of the L-shaped clamped sample and the properties of the paper, such as pulp, refining and grammage, have on the L-crush resistance and stiffness. The following mechanical properties are determined for each of the papers: Short compression strength, ring crush resistance, ring crush stiffness, bending resistance and thickness. Using the analysis of variance method, these parameters are also used to determine whether there are correlations between the mechanical properties of the paper and the measured values of the LCT. The aim is to optimize the L Crush Test method so that it can be used for the design of folding cores made of paper.

## **S02 | Modeling the mechanical response of fibers, paper, and board**

### **Reduced order multiscale modeling of paperboard**

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Paperboard is an important material for packaging food and beverages, with hundreds of billions of packages produced every year. Since quality of the packaging material is key, it is essential to understand the influence of fiber properties and fiber orientation on the mechanical response of paperboard. This is difficult because of the natural variability in the mechanical properties of paperboard fibers. Material models that take microstructure into account in the modeling framework can be used to redesign the paperboard structure and predict the quality of the packages.

Virtual modeling is therefore a powerful alternative to experiments, for gaining insight into the mechanical behavior of paperboard and predict its response in complex load cases. To this end, continuum based paperboard models have been used to predict the macroscopic mechanical response. Macroscopic models have successfully captured creasing and folding in industrial packaging applications [1]. Yet, a micromechanical model is needed for a deeper insight into the micromechanical response, and enables optimization of the material designs.

In this contribution, a multiscale framework is implemented, where the macroscopic response is determined entirely by a microscale representative volume element (RVE). The RVE is modeled with conventional continuum mechanics, where elastoplasticity is encompassed. To alleviate the inherent computational effort of multiscale analyses, an eigenstrain-based reduced order model (ROM) [2] is implemented. In this reduction, the RVE is divided into partitions, where plastic strain fields are assumed to be uniform for each partition.

The multiscale analysis successfully captures simple loading cases, such as uniaxial loading. This contribution provides a very promising framework upon which a more complex model will be developed.

[1] Robertsson K, Jacobsson E, Wallin M, Borgqvist E, Ristinmaa M, Tryding J. A continuum damage model for creasing and folding of paperboard, *Packaging Technology and Science*, Vol. 36, 2023.

[2] Fish J, Filonova V, Yuan Z. Hybrid impotent-incompatible eigenstrain based homogenization, *International Journal for Numerical Methods in Engineering*, Vol. 95, 2013.

### **A two-scale finite element model of paper materials based on a statistical physics microscale approach**

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Studying the mechanical behaviour of paper products is challenging due to their anisotropic response caused by the complex microscale composition governed by the network of cellulose fibres. To address this challenge, a two-scale finite element modelling technique inspired by the FE2 approach [1] is herein proposed, where a separation of length scales is postulated between the macroscale and the microscale. The method relies on a macroscale continuum finite element model of the paper component where at each Gauss point the tangent constitutive tensor is not assigned a priori, but it is computed from a statistical physics microscale model of paper. The statistical physics model [2] will provide the components of the stress tensor for any applied strain level by considering realistic number of fibres and their progressive nonlinear deformation during the loading process. This integration by considering detailed aspects at both macro and micro scales provides a more thorough understanding of the mechanical properties of these materials, offering potential improvements in predicting and utilizing the components made of paper with any geometry and subject to complex loading conditions. The mathematical formulation is implemented into the finite element analysis programme FEAP8.6 from the University of Berkeley, USA.

[1] I. Özdemir, W.A.M. Brekelmans, M.G.D. Geers, FE2 computational homogenization for the thermo-mechanical analysis of heterogeneous solids, computer methods in applied mechanics and engineering, Vol 198, 602-613, 2008.

[2] M. Fallah, H. Zarei, M. Paggi, A novel in situ micro-mechanical testing campaign on paper fracture and its statistical mechanics model, Euromech Colloquium 634 - Multi-physics of fibrous networks and fibre-composite materials, June 19-21, 2023, Eindhoven, the Netherlands

## **The mechanical behaviour of dry-formed materials - Modelling cellulose fibre materials with weak interactions**

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Dry-forming is a paper-forming technology that has been studied to a limited extent. In contrast to its wet counterpart, it requires no added water in the forming process. This leads to quicker forming of products and decreased energy consumption, as there is little water to evaporate. However, water is crucial in the formation of the molecular interactions that make up the fibre-fibre joints, which in turn build up the cohesiveness of the fibre network. Consequently, the formed material will be much weaker than traditional paper materials. Thus, the validity of common paper material models needs to be investigated.

The work presented here applies existing continuum paper models [1] to dry-formed cellulose materials and compares the results to previous experimental characterisation. The materials are, at varying density levels, subjected to in-plane tension, out-of-plane compression, and out-of-plane shear, as well as combinations of those. At first, the single-mode tests are used to find material constants through an iterative procedure. In the next step, coupling effects between loading modes are evaluated through simulation of the mechanical tests with the combined modes. The chosen models are then reevaluated, and suitable damage models are introduced

to account for the failure caused by a multiaxial stress state.

The results reveal the consequence of weak fibre-fibre joints on the overall behaviour of the network. In the absence of water and relatively weak joints, the failure mechanism is mainly governed by joint failure, even at high densities ( $>1000 \text{ kg/m}^3$ ). In contrast to conventional materials at these densities, the fracture observed here shows a behaviour distinct from the one typically observed in dense papers. For example, in the uniaxial test, this is manifested through pronounced strain softening beyond the stress peak point. Furthermore, the characteristic profile of the fracture path, discernible in both the in-plane and out-of-plane directions, suggests a fracture mechanism predominantly governed by shear forces. This is advantageous for the current application, as the softer behaviour makes the material suitable for forming. To accurately represent the evolution of material properties throughout the forming process, we propose a model incorporating parameter dependencies on material density.

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## **Modeling in-plane tensile properties of paperboard as function of gauge length using anisotropic damage mechanics and gaussian random fields**

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In-plane stress strain curves of coated solid bleached sulfate (SBS) paperboard were measured in both machine (MD) and cross (CD) directions as a function of gauge length from 10 to 100 mm. Results from 30 replicates for each gauge length provided average stress-strain curves, mean strength, and strength coefficient of variation. All experiments were simultaneously modeled with a gauge-length independent material model combining orthotropic elasticity, anisotropic plasticity, and anisotropic damage mechanics [1]. To fit all results, our modeling had to incorporate stochastic methods where stress to initiate damage was described by a Gaussian Random Field (GRF) with spatial correlations.

Two new outputs when using GRF methods are spatial correlation distance and coefficient of variation of the GRFs. These outputs provide structural information about paperboard products. The anisotropic damage mechanics used to fit experiments provided estimates of MD and CD paperboard toughness. The stochastic nature of both experiments and modeling, however, limited the ability of modeling to extract toughness from unnotched-specimen stress-strain experiments.

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## **An elasto-plastic material model for paper and paper-board at finite deformations**

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Paper and paperboard are widely used as writing, printing, and packaging materials, today. The exceptional mechanical properties and excellent recyclability of paper make it a promising substitute for traditional engineering materials such as metals or plastics. However, its intricate material behavior represents a current limitation to its wider application in engineering. This is due to the microstructural fiber network present in paper, which has a significant impact on macrostructural properties, including anisotropic elasto-plasticity.

In a continuum mechanical framework, paper can be considered as a homogeneous anisotropic material. Anisotropy is characterized by three principal directions, which are defined by the orientation of the fibers. In-plane, paper exhibits predominantly minor deformations, whereas significant deformations occur in the out-of-plane direction. It was demonstrated that the Poisson ratio in the out-of-plane direction is negligible, thereby enabling the decoupling of in-plane and out-of-plane behavior. Still, in order to address the complex deformations, for example, those occurring during forming processes, a unified model is required.

In the context of finite elasto-plasticity, the deformation gradient is split multiplicatively. This leads to the emergence of a non-unique intermediate configuration. Moreover, the derivation of frame-indifferent nonlinear constitutive laws for anisotropic materials requires the introduction of structural tensors. The thermodynamic consistency of the model is guaranteed by selecting an appropriate yield function, which is based on a modified version of the formulation proposed by Xia, Boyce, and Parks [1]. The model's validity is confirmed through several simulation results.

[1] Q. S. Xia, M. C. Boyce, and D. M. Parks. "A constitutive model for the anisotropic elastic-plastic deformation of paper and paperboard". In: International Journal of Solids and Structures 39.15 (July 2002), pp. 4053–4071. doi: 10.1016/ s0020-7683(02)00238-x.

## **2D non-linear material behavior and failure of loaded paper and board structures in finite element calculations**

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Efficient utilization of materials and lightweight constructions are fundamental principles observed in nature and are increasingly essential in today's technological advancements.

In this context, we introduce a non-linear elastic orthotropic material model tailored for paper and board, designed to facilitate precise engineering calculations. The majority of required material coefficients are derived from standard paper physics testing protocols. Our material

model assumes uniform behavior under tensile and compressive loading conditions, mirroring common practices found in the characterization of various composite materials. While this simplifying assumption warrants further refinement, it aligns with the level of detail commonly employed across material sciences. To facilitate computational analysis, we discretize the non-linear stress-strain curves of paper – both machine direction (MD) and cross direction (CD) – into  $n$  segments. Within each segment, the curves are approximated using linear interpolation techniques.

Finite Element (FE) calculations using standard software for analyzing Paper and Board structures should be carried out until structural failure is observed. However, employing non-linear material models often necessitates an extension of the FE software capabilities.

To accommodate these advanced models, the structure's geometry is discretized into hundreds of FE elements. Additionally, the loading process is divided into numerous small steps ( $m$ ), with each step requiring the creation of a separate FE model followed by computation. During each loading step, the FE model is adjusted to account for the deformed geometry from the preceding step. This adjustment involves updating the material coefficients based on the localized stress/strain preload by each element. Consequently, each finite element possesses its own unique load-dependent material properties. Throughout the calculation process, the boundary conditions remain constant, and subsequent load increments are defined. All calculation steps together captures the non-linear load-deformation behavior of the structure until failure occurs.

Remarkably, the efficiency of modern computational hardware ensures that each calculation step and the associated model-building process typically last only seconds, even on standard laptops. Consequently, the overall computation time remains manageable, typically measured in minutes.

A structure failure criteria after element overloading is proposed.

