CPP 37: Focus Session: Interactions Between Water and Cellulose II

Time: Thursday 16:15–17:15 Location: H34

Invited Talk CPP 37.1 Thu 16:15 H34

Modelling Hygroexpansion of Compression and Opposite Wood of Conifer Branches: Bridging the Gap between Molecular and Cell Wall Level — Marie Hartwig-Nair, Sara Florisson, Kristofer Gamstedt, and •Malin Wohlert — Dep of Materials Science and Engineering, Uppsala University

Softwood branches develop compression wood (CW) in the lower and opposite wood (OW) in the upper part exhibiting different hygromechanical properties and differ in structure at several length scales. Distinctive differences are found at cell level, cell wall level and at the level of chemical composition of the lignin and hemicellulose matrix.

The effect each of these respective differences have on tissue level of wood hygromechanical properties is not yet clear. Here, a hierarchical multiscale modelling approach is employed, where the impact composition, MFA and lignin chemical difference have on wood hygroexpansion is studied by the means of hierarchical modelling as support to tissue level experimental investigation of CW and OW hygroexpansion [1]. With atomistic models and Molecular Dynamics simulations of lignin at different levels of hydration, swelling coefficients for the different lignin matrices are obtained [2] and implemented in a Finite Element (FE) model of the cell wall. The FE model also accounted for differences in MFA and composition.

The results of the FE model will be discussed and connected to the MD and tissue level results.

[1] M. Hartwig-Nair et al., Wood Sci. Technol., 2024, 58, 887-906.
[2] M. Hartwig-Nair et al., Wood Sci. Technol., 2024, in press.

CPP 37.2 Thu 16:45 H34

Exploring Hygroexpansion of Cellulose Based Fibers via μCT — •Maximilian Fuchs[1,2], Raimund Teubler[2,3], Alexandra Serebrennikova[1,2], and Karin Zojer[1,2] — [1]Institute for Solid State Physics, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper — [3]Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Austria

Understanding the swelling of cellulose-lignin-based fibers is crucial for describing the processes involved in the uptake of water or other volatile organic compounds in paper. Microcomputed tomography (μCT) promises to monitor the hygroexpansion on a paper sheet level. However, extracting and analyzing individual fibers from the interwoven fiber network in these μCT images is challenging. We present a new approach to identify, extract, and analyze hollow fibers by focusing on the fiber lumen as the structural backbone. Using this approach, we quantify changes in fiber shape as the paper sheet absorbs water and another polar solvent, dimethyl sulfoxide (DMSO), from the vapor phase. We continue to observe these changes long after saturation, when no further mass is absorbed in the fibers. With both water and DMSO, the fiber wall thickness continues to increase even after reaching saturation. Furthermore, when exposed to water, the fibers tend to become rounder during swelling, suggesting fiber decollapse. In contrast, the data for DMSO indicates that the outermost fiber layer gets damaged, leading to unrestricted swelling once saturation is exceeded.

CPP 37.3 Thu 17:00 H34

Structure and dynamics of water adsorbed to amorphous cellulose: a comparison of experimental and simulated neutron scattering data — •Veronika Reich[1], Martin Müller[1,2,3], and Sebastian Busch[1] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum hereon GmbH, Garching, Germany — [2]Institute of Materials Physics, Helmholtz-Zentrum hereon GmbH, Geesthacht, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel

Neutron scattering experiments provide valuable insights into the nanoscopic properties of matter, a scale that is also accessible through Molecular Dynamics (MD) simulations. If the simulations reproduce the experiments, they can give greater insight into the material properties on the nanoscopic scale than traditional data analysis methods. In our work we establish a connection between published experimental data about water absorbed to amorphous cellulose from neutron experiments [1] and MD simulations. Special focus was put on the comparison of the structure factor of non-crystalline water and the dynamics as a function of temperature. The MD simulations were designed to be close to the experimental data from literature to achieve a meaningful comparison.

[1]Czihak, Christoph: Cellulose: Structure and dynamics of a naturally occurring composite material as investigated by inelastic neutron scattering, PhD thesis in material science, University of Vienna (Austria) and Institute Laue-Langevin (France), 2000