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## Assessment of paper curl predictions by two and three-dimensional fibre network models

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The exposure of paper sheets to through-thickness moisture gradients gives rise to non-uniform hygro-expansion, which in turn results in curl. The micro-structural origin of the hygro-expansion is relatively well understood: under the influence of absorbed water the fibres in the sheet swell by as much as 20%. Reliable quantitative measurements exist of the free expansion of individual fibres, as well as of isolated fibre-to-fibre bonds [1]. A more elusive question is exactly how this expansion of fibres and bonds is translated into sheet-scale expansion and curl - and how these mechanisms depend on the properties of the network. Methods proposed in the literature range from advanced computational multiscale models to more pragmatic approaches based on highly idealised representations. In the latter category, hygro-expansive coefficients for uniform wetting may be obtained from two-dimensional analyses of the network [2]. These can subsequently be injected into a simple continuum model of a sheet in bending. Our objective in this study is to assess the accuracy of curl predictions obtained via this two-step procedure. As a reference we use a three-dimensional finite element model of an idealised fibre network. We compare the expansivity under uniform wetting and the curl due to a moisture gradient as predicted by the analytical model with those obtained numerically from the three-dimensional finite element model. The results show that the inaccuracy of the curl prediction by the fully analytical model may be as high as 50%. However, if the expansivity extracted from the three-dimensional simulations under uniform wetting is inserted in the curl model, its inaccuracy drops to less than 10%. The continuum bending description hence performs adequately, provided it is based on a reliable estimation of the uniform expansion response

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## S03 | Moisture and temperature transport in paper and tissue

### High contrast analysis of cellulose nanofibril film structure and barrier properties

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Applications of cellulose nanofibril (CNF) films in the packaging industry are restricted due to their poor water vapour barrier properties [1]. This is due to our inability to link CNF film structures to their water vapour barrier capabilities, which is exacerbated by a lack of reliable bulk morphology characterisation methods [2].

Here, we demonstrate the combination of mercury intrusion porosimetry (MIP) and X-ray micro-computed tomography ( $\mu$ CT) to be an effective CNF film structure characterisation method. Mercury-intruded CNF films of varying grammage (151 g/m<sup>2</sup> to 266 g/m<sup>2</sup>) and layers (1 to 3) were analysed with  $\mu$ CT at 0.7  $\mu$ m voxel size. The mercury was easily distinguished in the reconstructed  $\mu$ CT data, illuminating the pore structure and obscuring all other artefacts. Detailed information on film thickness, porosity, and pore morphology could be determined in mercury-intruded films by  $\mu$ CT. This was not possible with non-mercury-intruded films.

Over 90 % of the identified pore networks were found to span the film thickness, even for films with grammage above 200 g/m<sup>2</sup>. We show that despite the formation of higher grammage and multi-layered films, the internal structure of the CNF films did not change significantly. This potentially explains the limited achievable water vapour transmission rates (WVTRs) produced by CNF films, as evidenced in our previous work demonstrating the WVTR plateau of 30 g/m<sup>2</sup> day for films above 300 g/m<sup>2</sup>. The MIP- $\mu$ CT method we developed will be applicable in analysing future cellulose-based films of varying structure, such as traditional paper, where comprehensive and robust film morphology characterisation is critical.

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## Absorption in paper: Where is the water? (Part 1)

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During this presentation, we discuss our latest research on understanding edge wicking in paper through the utilization of optical coherence profilometry, flow tracers, and x-ray microtomography [1, 2]. Our findings reveal a two-stage process of imbibition: first, percolation through the fibre wall, followed by the filling of external pore spaces. Self-similar behaviour is noticeable in all regions except in proximity to the wetting front. We also postulate the potential additional microscale mechanisms driving the need for the second part of our study.

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[2] Ferreira, E. S., Drummond, J., Veiga, A. T. V., Sibellas, A., Brown, S., Cranston, E. D., & Martinez, D. M. (2023). Mapping absorbency in cellulosic fibres with iron tracers. *Carbohydrate Polymers*, 120785.

## Absorption in paper: Where is the water? (Part 2)

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The water absorbency of paper-based products is a crucial material characteristic. The regulation of this property, whether to enhance or hinder it, involves understanding the microscale dynamics of imbibition, and currently, there is no consensus within the scientific community regarding this phenomenon. Notably, traditional imbibition models like the Bell-Cameron-Lucas-Washburn equation have been found to be potentially unreliable, and we propose that these models lack coverage of all the physical mechanisms needed to accurately characterize imbibition. To this end, we have performed a systematic study using X-ray microtomography, X-ray radiography, fluorescence microscopy, and backlight imaging to visualize the microscopic flow field for a range of fibrous materials in order to discern the effects of various physical and chemical treatments. In these experiments, microscale imbibition behaviours such as fibre swelling, interphase mass transfer, and partial saturation were observed, highlighting potential mechanisms to target when aiming to enhance or resist

imbibition.

## **A numerical model for the transport and drying of solutions in thin porous media - Coffee-stain effect and solute ring formation**

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We have developed a comprehensive numerical model for the transport and drying of solutions in thin porous media that consist of permeable fibers such as paper. We explicitly account for the gas-phase transport dynamics. Moreover, we introduce an empirical relation for the concentration- and molecular-weight dependence of the pore-fiber transport rate of the solutes. These two key elements enable us for the first time to realistically model two important phenomena relevant to inkjet printing technology. The first is the equivalent of the coffee-stain effect for dilute solutions in porous media. The second is the formation of solute rings for concentrated aqueous mixtures of compounds with a molecular weight significantly above that of water. Whereas the first is governed by spatially non-uniform solvent evaporation, the second case is dominated by solvent-mediated pore-fiber transport. We achieved a good qualitative agreement with the available experimental data.

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## **Paper fibers beyond saturation: $\mu$ -ct analysis of prolonged structural changes**

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The uptake of polar volatile compounds such as water or dimethyl sulfoxid (DMSO) by paper is a complex interplay between sorption in the cellulose-lignin based fibers, diffusion, and capillary transport. We aim at distinguishing the relative impact of sorption and of capillary transport on the microstructure of paper by exposing strongly hydrophobized paper to either the vapor phase or the liquid phase of the compounds, while monitoring the uptake and swelling. DMSO is chosen because it is expected to enter inter-fiber pores and thus capillaries, which are inaccessible to water in strongly hydrophobized papers. Microcomputed tomography ( $\mu$ -CT) allows us not only to locate liquids within the pores, but to quantify changes in the microstructure, i.e., in fiber volume and in volume of pores between the fibers, as the uptake evolves over time.[1]



This gives us the possibility to relate volume changes to the amount of volatiles incorporated. We find that capillary transport greatly accelerates uptake; while a few days are sufficient to saturate paper with liquid DMSO, an uptake by vapor requires several weeks to saturate paper. The extent of swelling of the fiber and the inter-fiber pores depends on whether the paper was exposed to liquid or vapor. However, a pore network analysis of the reconstructed  $\mu$ -CT images reveals that the structural changes in the initial stage of exposure are similar for both exposure scenarios. The long-term behavior shows similarities regardless of whether liquid or vapor, DMSO or water is considered. Long after the mass uptake is complete, i.e., saturation is reached, the volume of fibers and pores continues to change. This long-term expansion, which involves a redistribution of the volatiles in the fiber walls, is likely due to a progressive detachment of fibril bundles.

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## Investigation of capillary rise height under rotational conditions

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The aim of our project is to gain a better understanding of capillary rise in paper-based materials in order to determine different material properties, such as pore radius, porosity, contact angle and fibre roughness. With our self-developed rotation device, the equilibrium state, which occurs under rotational conditions during the imbibition of water in paper, is investigated for different rotational speeds. This approach was developed in order to be able to neglect various effects that play a role in the dynamics of imbibition. Nevertheless, previous work has shown that it is not sufficient to consider only capillary and centrifugal force for the theoretical modelling of the capillary rise height [1]. We extended the model to include the effect of angular velocity dependent evaporation and found a good agreement between the measured data and the model. In order to verify the evaporation rate resulting from the fitting of the model to the data of the rotation device, a vertical imbibition experiment is also carried out, in which the evaporation rate is determined gravimetrically under controlled humidity. In addition, the surface or fibre roughness has also been integrated into the model. In order to demonstrate their influence experimentally, roughened glass capillaries and porous glass were rotated in addition to paper substrates. Thirdly, we investigated the question of whether, despite the equilibrium state of the imbibition, (local) currents occur under rotational conditions that can also have an influence on the exposure distance. This question was experimentally realized with fluorescent particles added to the liquid and coaxial zoom optics.

[1] Postulka N., Meckel T., Biesalski M., Porosity Centrifuge: Determination of Pore Sizes of Swellable Porous Materials under Hypergravity, Langmuir, 37, 2021.

## Limiting factors for microcomputed tomography monitoring of water transport through paper

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While microcomputed tomography ( $\mu$ -CT) can be a powerful tool for investigating liquid water uptake in paper, this technique has inherent limitations for time-resolved measurements. These limitations are related to aspects such as the minimum acquisition time, exploitable absorption contrast, and degradation in combination with the paper grade, which may have, for example, fillers or certain sizing. Each aspect is ultimately linked to a sufficient spatial resolution, which is essential for distinguishing fibers, the pore space between the fibers, and the location of liquid within the pore space. The minimum acquisition time depends on the sizing. While hydrophobic papers can stretch the uptake over hours, hydrophilic samples incorporate water in the order of minutes, causing rapid changes in the microstructure. Such changes cannot be recorded quickly enough with a  $\mu$ -CT measurement, resulting in blurred 2D images and reduced spatial resolution in the reconstructed image. Fibers have a rather low absorption contrast, so that fillers with their comparatively high absorption contrast obscure the fibers. This contrast can be enhanced by adjusting the acquisition times, which in turn compromises the spatial resolution. If such contrast enhancement is not possible, the partially obscured fibers enter the 3D reconstruction like blurred features and thus reduce the spatial resolution, regardless of whether the samples are dry or wet. In addition, samples immersed in water can degrade rapidly under certain conditions.

## Web structural changes that occur in paper towels upon the imbibation of water

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Paper towel products, a subset of hygienic papers, includes kitchen towel and away from home hand towel paper grades, where the end use properties of water absorbency and wet strength are of paramount importance. End use performance depends on the rate of water absorption and specific water holding capacity when used to dry surfaces such as countertops or hands. Maintaining strength during wiping is essential, and achieved through the use of wet strength resins. Of secondary importance is softness or hand feel that results from web bulking and fiber flexibility, which have a positive effect on value ranking. Creating a structure with the counteracting properties of strength and bulkiness, the latter caused by reduced bonding and open pore structure, has been attained using a variety of manufacturing processes. These include creping, through air drying, embossing patterns, multi-ply layering and chemical treatments. And while the complex structures of these products have been revealed using

modern 2D and 3D microscopic techniques, there is an absence in the literature of dimensional changes that occur upon wetting with water. The fragility of the web precludes analysis post drying, since the surface tension of the water collapses the structure. The investigation discussed in this presentation pursues the examination of the structure of paper towels in the wetted state or dried in a manner that preserves the wet web structure.

Two approaches were used to map the 3D structure of the web, before and after wetting. The first uses liquid exchange to replace the interstitial water with solutions of ever decreasing surface tension. The final step for drying occurs with a liquid with sufficiently low surface tension so that the delicate wet web structure is preserved. The structure is analysed before and after wetting using 3D Xray microscopy and Twin Laser Profilometry. A second approach uses the non-contacting TLP profilometric technique to map the two external surfaces of the web in situ before and while in the wetted state. Dimensional changes that occur upon wetting are quantified using digital volumetric correlation analysis. Of interest are the changes that occur around, and as a result of, specific induced structural features, such as TAD domes or crepe lines. This presentation will report experimental constraints and limitations of the methods for a select set of samples.

## **A thermo-hygro-mechanical material model for paper and paperboard**

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Paper and paperboard are recognized as sustainable materials due to their biodegradability, recyclability, and reusability. While they are predominantly used in the packaging industry, the ongoing environmental challenges may expand their application in other sectors. A critical aspect of these materials is their behavior under combined thermo-hygro-mechanical loads.

To address this, we have developed an innovative material model that simulates the mechanical behavior of paper and paperboard under varying temperature and moisture conditions. Interactions between elasto-plastic deformation, moisture diffusion, and heat conduction as well as accounting for the reduction in stiffness and strength as moisture and temperature rise were integrated into the model. Temperature-induced expansion, as well as swelling and shrinkage were also considered. Furthermore, the effects of energy dissipation and drying on the material's temperature and moisture fields were taken into account. Formulated within a thermodynamically consistent framework, this model is applicable to finite deformations. The necessary material parameters were identified through conventional experiments. The model's effectiveness was demonstrated through various numerical examples.

The material model has the potential to significantly benefit the packaging industry by optimizing manufacturing processes and making paper and paperboard more attractive for broader use.

## **Paper curl at different time scales: seconds, minutes, weeks**

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The dimensional stability of paper during printing is crucial for ensuring production quality and runnability. However, inkjet printing faces inherent challenges due to the hygroscopic nature of paper and the use of water-based inks. We are starting by discussing the root causes of paper curl due to wetting, drying and paper two-sidedness. Special focus is given to the fundamentally different drivers for the curl immediately after wetting and the resulting permanent curl after redrying. We then move on to the analysis of long term curl, which develops over weeks. Despite freshly printed sheets are flat, a considerable development of paper curl is often observed during storage. In this study, we establish the link between the migration of ink co-solvents and the long-term curl development of printed paper. A4 paper sheets were sprayed with a water-glycerol model ink and changes in the sheet's curvature were monitored using a 2D-laser sensor. We also investigated glycerol migration by splitting the sheets into layers and determining the glycerol distribution using high-performance liquid chromatography. Our results demonstrate the development of curl during storage as well as glycerol migration in thickness direction of the sheet, both on a comparable timescale. We thus propose that long term curl in inkjet printing can be caused by z-directional migration of the co-solvent (glycerol) over time. Finally we are discussing the role of fiber bonds in the development of paper curl.

## **Moisture transport and swelling in paper sheets: a strategy based on a multi-phase flow approach**

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Paper is a natural material composed of fibers and pores. This porous structure is highly sensitive to fluctuations in moisture content. When paper is used for digital printing, fluctuations in the moisture content may produce a hygroexpansion of the material. If the printing process is not properly controlled, unacceptable deformations may result. In this work, we implement a computational model to study the moisture transport and swelling in paper. Paper is modelled as a multi-phase material, by means of the hybrid mixture theory [1]. The advantage of this approach is that balance equations can be solved for phases and constituents. Therefore, the constitutive laws and mechanisms driving the flow needs to be defined at the smaller scales, which allows a better correspondence between our simulations and the underlying physics of the problem. An application of the hybrid mixture theory can be found in [2], where a triphasic model was derived to study porous cellulose networks. Here, we adapt this model to study paper. The novelty of our work is that the constitutive relations are derived from physical prin-

ciples and assumptions at the microscale level. We model paper as a structure composed of two phases: fibers and inter-fiber water. Moreover, we assume that fibers are composed of the solid skeleton and intra-fiber water. Liquid transport is modeled using unsaturated flow theory. The moisture transport in pores and fibers is assumed to be driven by the chemical potential. When paper is in contact with water, the pores are filled first because of capillarity. The pores are modelled as tubular structures with different radii. Water fills the smaller pores first and then the larger pores, which is consistent with the microscopic reality of the problem. Some of the water in the pores is absorbed by the fibers. By solving analytically a single fiber problem, we found an expression for the mass exchange between fibers and pores. Water captured in fibers produce swelling in them. Swelling and mechanical deformations are modelled using a linear elastic law. The performance of the model is verified by using experimental data on plain paper.

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## **Integrating reactive diffusion and swelling in Cellulose-based porous media through physics-informed neural networks**

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The simulation of reactive diffusion of fluids through porous media poses significant challenges, especially when dealing with the complex geometries and dynamic changes within real-world porous media, such as swelling of the solid matrix in paper.

Conventional numerical solvers often struggle to accurately and tractably represent these complexities. This study leverages state-of-the-art extended physics-informed neural networks (PINNs) to develop a mesh-free modeling framework to investigate the reactive transport of moisture and volatile organic compounds through the intricate microstructure of paper. The application of PINNs allows the implicit inclusion of experimentally observed changes in the geometrical properties of the paper matrix in the formulation of the governing partial differential equations.

Consequently, this approach facilitates the study of the spatio-temporal evolution of migrant concentrations within the porous environment of the paper, taking into account the dynamic adaptation of the material geometry through processes such as swelling or shrinking to the current state of adsorption. To the best of our knowledge, this is the first demonstration of the use of PINNs to account for adaptive geometries during transport.

## **Tomographic investigation of liquid distribution in partly-saturated fibre networks under different strain states**

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In paper manufacturing, efficient wet pressing is crucial for achieving an economical and energy-efficient process. Wet pressing of paper can be described as a transport process, where the web and press felt constitute a layered porous media that is compressed by an external load, where water flows from the paper web into the voids of a press felt. After the initial dewatering of the paper web, partly saturated conditions of the wet fibre networks are present where part of the water was substituted by air during the elastic re-expansion of the networks. At a subsequent compression (e.g., in a second press nip), the compaction of the paper web and press felt causes a change in the distribution of pores and pore sizes [1], resulting in local changes in the capillary pressure of the network. Furthermore, air can be trapped inside the pores of the networks, clogging the water flow paths [2]. Consequently, the overall permeability of the networks changes, which can significantly influence the dewatering efficiency. In our study, we demonstrate a novel method to study the distribution of inter-fibre water in partly saturated fibre networks under different strains with tomography. Visualizing water, fibres, and air simultaneously in a tomographic image is difficult due to similar attenuation coefficients, so choosing a suitable contrast agent solution that behaves similarly to purified water within the porous network is studied in depth. This allows for a sufficient distinction between the three phases within one scan, enabling the study of the realistic water distribution in partly saturated fibre networks under varying strain conditions. The results emphasize the influence of the microstructure on the resulting fluid distribution and show how the fluid particle size decreases with increasing strain of the network.

[1] Chevallier, P. and Silvy, J., La perméabilité directionnelle des feutres de presses humides. La papeterie, 5. 1988.

[2] Vomhoff, H., Dynamic compressibility of water-saturated fibre networks and influence of local stress variations in wet pressing. PhD Thesis. Royal Institute of Technology, Stockholm, 1998.



## S04 | Pulp and paper engineering

### Characterisation and effects of micro- and nanoscale components and their impact on the efficiency of chemical additives

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The presence of microfibrillated cellulose (MFCs) and cellulose nanofibers (CNFs) in paper pulp significantly affects the final paper properties. Despite the intense academic attention and promising possibilities, the micro- and nanocomponents have yet to be thoroughly investigated and integrated by the industry. The lack of uptake by sector is primarily the result of the challenges associated with studying these fine materials [1]. We propose to develop a straightforward methodology to study the effect of the micro- and nanoscale components. The methodology is based on flow pulsation, where the CNFs align at a higher flow rate, followed by decay due to Brownian motion at lower flow rates [2]. Using Polarised Optical Microscopy (POM), the measured time-dependent quantities, such as birefringence, particle content, and patterning, can be combined to get the sample fingerprint. The setup includes a light source, two polarization filters, and a camera. Furthermore, the setup is small and automated by Raspberry Pi to facilitate portability and fast data processing. We investigated MFC's fine samples with different coarseness; repetitive results show unique decay profiles for different samples, indicating the different sample compositions. The work serves as a basis for analyzing industrial white-water samples and better understanding the impact on dosage and retention in papermaking.

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[2] Rosén, Tomas, Nitesh Mittal, Stephan V. Roth, Peng Zhang, Fredrik Lundell, and L. Daniel Söderberg. "Flow fields control nanostructural organization in semiflexible networks." *Soft Matter* 16, no. 23 (2020): 5439-5449

### Energy optimization of pressure screen rotor via a CFD virtual test bench - best practice

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Pressure screen rotor adaptations lead to a numerical reduction of 20% in energy consumption. Pressure screens play a vital role in paper mills. They are positioned at different stages of the process and their main function is separating fibers and contaminants from the pulp mixture. In this vital role the energy consumption of screens contributes significantly to the overall

energy profile of mills.

The rotor as driving element associated with the pumping and movement of pulp through the screening process is one of the parts where optimization leads to a significant reduction in energy consumption and increase the mechanical efficiency of the screen.

To address this optimization task ANDRITZ AG and bionic surface technologies GmbH created together a validated virtual test bench where different rotor types and geometrical adaptations of rotor parts were studied and a digital twin developed.

For this virtual test bench we use computational fluid dynamics (CFD) where the rotor and rotor adaptations could be exchanged.

The simulation approach for the pressure screen virtual test bench is a single phase fluid model of pulp at its inflow consistency including non-Newtonian behavior. We developed a geometrical approach to exchange in an easy way different rotor types and rotor adaptations. The screen is represented as a complete 3D geometry and includes all necessary flow streams (feed, accept, reject). The model allows to specify the contribution of each rotor part (foils, foil arms, cylinder) in percentage of the total power. A critical point in realistic modelling of the flow is the geometric resolution of the wire bars within the model. Only the geometrical resolution of the wire bars along the perimeter allows to resolve the local flow interaction between the rotor and the screen basket. Of special interest are the small vortices at the bars' heads which directly related to the screening functionality. With our virtual test bench we are able to resolve this flow behavior and draw conclusions.

While comparing different geometry changes of a screen rotor an indication not only of the mechanical power consumption but also of the screening efficiency is of interest. The virtual test bench allows to plot the pressure and velocity distribution in the gap between screen basket and rotor. Comparing pressure distribution along the foils and its changes.

During the optimization process the cross section of holding bars, the gap thickness and foils were changed. Reduction of 20% in energy consumption could be achieved numerically with these changes.

## **Correlation of near-infrared spectroscopy with wood species and lignin content**

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The continuous kraft cooking digesters in the fiberline are facing challenges that impact the quality of the final product. Therefore, it is essential to enhance the control over digestors by integrating advanced techniques such as near-infrared (NIR) spectroscopy, model predictive control and machine learning production models. The objective of this study is to use NIR spectra to predict the amount of lignin in hardwood and softwood samples, to optimize the continuous cooking process in digesters by predicting lignin content based on spectral patterns [1]. We investigate the correlation of NIR spectra with the amounts of lignin relative to other

constituents i.e., cellulose, hemicellulose, and water in wood chip samples of different coarseness from different wood species, forming a dataset with NIR spectra and lignin content. Partial least square (PLS) regression is applied to the raw NIR data to build a model, which forecasts the lignin fraction. As a linear calibration method, PLS regression effectively reduces data dimensionality using a machine-learning technique and performs regression simultaneously [2]. The identified set of latent variables captures the most potent predictors in the data set, with the first latent variable accounting for most of the variance. This method allows for automatic extraction of specific wavelengths of absorption, which is then used to predict wood species needed for the simulation model and process control. The absorption wavelengths automatically identified by PLS regression correspond consistently with the wavelengths associated with lignin, hemicellulose, and water. These identified wavelengths serve as an essential factor in the model's process of determining the lignin content within the analyzed samples. The approach presented here offers a valuable tool for predicting the lignin content, promising improved efficiency and cost-effectiveness in the wood digestion process.

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[2] Rosipal, R., & Krämer, N. "Overview and recent advances in partial least squares." *International Statistical and Optimization Perspectives Workshop* Subspace, Latent Structure and Feature Selection", Springer Berlin Heidelberg, pp.34-51, 2005.

## **Faster substitution with forest-based high yield energy-efficient packaging**

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Unlike fossil-based plastics, wood-based packaging materials can be produced eco-friendly by using residuals from wooden houses, such as wood chips from sawmills and pulpwood from well-managed growing forests in northern Europe. The use of these woodchips to produce chemithermomechanical pulps (CTMP) paperboard and liquid packaging requires a reduction in electric energy consumption during fiber separation, since the content of lignin sulfonate within fiber walls and mid-lamellae affects fiber properties. As a result, it is imperative to optimize the impregnation methodology of sodium sulfite in wood chips to achieve evenly distributed softening properties preferably at the level of individual fibers. The long-term goal is to understand how to produce paperboard middle layer CTMP at less than 200 kWh/t rather than the present 500-600 kWh/t [1]. By using XRF (X-ray Fluorescence) techniques developed in-house and validated by beamline measurements, we have been able to determine how the sulfonated lignin is distributed both on individual fibers and between the fibers [2]. It also seems possible to enhance the surface area of lignin-rich pulp fibers while losing minimal bulk by refining them by means of well optimized low consistency refining. We have aimed to achieve extremely efficient separation of coniferous wood fibers by co-optimizing the sulfonation and the temperature in pre-heater and chip-refiner. Furthermore, we have studied the influence

of lignin softening behavior and possible crosslinking after defibration i.e., in following unit operations as pressing, peroxide bleaching and drying. In defibration during chip refining, the maximum softening of wood fibers is preferred to maximize fiber preservation and minimize energy consumption. However, it is preferable to maximize the stiffness of finished pulp fibers to reduce bulk loss during paperboard production. We believe that strong and lightweight composite packaging structures can be manufactured in an environmentally friendly and low-energy-consuming manner.

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[2] Norlin, B., An, S., Granfeldt, T., Krapohl, D., Lai, B., Rahman, H., Zeeshan, F., & Engstrand, P. [2023]: Visualization of sulfur on single fiber level for pulping industry, Journal of Instrumentation, vol. 18: 01.

## **Research on the drying methods and parameters during the drying process of pulp fiber**

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At present, the drying methods of pulp fiber mainly adopt air drying and oven drying. These methods are backward. The vacuum freeze-drying has a wide range of applications in pulp fiber. The moisture in the fiber cell wall can sublime from the solid state to water vapor directly [1]. The fiber is not affected by surface tension during the drying process. This method can reduce the damage to the microstructure of pulp fiber cell walls. Although the freeze-drying is a more suitable drying method, the study on the parameters of freeze-drying is scarce. In order to obtain a more realistic surface morphological structure of pulp fiber, this paper investigated the effects of different drying methods on the drying time and quality of pulp fiber. The study focused on different values for the following parameters: heating plate temperature and vacuum degree of drying chamber. The responses measured included: freeze-drying time and the quality of pulp fiber. In addition, optimal drying conditions for pulp fiber had been determined. The results indicated that it can better observe the original morphology of pulp fiber by the vacuum freeze-drying method. The eutectic point of pulp fiber was  $-4.1^{\circ}\text{C}$ , and the pre freezing temperature was  $-25^{\circ}\text{C}$ . The results highlighted that the optimum conditions were:  $35^{\circ}\text{C}$  and 3mbar, respectively, for, heating plate temperature and vacuum degree of drying chamber. The parameters obtained in this article were beneficial to observing a more realistic surface morphology of pulp fiber and provided basic support for the forming process of paper.

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## S05 | Advances in new paper-based materials

### Novel foldable lightweight design structures

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A highly multi-disciplinary approach has been applied to investigate possible product concepts, to develop experimental and simulation tools and to build up knowhow on the properties of varied tessellations. Ultimately, the novel folding technology will enable industrial-scale production of never-before-seen structures for a wide variety of applications related to the paper and packaging industry, as well as in other industry areas.

A folding technology based on simple (origami) tessellation designs and bio-based raw materials has been developed for a large-scale industrial production. An important aspect has been the continuous folding technique applied to flat cellulose-based webs to form material-efficient repeated patterns for wrapping, shock-absorbing frames or panels. Internationally, an interest in origami-based folded structures has grown steadily over the recent years but has concentrated on other industrial sectors such as aerospace.

Our main scientific focus has been on optimizing key relations between mathematical, mechanical, design and engineering aspects of the potential tessellations and relevant material parameters. Mechanical FEM simulations and visual folding simulations have been applied to predict the performance of different repeated tessellation designs. Design and research of conceptual product applications has produced some visually prominent solutions that have been publicly introduced in design exhibitions.

The main objective of the Fold project (<https://fold-project.com/>) was to take the folding technology to a sufficient level of maturity that the participating companies will be able to enter the market after their own internal or collaborative development rounds.

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[2] Kankkunen T., Niiranen J., Kouko J., Palmu M., Peltonen, K., Parametric linear finite element stress and stability analysis of isotropic and orthotropic self-supporting Miura-ori structures, *Mechanics of Advanced Materials and Structures*. 29(27):5808-5822, 2022. <https://doi.org/10.1080/15376494.2021.1965679>

## Advanced paper-based materials for dry 3D forming

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Paper-based packaging materials need to perform well in demanding dry 3D forming process conditions. This study covers some of the key factors affecting the extensibility of paper-based materials and presents a laboratory-scale development and pilot-scale results of a press-formable material concept. Low consistency and high consistency refined bleached softwood kraft (BSK) pulp was used in the experiments. The materials were formed using water-laid and foam-laid web forming using a laboratory sheet moulds and a pilot paper machine. Polyvinyl alcohol (PVA) fibres and a foamable latex were used for conceptual testing purposes as strengthening components and the latter as a foaming chemical. Anionic sodium dodecyl sulphate (SDS) was used as another foaming chemical. In this study, over 30% and significantly above 50% elongation was reached with BSK-based materials in laboratory and in pilot scale, respectively. In-plane compaction was the most significant factor regarding the elongation, but it also decreased the strength of the materials in the direction of compaction. Foam-laid BSK with thermoplastic binder chemicals and fibres produced greater extensibility and better press-forming performance compared to water-laid BSK material. The experimental data closely followed the theoretical relationship between shrinkage and elongation. 3D forming performance of the dry paper sheets was tested using fixed and sliding blank methods. In addition to high elongation, optimal strength was needed for the best press-forming performances. The dry paper sheets performed well enough in 3D forming, that they would be applicable to many consumer package applications according to their extensibility.

[1] Kouko J., Tanninen P., Leminen V., Barbier C., Karlsson C., Pesonen A., Hjelt T., Foam-laid extensible paper for improved extensibility and press-forming performance, *Cellulose*, Vol. 31:6955-6973, 2024. <https://doi.org/10.1007/s10570-024-06011-7>

[2] Kouko J., Hjelt T., Pilot made highly extensible paper for dry 3D forming, *TappiJ*, (under review process for TappiJ).

## Paper-based 3D cell culture with scaffold and fluid transport functions

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The paper-based 3D cultivation of mammalian cells has been published long ago (1). In these works, mainly the scaffolding properties of paper have been exploited. Surprisingly, however, the diverse microfluidic properties of paper have – to data – only been used to a limited extent for this application (2). But precisely this property could solve a major problem in the 3D cultivation of mammalian cells, namely supplying oxygen and nutrients to cells that grow into clusters beyond the 200 - 300  $\mu\text{m}$  range. Above this size, diffusion is no longer sufficient to supply cells adequately, but micro tissues or organoids beyond this size are necessary, to

become meaningful enough in e.g. toxicity tests to one day replace animal models. Here we aim to develop new types of paper assemblies which functionality. By cutting and hydrophobic functionalization of paper sheets with high spatial precision, the passive, capillary-driven liquid transport can be well controlled, both in direction and speed. In addition, the ability to integrate hollow fibres and microcapillaries. In addition, the option to produce hybrid papers with hollow fibers and microcapillaries further expands the possibilities for tailoring the desired microfluidic properties. Using this toolset, we are able to cultivate cells over a period of - at present - three weeks in a fully passive capillary driven paper assembly.

[1] Ratmir Derda, Anna Laromaine, Akiko Mammoto and George M. Whitesides, Paper-supported 3D cell culture for tissue-based bioassays, PNAS, 106 (44) 18457-18462, 2009.

[2] Sabrina M. Cramer, Tyler S. Larson and Matthew R. Lockett, Tissue Papers: Leveraging Paper-Based Microfluidics for the Next Generation of 3D Tissue Models, Anal. Chemie, 91, 17, 10916- 10926, 2019

## Development of paper composites for aluminum-air batteries

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Metal-air batteries have emerged as promising options in energy storage devices due to their notable attributes, such as high energy density, capacity, and cost-effectiveness. Moreover, they operate without emitting hazardous substances, addressing concerns associated with conventional Li-ion batteries. Among the various metals considered for energy storage, Aluminum stands out as an appealing choice due to its abundance in the earth's crust, cost-effectiveness, high theoretical gravimetric capacity ( $2.98 \text{ Ahg}^{-1}$ ), high theoretical potential (1.66V in saline and 2.35 V in alkali electrolyte), and eco-friendliness. This research aims to develop an Aluminum-Air battery compatible with traditional paper recycling processes. These batteries are thin, flexible, and have minimal environmental impact. The present study investigates the interaction between paper substrates containing different additives and a conductive coating. This innovative conductive coating eliminates the need for organic solvents, resulting in an entirely aqueous formulation. The conductivity of these coatings and the performance of the cathode/paper composites as an Aluminum-Air battery are measured.

Previous work in this area has primarily focused on coating formulation to create conductive papers. This research aims to understand the role of the paper when used with a non-solvent-based conductive coating formulation. This work explores the effects of fiber composition, refining, internal sizing, and wet strength. The results indicate the paper itself plays a significant role in determining the effectiveness of the conductive coating. The research points to the ability of these papers to be used as both an electrode and membrane separator in power applications. Furthermore, the formulations of the coating material and the paper make it possible for power sources created using these materials to be compatible with recycling operations. Results show the paper can achieve high conductivity values using the approaches described.

This work lays the foundation for developing single-use power sources enabling smart pack-

aging that can be recycled. Basic air-aluminum batteries are demonstrated using the new paper-based electrode materials. The role of electrolytes is explored as well. These electrodes represent a means to provide more environmentally friendly materials for the electrically powered economies of the future.

## **Advances in papermade materials for energy conversion processes**

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Regarding forward to a hydrogen economy dramatically cost reduced technology components are necessary to achieve economic sustainability and wide acceptance for market entrance and establishment.

Using pulp for designing and creation of novel structured and cost efficient high performing material components in reaction techniques and energy applications in this context is topic of this PTS contribution “Advances in papermade Materials for Energy Conversion Processes”.

The talk enables insights in research projects on how paper technology is being under investigation to create novel structured functional specialty paper materials for several hydrogen technology applications respected hydrogen generation, usage and conversion in energy transition context.<sup>[1]</sup>

[1] M. Rentzsch, S. Schramm, M. Zahel. Auf dem Weg zur Wasserstoffwirtschaft, Wochenblatt Papierfabrikation, 04, 2023.



## S06 | Barriers and coatings

### Characterization of cellulose surfaces with white light interferometry

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Cellulose, a fundamental component of plant cell walls, plays a crucial role in industrial, biotechnological, and environmental sectors. This study focuses on the development of an advanced methodology for the surface analysis of processed cellulose using White Light Interferometry (WLI). In white light interferometry, white light is divided into different beams, each traveling on separate optical paths. These beams are then reflected from the surface of the examined object and recombined. Due to the different wavelengths of various colors in white light, interference occurs when the beams recombine with the reference beam. Analyzing this interference pattern allows for the precise measurement of the optical distance between the object's surface and the interferometer's reference point and for each pixel in the optical image the surface height is determined.

Here we apply WLI measurements to processed cellulose sheets in order to reveal and quantify its topographic features, deriving quantitative information about the different length scales of surface roughness and the distribution of morphological features. The results from WLI measurements are validated with Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). From this comparison the limits and opportunities for WLI based cellulose characterization emerge.

Finally, we investigate how the surface morphology impacts on cellulose barrier properties of processed cellulose. To this end we characterize the water-uptake and measure the dynamic contactangle of sampes and compare the findings to the data on surface metrology.

### Moisture performance of silica-paper hybrids in the hygroscopic range

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Moisture-variable vapor retarders, crucial in construction, are traditionally made from plastic-based materials, raising environmental concerns due to the use of fossil materials. This study explores the potential of functionalized papers, particularly silica-paper hybrids, as sustainable alternatives. [1] The research delves into the moisture properties of sol-gel coated linters-papers, considering static contact angle, water vapor permeability, and sorption behavior following DIN EN ISO 12571. [2] Results challenge the assumption of static contact angle as the sole indicator of water vapor permeability and reveal distinct sorption trends among coatings. Notably, silica-

coated papers, especially those with a 0.8 TEOS dense coating, exhibit lower mass change than uncoated paper. While minimum mass change in sorption often correlates with high static contact angle results, exceptions such as 0.8 TEOS dense emphasize the intricate relationship and challenge these assumptions. The study addresses hysteresis, noting the lower hysteresis of mesoporous coatings in comparison to dense coatings and implying benefits in moisture release. Findings underscore the need for a nuanced understanding of coating characteristics and their impact on sorption, highlighting the limitations of static contact angle tests in predicting the sorption behavior of coated papers. In order to better assess the relationship between the coating content of the papers and their specific sorption properties, further investigations, such as the measurement of specific surface properties (e.g. specific surface area), are required

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[2] Deutsches Institut für Normung e.V. 2022. Wärme- und feuchtetechnisches Verhalten von Baustoffen und Bauprodukten. Bestimmung der hygroskopischen Sorptionseigenschaften (ISO 12571:2021); Deutsche Fassung EN ISO 12571:2021

## Experimental investigations into fold cracking of double coated barrier dispersion coatings

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The trend for replacing single-use plastics with fibre-based barrier board packaging has prompted significant research into dispersion coated barriers, as well as laminated boards (produced using conventional or biodegradable plastics). Minerals have been shown to be suitable additives to these coatings for improving barrier performance through surface chemistry and by increasing the tortuosity through the layer. They also improve the cost effectiveness by reducing material cost, improving drying rate and functional material hold out. Minerals can improve the barrier handling, rheology and reduce “stickiness” and blocking of the films. Fillers in extruded films, can improve adhesion of the film to the board [1].

One challenge is reduction of cracking at the fold during converting and the subsequent loss of barrier performance. In this work we systematically looked at the impact of mineral type and level and coating application method in a precoat layer before top coating with a barrier dispersion coating. Barrier results presented include moisture vapour transmission rate MVTR, blue stain in IMS and viscous vegetable oil penetration and Cobb water absorption.

Traditional cracking at the fold evaluation used for graphic printing showed that all of the samples gave good performance and no cracking was visible after folding. When the barrier tests were carried out on the precoat layers alone, all failed, showing the requirement for a topcoat barrier layer. After the topcoat application differences were observed in the performance, depending on the folding (degree of folding and inside or outside of the fold), the mineral type and level, the fluid used in the test and on the precoat application system.

In summary we show the importance of consideration of application method & converting on

final barrier performance, and specifically showed:

- A minimal difference in barrier properties with mineral loading, as the precoats were fully bound. The Cobb values were marginally worse at 60 pph pigment.
- Good barrier performance on the samples when flat or creased at 90°.
- The outside of the fold when the papers have been creased at 180° was most problematic, and the “stretching” of the coating more critical than “compression”.
- The MVTR of the flat samples was best for the blade coated precoats, due to better particle alignment. However, this was not the case after folding.
- In the unfolded Cobb test, the platey talc was the best, followed by the platey kaolin and then the less platey kaolin. However, after creasing, the opposite trend was seen.

[1] Helanto, K. Pilot-scale filler-reinforced biodegradable coatings for paperboard packaging, Doctoral Thesis 154/2023 Aalto University, (2023).

## Effect of particle size in the properties on cellulose nanofiber/lignin particle composite

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Cellulose nanofiber (CNF) has been studied as a bio-based material to replace petroleum-based packaging materials thanks to its excellent physical properties, but the use has been limited, because the properties can be deteriorated under high moisture due to the hydrophilicity of CNF [1]. Lignin is another polyphenolic bio-based resource from plant biomass and its inclusion potentially improve material hydrophobicity [2].

In this study, composite sheets based on CNF and lignin particles were prepared via spray deposition and the effects of the size and amount of lignin particles on the properties of the composite sheets were investigated. As lignin particles, three different sizes (lignin macroparticle (LMP) and two different size lignin nanoparticle (LNP)) were tested. The water vapor permeability (WVP) of the sheet including LNPs could be reduced by 25% compared to CNF alone sheet, despite its lower density. SEM and AFM with infrared spectroscopy analysis revealed that LNPs migrated to the top surface of the sheet during drying forming a barrier layer which is likely to reduce WVP. The layer of LNPs increased the water contact angle as well. Overall, the results of this study provide a fully bio-based option that could be used as a packaging material.

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[2] Wen Y., et al., Preparation and Characterization of Lignin-Containing Cellulose Nanofibril from Poplar High-Yield Pulp via TEMPO-Mediated Oxidation and Homogenization, ACS sustainable chemistry & engineering, Vol. 7(6), pp. 6131-6139, 2019.

## Transparent plasticized cellulose nanocrystal films for high-performance barrier

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Paper-based cellulose nanocrystal (CNC) films can be used in multiple industries as a sustainable replacement for fossil-based plastics. However, their applications are currently restricted by their low barrier properties and brittleness. Tailoring the properties of CNC is critical to sustainably develop their commercial applications. In this study, high-barrier bioplastic films of maltitol, a green polyol plasticizer, and CNCs were prepared using a spray deposition technique. The results showed that the addition of maltitol increased the gas barrier properties, maximum tensile strength, elongation, and translucency of the CNC film. The barrier properties of CNC films plasticized with maltitol were significantly improved over CNC. In particular, films containing 30 wt.% maltitol showed a water vapor permeability of  $3.67 \times 10^{-12}$  (g/Pa.s.m) and oxygen permeability of 4.75 (cm<sup>3</sup>.μm/m<sup>2</sup>.day.Pa) at 50% relative humidity (RH) and 23°C, corresponding to 94% and 78% reductions over CNC films, respectively. The contribution of structural properties and the number of free hydroxyl groups on the barrier properties in the plasticized film was investigated. Both gas porosimetry measurements and cross-sectional SEM microimaging revealed a denser and more aligned layered structure of the film with lower porosity in plasticized samples compared to pristine CNC. The change in the number of free hydroxyl groups and the probability of their interaction with moisture was measured by plotting thermodynamic and kinetics isotherm graphs of the moisture sorption of the films at different RH. The analysis showed at 50% RH plasticized CNC films absorb less moisture over a longer time period, demonstrating that there are less accessible free hydroxyl groups in these films compared to control film, as the hydroxyl groups of the CNCs tend to interact with those of maltitol. In conclusion, the integration of exceptional transparency, barrier properties, and flexibility in maltitol-plasticized CNC film, utilizing a green and food-safe plasticizer, presents highly promising and sustainable solutions for diverse packaging applications, particularly in food packaging requiring superior barrier performance and flexibility. This new development enables the precise modulation of mechanical, optical, and gas barrier properties in bio-based CNC films, facilitating the engineering of high-performing and environmentally sustainable products.

## Barrier coatings made from lignin and fatty acids

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The use of sustainable packaging materials is increasingly coming into focus. One approach to this is the use of cellulose-based materials such as paper, cardboard or carton. Due to their hydrophilic nature and porosity, they are highly permeable to gases and water vapour and even

lose their stability when exposed to moisture. By using bio-based polymer coatings such as lignin, the barrier properties can be drastically increased. Here, we present barrier coatings made from lignin esters and bio-based additives. Through application of the lignin ester as coating material the water vapour barrier properties of clay coated kraft paper increases by more than 50%. However, the introduction of additives, such as long chain fatty acids, to form binary coating systems show a further increase of the barrier properties. Water vapour transmission rate values of less than  $20 \text{ gm}^{-2}\text{d}^{-1}$  under tropical climate conditions can be achieved. SEM analysis show that the lignin esters can form homogeneous films while the additives form crystalline structures.

[1] Bartels, K., Trosien, S., Biesalski, M., Wildberger, M. (2023). WO2023134835A1.

## S07 | Paper as stochastic material

### Describing fiber orientation in paperboard using micro-CT scans and statistical analysis

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Micro-CT scanning of paperboard offers comprehensive possibilities for examining the structural composition on the microscale. As a direct method, the fiber orientation distribution (FOD) can be derived directly from the images and no detours via radiation or acoustic measurements are necessary. In addition, the entire body, including the core, can be analyzed without destroying the sample. This enables a detailed analysis of the FOD, which is one of the most important influencing variables for paper properties such as stiffness and strength. In this work, the reconstructed scans of three-ply paperboard were discretized and the fiber orientation tensors were calculated for each element. Based on the direction of the first eigenvector of the fiber orientation tensors, the FOD was drawn. It was functionally approximated by periodic and non-periodic probability density functions (PDFs) using statistical tests. This offered the possibility to use them directly in numerical models. Furthermore, structural differences between the samples could be analyzed using the functional parameters. It was shown that the von Mises PDF is best suited to describe the FOD in the core of the paperboard, while the Elliptical PDF is best suited for the outer plies. Furthermore, it was found that the fibers in samples from the paper roll center were more irregular distributed than those in samples from the paper roll edge. These findings help to create more realistic and accurate fiber network models that can be used to investigate the effects of microstructural properties and mechanisms on macrostructural material behavior.

### Uncertainty quantification in multiscale simulation of fibre-based materials

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The base structure of many fibrous materials, such as paper, is the fibre network. The small fibres bonded to each other due to hydrogen bonds are its main constitutive. The fibre network presents heterogeneity, structural disorderliness [1], and anisotropy [2], which result in difficulties in accurately predicting its mechanical performance.

Direct simulation of fibre networks can capture the complicated mechanisms of failure to different degrees depending on the employed method. However, it cannot be used for product development due to the overwhelming computational cost required to capture the relevant product size.

In this study, an efficient uncertainty quantification method in multiscale simulation of fibre-based materials is proposed. We address three main challenges: i) proposing a computationally feasible simulation approach for stochastic failure of fibre-based materials at sizes relevant to product scale, ii) capturing the size-dependent nature of the strength of fibre-based materials based on the proposed simulation framework and iii) quantifying the influence of disorder on the stochastic response of fibre networks. For the first time, it is shown that the natural disorder existing in the network accounts for 30% of the experimentally observed stochasticity in the mechanical response.

[1] Mansour R., Kulachenko A., 4 - Stochastic constitutive model of thin fibre networks, In: Elsevier Series in Mechanics of Advanced Materials, Elsevier, 2022. <https://doi.org/10.1016/B978-0-12-822207-2.00014-3>

[2] Alzweighi, M., Mansour R., Kulachenko A., Evaluation of Hoffman and Xia plasticity models against bi-axial tension experiments of planar fiber network materials, International Journal of Solids and Structures, 238, pp.111358, 2022

## Modeling statistical fluctuations in paper on multiple scales

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The substitution of resource-intensive materials, such as plastics and concrete, with paper or other natural fiber-based materials presents a significant opportunity to advance sustainability. Despite their longstanding history, knowledge of the mechanical properties of these natural materials remains incomplete.

Paper, distinct from other composite materials, exhibits significant fluctuations due to its natural origin. These fluctuations, along with its anisotropic behavior, originate from the unique geometric and material properties of its microstructure, i.e., its fiber network. Consequently, a multiscale modeling approach is essential to capture the complex characteristics of this material. Several methods of modeling fiber networks for paper have been developed. However, generating detailed networks is a challenging but necessary task for accurately modeling the material behavior of paper. Moreover, bringing these fluctuating microstructural properties into macroscale simulations introduces additional complications.

To address these challenges, we present an automated approach for generating synthetic fiber networks based on statistical analyses of real paper samples. This methodology enables us to introduce stochastic fluctuations in the geometric and material properties of the fibers. Using this approach, we are able to analyze the statistically fluctuating mechanical behavior of the networks through virtual microstructural experiments. We use these experiments to inform a macroscale material model that incorporates fluctuating material properties via spatial random

fields.

In this work, we produced multiple synthetic fiber networks and tested their mechanical responses. Then, we analyzed the statistical variations from these virtual experiments to inform our stochastic macroscale material model. Finally, we simulated different structural examples using this macroscale model.

The combination of our automated generation process for detailed microstructures of paper and the chosen stochastic macroscale model provides a powerful toolbox for analyzing the multiscale material behavior of paper. This approach allows us to examine intricate structural problems and contributes to a better understanding of the complex mechanical response of paper.

## Impact of local structure variations on air flow through porous sheets

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Predicting the rapid transport of gases through inherently inhomogeneous paper sheets is challenging. Since the flow is dominated by a few effective paths, a prediction must be able to find and account for these paths in the pore space of the 3D microstructure; flows driven by pressure gradients, even laminar ones, may choose paths, that differ from those preferred by diffusion or capillary uptake. Transport simulations on representatively chosen microstructures can provide these pathways. In view of the strong local variations in the microstructure of paper, it is worth looking at such simulations retrospectively: Which combinations of local structural properties favour these pathways? How likely are such favourable combinations to be realized in a paper sheet? To address these questions for air transport through paper sheets, we combine insights from computational fluid dynamics and pore network simulations with a copula-based statistical analysis revealing the pairwise interdependence of transport-relevant local descriptors of the 3D microstructure. The model paper grades considered are softwood fibre sheets without fillers before and after uniaxial compression. Their microstructural variations are resolved by means of  $\mu$ -CT 3D imaging[1]. Compression preserves the fibre stacking, but converts large variations in sheet thickness into large variations in density, and is therefore expected to localise the air flow and alter the relevant pathways. The work was performed in the Christian Doppler Laboratory for mass transport through paper.

[1] Neumann, M., et al., Capturing centimeter-scale local variations in paper pore space via  $\mu$ -CT: A benchmark study using calendered paper. *Microscopy and Microanalysis*, 27, 1305-1315, 2021.



## **S08 | Structural performance of structures made from paper-based materials**

### **The influence of structural buckling on the compressive strength of paperboard structures as illustrated with the ring crush test**

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Differentiating the contributions of material and structure to the edge-wise compressive performance of fiber-based packaging is essential to developing pathways to develop improvements in pulps and paperboard. In order to obtain an “intrinsic strength” it has been noted that small-span lengths are required to minimize buckling. Two examples are the short-span compressive strength (0.7 mm free span length) and the ring crush compression strength (0.64 mm free-span length). The majority of packaging will have free span lengths much greater than these tests spans so one-might question the applicability of these tests.

The hypothesis that was evaluated, explored, and reported here was as follows: the compressive strength of a package results from buckling of imperfect structures made from inelastic materials rather than from reaching a stress-level corresponding to some prescribed failure criteria. To explore this hypothesis, the ring crush test itself was taken as structure and simulated using finite element analysis (FEA).

For the FEA, the material was taken to be linear-elastic with strain-hardening plasticity having a transition zone of decreasing tangent modulus to some final non-zero slope. No failure criteria were prescribed for the material. Linear-elastic buckling mode shapes and corresponding elastic buckling loads were determined from eigenvalue/vector analysis. Several of these modes were chosen to introduce imperfections into the geometry. A nonlinear static analysis was then performed where the displacement of the top edge was increased.

In the 1950's a set of modified ring crush tests that yielded significantly higher strength values than the standard ring crush test were performed at the Institute of Paper Science (IPC) [1]. Using the MD/CD elastic moduli reported in the IPC report and a conservative estimate of plastic yielding, the FEA simulation of the modified ring crush test had good agreement with the IPC results for both peak load and shape of the curve. The simulation revealed how the plasticity and the scale of initial imperfections influence the load-deformation curve of the test resulting in loss of initial stiffness as well as a peak load or ring-crush strength.

The presented analysis suggests that the ring crush test was always dominated by buckling rather than intrinsic compressive strength and the shape of the stress-strain curve is more important for compression than intrinsic strength.

[1] Institute of Paper Chemistry, Effect of Specimen Height on Modified Ring Compression, PROJECT 1108-4, Report to the Technical Division of the Fourdrinier Kraft Board Institute, 1965.

## **Biomimetic crosslinking mechanisms of spray-coated nanocellulose coating for mechanical robustness**

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Despite the variety in functionalities offered by spray-coated nanocellulose coatings, the applicability onto various substrates and mechanical robustness should be enhanced to increase functional lifetime. In first instance, interphase adhesion of cellulose nanofibril (CNF) layers to glass and polymer substrates was strengthened by applying a bio-inspired adhesive interlayer based on catechol-chemistry, as the beneficial compatibility between polydopamine and cellulose has been widely recognized [1]. Boric acid (BA) was also individuated as ideal linker between polydopamine and cellulose. Covalent bond formation was envisioned through sequential esterification reactions with the catechol and sugar units. The influences of various application procedures (e.g., dip- or spray-coating) were evaluated and linker concentrations were optimized to result in better adsorption of a primary nanocellulose layer in wet conditions and higher mechanical resistance after drying. Secondly, different model coating systems were developed in combination with BA as internal crosslinker [2], which was organized either in layer-by-layer or homogeneously mixed coatings with different CNF:BA concentration ratios. The mechanical resistance of CNF:BA coatings was evaluated through nano-indentation, scratch resistance and rubbing tests, indicating significant improvement in mechanical durability for given crosslinker concentrations. The favourable crosslinking of organo-boron compounds with biopolymers can be attributed to the formation of a complex network structure with ortho hydroxyl groups, thereby strengthening the intermolecular bonding in the nanocellulose network. Results are under further development in the Triple-A-Coat Project (EU 101057992) through incorporation of anti-microbial properties.

[1] Samyn, P. Polydopamine and Cellulose: Two Biomaterials with Excellent Compatibility and Applicability, *Polymer Reviews*, Vol. 61, 814-865, 2021.

[2] Wang, Y., Zhang, C., Xu, N., Lan, J., Jiang, B., Meng, L. Synthesis and properties of organoboron functionalized nanocellulose for crosslinking low polymer fracturing fluid system, *RSC Advances*, Vol. 11, 13466-13474, 2021.

## **S09 | Manufacturing and forming processes for paper-based materials and structures**

### **In-situ process monitoring in deep-drawing of paper using partially transparent tools**

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The production of three-dimensionally formed packaging from paper by deep drawing leads to the occurrence of wrinkles, which result from the high tangential compressive stresses in the flange area and the limited flowability of the material. Wrinkles, although mostly tolerated in industry, end in both a reduced visual appearance and a reduction in usability for packaging, for example when gas-tightness is required.

Previous research efforts have been limited to determining the wrinkle distribution after completion of forming and removal of the formed part[1]. Consequently, the possibility of understanding the sequence of formation of individual wrinkles in the inhomogeneous material is lost. To remedy this situation, a method for local in-situ process monitoring is presented.

Using a transparent die and an industrial camera, the flange area can be observed during the forming process. An image processing algorithm based on the brightness gradient, is applied to analyse the local development of the deep drawing process from the continuously recorded image data.

The method described can be used to analyse the draw-in behaviour and wrinkle formation locally and continuously over the drawing depth. It can be seen that the blank holder force influences the draw-in and the wrinkle pattern both locally and over the drawing process. A more precise understanding of the wrinkle formation will allow for more efficient process control in the future.

[1] Hauptmann, Marek et al.: The role of material composition, fiber properties and deformation mechanisms in the deep drawing of paperboard. In: Cellulose 22, Nr. 5, 2015, S. 3377–3395

### **CFD simulation of fiber transport and laydown in dry paper web laying using airlaid techniques**

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Paper production traditionally involves a wet process, where cellulose fibers are dissolved in water. While water facilitates uniform web laying and enables fibers to swell, resulting in stable webs by promoting the formation of bonds between individual fibers, the subsequent drying

phase requires substantial thermal energy. Research aims to reduce water retention in fiber networks, improve drying efficiency, and explore alternatives with lower enthalpy of evaporation. Our focus lies in completely eliminating water from the web laying process, drawing inspiration from the airlaid technique used in the textile industry, where short fibers can be processed into a nonwoven [1]. In the paper industry, this method is already utilized, for example, in the production of paper napkins.

To achieve stable and uniform paper fiber webs, it is crucial to obtain a detailed understanding of the underlying fluid flow (particularly turbulence) and fiber transport within the forming head. Therefore, Computational Fluid Dynamics (CFD) simulations offer the possibility to investigate the three-dimensional flow field, as well as the transport of fibers and the laydown process [2]. This enhances the overall understanding of the process and will be utilized in the development of a new prototype machine for the airlaid process in paper production. Modeling fiber bending, twisting, and interactions, including agglomeration, poses challenges and computational expenses. Parameters such as Young's modulus require in-depth investigation for accurate representation of fiber behavior. Because of computational limitations, only a subset of the process will be simulated at the fiber level using a Lagrangian model. This subset, based on the Discrete Element Method, will serve as a representative part for validating a simplified Eulerian multiphase model, where the fibers are considered as a continuum. This approach balances detail level, computational costs and computation time, aiding in the design of optimal fiber deposition methods

[1] Brydon et al. (2022). Drylaid web formation. In Handbook of nonwovens (pp. 89-180). Woodhead Publishing.

[2] Gramsch et al. (2015). Optimizing spunbond, meltblown, and airlay processes with FIDYST. Melliand International, (2).

## **Universal method for predicting the formability of paper-based materials in deep drawing and hydroforming**

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As part of the research project, a systematic investigation of the formability of different papers in active media-based forming and compression deep-drawing with a specific surface was compared for the first time. An optimized forming result was achieved for each paper through comparable variation of the process parameters blankholder force and forming pressure. To systematically evaluate the geometric forming quality, a method was developed that extracts the different geometric features from digital images of the molded parts. This showed that the forming quality of the papers examined varied and that not all geometric features could be meaningfully determined. The most suitable characteristic that can be determined and used for evaluation independently of the forming quality was identified as the degree of filling of a

virtual cut, also known as surface filling, through the sample in the case of active media-based deep drawing. In compression drawing, the evaluation of the folds, particularly the starting height of the fold formation, has proven to be a suitable criterion.

## **Failure analysis and avoidance in corrugated board creasing using numerical prediction models**

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Using comprehensive material models, modern simulation programs now enable comparatively simple modeling of forming processes in paper processing. The models created for mapping the die-cutting groove of single-wall corrugated cardboard showed good qualitative agreement with the laboratory samples in terms of the deformations that occurred. The finite element method is suitable for analyzing geometric influencing factors under non-linear conditions. Accordingly, the models are particularly suitable for relative comparisons to optimize geometric parameters. These can be the geometries or the feeding path of the creasing tools, the applied creasing forces or the structure of the corrugated board itself. In addition, geometrically induced weak points in the workpiece can be reliably identified using the models and local failure can be predicted. The creasing models are not suitable for quantitative predictions or comparisons of the occurring material stresses due to the boundary conditions. However, limit loads on the structure, for example the liner, could also be estimated using relative comparisons.

With regard to processing, the model shows that for parallel creasing, inserting the creasing rule on the wave crest is associated with the lowest stress on the workpiece. The corresponding positioning of the creasing tools would ensure the best possible avoidance of ceiling cracks, any associated optimization of material usage and generally consistent creasing results.

## **Numerical and experimental analysis of multi layered paperboard forming**

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Forming paper-based products poses significant challenges, such as maintaining geometric integrity, managing springback, and overcoming instability limits. These obstacles arise due to the unique material properties of paper, which are characterized by high anisotropy, inhomogeneities, and limited flowability of the fiber composite. Additionally, paper usually consists of multiple tightly bonded layers, which can amplify some of the challenging properties.

One approach to tackle these challenges is to collectively form several papers, allowing a customized material composition for each product. By utilizing the mutual support within the fiber network[1], deliberate material selection and orientation can affect forming properties.

Research on the effect of the layer structure, both numerical and experimental, has yielded some very promising results. In deep drawing processes, individual papers can be securely bonded without the need for adhesives. Under certain process parameters, the bond strength even exceeds the material strength. Additionally, joint forming enhances the pressure stability of paperboard packaging, providing superior product protection compared to those of industrial layered papers of similar thickness. Furthermore, a new way to reduce anisotropic springback has been found by varying the fiber orientation throughout the layers.

The presentation will demonstrate how the bonds are formed and show visible differences between the formed layered and non-layered products. It will also discuss how the layer selection can be optimized for different geometries, using numerical analysis.

[1] Franke W. et al., The effects of pretreatment and coating on the formability of extrusion-coated multilayer paperboard-plastic composites, *Packaging Technology and Science*, Vol. 34, 2021

## Piezoelectric paper development and applications

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Functionalized paper has been of interest as a flexible and biodegradable platform for diverse applications in analytical experimentation in recent years. Here, we demonstrate the formation of piezoelectric paper through integration of piezoelectric nanomaterials ( $BaTiO_3$ ) within the paper matrix to realize different sensor types. Highly refined (400 kWh/t) cellulose fibres were functionalized with 300 nm  $BaTiO_3$  nanoparticles using a layer-by-layer process, suitable for industrial paper-making processes [1]. We rendered the  $BaTiO_3$ -functionalized fibre suspension into paper composites that were better loaded with the piezoelectric nanomaterial across its thickness compared to [1], resulting in improved adhesion between nanoparticles and fibres. Electrodes were patterned on the paper composite substrate surfaces via gold evaporation through a shadow mask. The subsequent corona poling of the paper composite substrates at the Curie temperature ( $\sim 120^\circ\text{C}$ ) of  $BaTiO_3$  aligned its polarization axis along the substrate surface normal, yielding a piezoelectric coefficient of up to  $d_{33} = 25.4 \text{ pC/N}$  which stayed stable over a time period of about a month. We characterized an accelerometer made from the piezoelectric paper substrate by subjecting it to vibrations over a range of frequencies; its transfer behaviour corresponded to the expected behaviour of the corresponding electromechanical model. We also implemented an air quality sensor based on a piezoelectric paper substrate to measure the mass of particulate matter per volume of air. As air is drawn through the paper substrate, the paper acts as a filter, and the deposited particles increase the mass of the paper. The paper sample is brought to vibrate through piezoelectric actuation; as particles deposit on the paper, a shift in the resonant frequency is observed.

[1] K. Sankaralingam et al., Piezoelectric Paper: Large-Scale Compatible Manufacturing Process and Sensor Demonstration, *Technical Digest of the 2022 Solid-State Sensors, Actuators and Microsystems Workshop*, Hilton Head Island, SC, USA, June 5-9, 2022, pp. 423-426.

## **S10 | Recyclability and recycling processes for pulp and paper**

### **Towards sustainable paper recycling: A method for assessing the effects of non-wood fibers**

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In recent years, new types of fiber have increasingly entered the market to meet the demand for sustainable products and to develop alternatives to the increasingly scarce raw material, wood. Examples of this include grass paper, straw pulp, miscanthus, or silphia pulp, and algae papers. Products made from these materials are sometimes advertised as recyclable through the recovered paper cycle, or consumers dispose of the products in the blue bin due to their similarity to paper. Previous studies show that some of these fibers are rejected in the recycling process due to the dimensions of the fibers. Others have poor binding properties and significantly poorer optical properties compared to conventional fiber materials [1]. Little is known about other factors, such as the influence on process water, interactions with common additives, and behavior in dry sorting (NIR sorting) and their influence on recycling. To date, there is no method to evaluate the influence of such fiber materials on the recovered paper cycle. It is, therefore, currently not possible to distinguish between more and less recyclable fiber materials. This work aims to develop a novel test method for assessing the circularity of alternative fiber materials, to obtain data using this method, and to develop a proposal for a corresponding evaluation scheme. The parameters that will be evaluated include the behavior of the fibers in hole and slot screening during stock preparation, the effect of pulping on the strength and morphology of the fibers, the effect on process water, the degradation of fibers during multiple recycling cycles and the effect on strength through additives.

A systematic series of tests will examine the influences of different concentrations of the non-wood fibers in recycling. Based on these results, a proposed test method can be created that considers the behavior of non-wood fibers and how to determine their suitability for recycling. The outcomes will aid in identifying recyclable and non-recyclable fiber materials and mitigating challenges in pulp and paper manufacturing facilities handling recycled paper. Insights gained from this research will also contribute to advancing sustainable practices in the paper industry and fostering a circular economy model.

[1] Liu, Z., Wang, H., & Hui, L., *Pulping and Papermaking of Non-Wood Fibers*, Intech Open, 2018. DOI: 10.5772/INTECHOPEN.79017.

### **Recyclability scoring of biowax-impregnated transparent papers**

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Papers are preferred flexible and renewable substrates for packaging, biosensors, or electronic devices [1], where high transparency is required to meet consumer preferences or provide better performance. The opacity of conventional papers originates from the interaction of light with the heterogeneous structure of a paper fiber network, causing scattering effects at the fiber-air interface and differences in refractive index between cellulose and air. Therefore, the impregnation of a porous paper structure with transparent agents such as, e.g., oil, resins, wax or synthetic polymers beneficially improves transparency [2], as penetration of the liquid substance allows to fill the micro-voids between fibers with a material of comparable refractive index. The selection of hydrophobic waxes may simultaneously improve the water resistance and barrier properties of the paper sheet. However, making a more dense and water-resistant internal structure of the paper with intimate interaction between cellulose fibers might pose challenges in the recycling of transparent papers, where fiber clogging and permanent deposition of wax onto recycled pulp fibers are to be expected. In this study, a set of biowaxes was screened to evaluate the influences of their intrinsic properties on the processing conditions and transparency of impregnated papers. In contrast with traditional fossil-based paraffin wax, however, high transparency and hydrophobicity was obtained for selected biowaxes. Most important, the influences of biowax content (g/m<sup>2</sup>) and number of impregnation steps on paper recyclability were assessed according to the recent Harmonized Cepi Recyclability Laboratory Testing Method for standard pulp mills (v2), indicating positive total recyclability scores (T = 84 to 94), with extremely high total fiber yield (> 98%). Therefore, it seems that intrinsic properties of a biowax with given hydrophobicity and crystallinity are critical in optimizing the impregnation and recycling process.

[1] Zhu, H.; Fang, Z.; Preston, C.; Li, Y.; Hu, L. Transparent paper: fabrications, properties and applications, *Energy Environ. Sci.*, Vol. 7, 269-287, 2014.

[2] Guan, F.; Song, Z.; Xin, F.; Wang, H.; Yu, D.; Li, G.; Liu, W. Preparation of hydrophobic transparent paper via using polydimethylsiloxane as transparent agent, *Journal of Bioresources and Bioproducts*, Vol. 5, 37-43, 2020.

## **Life cycle assessment of black liquor gasification and combustion process by simulation**

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We conducted a thorough analysis of the black liquor gasification and combustion processes using Aspen Plus process simulation software. By varying levels of oxygen input, four scenarios were considered in the study. Subsequently, GaBi software was employed to conduct a life cycle assessment (LCA) for the proposed four scenarios, enabling a comparison of environmental impacts, electricity generation, and costs across different oxygen inputs.

Firstly, the software of Aspen Plus was utilized to simulate the gasification and combustion process of black liquor, employing a base input flow rate of 11,200 kg/hr. The physical properties of the black liquor were derived from literature and classified as unconventional solids. The gasification simulation was conducted using the default reactors of RYield and



RGibbs in Aspen Plus, primarily yielding combustible gases of hydrogen, methane, and carbon monoxide. These gases were subsequently subjected to the combustion process using the RGibbs reactor, generating heat to drive a steam turbine for electricity generation. To evaluate the impact of oxygen concentration on power generation and gas emissions, the oxygen inputs ranging from 160 kmol/hr to 220 kmol/hr were introduced during simulation. Subsequently, the data from Aspen Plus was analysed and input into GaBi software for life cycle assessment, encompassing the processes from diluted black liquor generation to complete gasification and combustion. Eventually, for the generated data by GaBi software, from the points of view of LCA, the black liquor gasification and combustion processes were evaluated by the indicators of global warming potential (GWP), photochemical ozone creation potential (POCP), acidification potential (AP), eutrophication potential (EP) and human toxicity potential (HTP).

The study results showed that: (1) An increase in oxygen input led to an augmented electricity generation from the steam turbine, albeit with higher GWP and increased costs. This phenomenon was attributed to the heightened oxygen input promoting more thorough gasification and combustion reactions, resulting in the release of additional fixed carbon elements into the atmosphere, thereby exacerbating the greenhouse effect. (2) For every 20 kmol/hr increase in oxygen, the average GWP rose by 8.67%, while electricity generation and costs surged by 12.58% and 12.51%, respectively. Notably, the growth rate of greenhouse gas emissions is not as high as the growth rate of electricity generation and costs. (3) An increase in oxygen input led to a decrease of POCP, primarily attributable to reduced emissions of hydrocarbons such as methane. The heightened oxygen input facilitated more comprehensive combustion of methane, thereby curbing methane emissions. Specifically, for every 20 kmol/hr increase in oxygen, the average POCP decreased by 39.82%. (4) With the increasing oxygen input, the indicators of AP, EP, and HTP exhibited no significant variations, which are primarily influenced by the quantity of sulphur elements, such as  $H_2S$ ,  $SO_3$  and  $SO_2$ .

## Study on tackiness and strength contribution of micro-stickies with the treatment of deposit control agents

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Stickies deposition is a major problem in the utilization of secondary fibers. A variety of deposit control agents have been developed to cope with it, but the problem of how to evaluate the effects of the control agents on the tackiness change of stickies in a quick and convenient way remains weakly tackled. In this study, four stickies control agents, a polyamine, a highly cationic starch, a silane coupling agent and a talc, respectively, were applied to a simulated recycled pulp consisted of wood fibers and model micro-stickies; then the chemically-treated pulps were dried in small dishes made from stainless steel film simulating metal surfaces or PET film simulating fabric cloth surfaces. "Stickies-substrate" double-layered test specimens could

thus be easily made by proper cutting (sometimes “stickies-substrate-stickies” triple-layered specimens were also made by covering another film on the top the stickies layer, followed by drying and cutting). Then internal bond strength testing were carried out conveniently. The results indicates that the method was capable of rapidly and simultaneously evaluating the tackiness change and strength contribution of the control agents treated microstickies, which is not only suitable for clarifying the different stickies controlling effect incurred by using different control agents, but also beneficial in helping clarifying their different functioning mechanisms.

[1] Yun Wang, Cornellius Marcello, Neha Sawant, et al. Identification and characterization of sticky contaminants in multiple recycled paper grades. *Cellulose*, 2023, 30 (3): 1957-1970.

[2] . D. W. Francis, M. D. Ouchi. Effect of dissolved and colloidal solids on newsprint properties. *Journal of Pulp and Paper Science*, 2001, 27 (9): 289-295.

## **S11 | Energy saving and emission reduction methods**

### **Modelling and simulation of multiphase flows inside a dryer section hood as part of a paper machine**

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Most of the primary energy consumption of a paper machine arises during the drying process to evaporate the water contained in the moist web. A significant amount of thermal energy exits the dryer hood as latent heat in the water vapour towards the heat recovery unit. This air/vapour mixture contains about 0.15 kg vapour per kg dry air at a temperature of 80°C, which corresponds to a dew point of approximately 60°C. One way to maximise the potential heat recovery is to increase the vapour content of the exhaust air by reducing the fresh air supply. Such an approach maintains a high dew point, but also expands the risk of condensation inside the dryer section. Unintentional condensation affects the drying hood performance. In the worst case, water droplets collide with the paper surface, triggering a web tear-off.

Our research focusses on the development of a numerical dryer hood model. Industry insights provide the basis for creating a simplified geometric CAD model. As a simplification, boundary conditions describe the moist paper web. A multiphase flow simulation replicates the dry air, vapour and liquid phase inside the enclosure. In addition, condensation and evaporation models reproduce the heat and mass transfer between the different phases. The complete model will be validated with data from the industry regarding the moisture and temperature profile of the paper web and the conditions inside the drying hood. In the long term, the model enables the virtual testing of active and passive installations to identify condensation zones and achieve a higher vapour content for potential energy savings. Overall, the results contribute to the design guidelines of paper machine hoods [1].

[1] TIP 0404-24 Guidelines for the design, operation, performance evaluation, and troubleshooting of a paper machine hood and air systems. Technical Information Paper, 2021.

### **Functional fillers for the reduction of carbon footprint of paper**

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During recent years, the consideration of carbon dioxide equivalents became the focus of global initiatives and national regulations [1]. As the paper and board producing industry is among the main six emitters of greenhouse gases of the industrial sector, GHG reduction regulations triggered many initiatives among which the replacement of raw materials with high carbon

footprint is seriously considered. This article shows that the careful choice of functional pigments can support the carbon footprint reduction of paper and board.

Behind cellulose, functional pigments represent the second biggest ingredient in paper formulations which brings considerations around the right choice of pigments into a very important position. It can be shown that the application of standard ISO methods deliver a typical carbon footprint for a dry ground calcium carbonate with a particle size of 2.5 to 5.0  $\mu m$ : 54.2 kg  $CO_2eq$ /ton. This means that calcium carbonate pigments have an extremely low carbon footprint. Consequently replacing other ingredients contribute to remarkable reductions of the carbon footprint of an overall paper formulation [2].

Core of this article highlights a full-scale commercial paper mill trial where titanium dioxide ( $TiO_2$ ) was replaced with ground calcium carbonate (GCC) in the white top ply of a 135  $gm^{-2}$  white kraft liner. It can be shown that this replacement leads to a significant improvement of carbon footprint (by -35%) and that carbon footprint reducing measures can be done without compromising on quality!

[1] He. B., Liu, Y., Zeng, L., Wang, S., Zhang, D., Yu, Q., Product carbon footprint across sustainable supply chain, Journal of Cleaner Production, 241, 118320, December 20, 2019.

[2] Hertwich, E. G., Wood, R., The growing importance of scope-3 greenhouse gas emissions from industry, Environmental Research Letters, Vol 3, Nr. 10, 104013, October 05, 2018.

## **S13 | Paper chemistry and chemical engineering of lignocellulosics**

### **Inkjet papers show delamination during microcomputed tomography investigation**

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While microcomputed tomography ( $\mu$ -CT) can be a powerful tool for investigating liquid water uptake in paper, this measurement technique can also pose problems: Inkjet papers of different sizing degree containing calcium carbonate fillers were immersed in water to monitor the uptake of liquid water in a time-resolved manner using the  $\mu$ -CT. During image acquisition, the unsized and low sized paper grades showed delamination. The strongly sized sample showed gas bubbles forming on the surface in addition to a slight delamination. When the experiment was repeated with a strongly sized paper without fillers, neither delamination nor bubble formation was observed. Rather, irradiation of calcium carbonate powder mixed with water during the  $\mu$ -CT measurement resulted in bubble formation. This suggests that the fillers in the paper promote hydrolysis when in contact with water [1]. The radiolytic gas released is likely hydrogen.[1] Delamination and bubble formation occurs only when a filler-containing paper immersed in water is exposed to X-ray radiation in a  $\mu$ -CT machine and with the paper sample in close proximity to the X-ray source. Since such close proximity is a prerequisite for spatially resolving pores in paper using  $\mu$ -CT setups without an X-ray focusing unit, fillers are expected to compromise high resolution measurements of water distribution in paper in  $\mu$ -CT instruments.

[1] Costagliola A., Vandenborre J., Blain G., Bat V., Haddad F. and Fattahi M, Radiolytic Dissolution of Calcite under Gamma and Helium Ion Irradiation, The Journal of Physical Chemistry, Vol. 121, 2017.

### **Potential of flow cytometry to detect microplastics and -stickies in paper recycling water**

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The recycling of paper, especially paper packaging with a barrier coating, involves water-based processes that are susceptible to contamination by microplastics, stickies and particles arising from coated materials. These contaminants negatively impact product quality, processing efficiency and the overall sustainability of paper recycling. This study explores the application of flow cytometry as a promising technique for the rapid and efficient detection of small

microplastics or -stickies in water used during paper recycling.

Microplastics (particles  $<5$  mm) and –stickies (hydrophobic particles  $<100$   $\mu\text{m}$ ) originating from recycled paper materials pose a challenge to maintain the purity of process water in paper recycling. Conventional detection methods for such particle types are often time-consuming, labor-intensive and may not have the sensitivity required for accurate analysis.

Flow cytometry, traditionally used in cell biology and medicine, offers the advantage of high-throughput analysis. In addition, the flow cytometer has the ability to characterize particles based on size, shape, and fluorescence properties. This study evaluates the feasibility of adapting flow cytometry to quantify and differentiate microparticles in water samples obtained from paper recycling processes.

Preliminary results show the ability of flow cytometry to rapidly detect and quantify microparticles, which may provide the first valuable insights into the contamination levels within recycling water. In addition, the study addresses potential challenges and limitations associated with flow cytometry, including the need for standardized protocols and calibration methods. Recommendations for optimization and future research directions are discussed. The goal is to establish flow cytometry as a reliable tool for monitoring and controlling microparticle contamination in paper recycling water systems.

In conclusion, the application of flow cytometry is a promising method for the assessment of microplastics, stickies, and barrier-coated paper particles in paper recycling process water. It offers a faster and more efficient alternative to conventional methods. Implementation of this technique could contribute to the improvement of the industrial efficiency in the paper industry and the environmental sustainability.