Contribution ID: **603** Type: **Poster (+) Presentation**

Hygromechanical Properties of PEG-Treated Archaeological Wood: Molecular Simulation and Poromechanics

Tuesday, 1 June 2021 19:00 (1 hour)

Archaeological wood of shipwrecks buried for centuries under sea sediments is highly degraded due to the chemical changes and material loss. Uncontrolled or rapid drying of such artifacts results in drastic distortion and collapse of material due to high drying stress, therefore consolidation methods and drying processes have been developed to preserve these culturally valuable artifacts. As a consolidation technique used for both Swedish warship Vasa [1] and Henry VIII's warship the Mary Rose [2], polyethylene glycol (PEG) solution was sprayed for decades on the surface of both shipwrecks to penetrate the wood and stabilize the wood structure [1]. While the experimental results show higher stability in PEG-treated samples [1], many questions regarding the impact of PEG polymers on the stability of wood polymers remain unanswered due to the microscopic nature of complex nanoscale phenomena involved. In this study, we combine the data obtained from molecular dynamics (MD) and grand canonical Monte Carlo (GCMC) simulation with a poromechanical model to examine the PEG-cellulose synergic interaction in amorphous mixtures as observed in sorption isotherms, mechanical moduli and hydrogen bonding network. To this aim, mixtures of amorphous cellulose and PEG200 are constructed as simple models representing the interaction of PEG200 consolidant with cell wall holocellulose component. Mixtures with different mass ratios of cellulose and PEG are modeled using the OPLS-AA force field and prepared by high-temperature relaxation followed by quenching at room temperature. Hybrid MD/GCMC is then employed to obtain the sorption isotherms and PEG-cellulose mixtures at different levels and regimes of hydration. Following the GCMC simulations, mechanical tests are performed on resultant structures to examine the sorption-induced mechanical softening in the wood structure for both treated and untreated samples. The data are then introduced into a poromechanical model which allows analyzing the change in the coupling between sorption and deformation by adding PEG to cellulose. The presented model, methodology, and the choice of simulation parameters such as system size are validated through comparison with available simulation and experimental data on amorphous cellulose sorption isotherms and mechanical properties. As indicated by sorption isotherms and swelling curves, the PEG-cellulose mixture shows deviation from the ideal mixture rule referring to a synergic interaction between PEG and Cellulose. This synergic behavior can be examined by investigating the confinement of PEG molecules in the nanoporous structure of amorphous cellulose and by the hydrogen bonding network between cellulose and PEG. The PEG molecules rearrange the existing hydrogen bonding network by forming new hydrogen bonds with the cellulose chains reducing the sorption sites available for moisture adsorption. In addition, the amorphous cellulose limits the free swelling of PEG observed in its pure liquid form. These two mechanisms can describe the reduction in moisture content and its outcome: less swelling/shrinkage in treated samples and thus higher stability in museum conditions.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

[1] E. Hocker, G. Almkvist, and M. Sahlstedt, "The Vasa experience with polyethylene glycol: A conservator' s perspective,"J. Cult. Herit., vol. 13, no. 3, pp. S175–S182, 2012.
[2] E. J. Schofield, R. Sarangi, A. Mehta, A. M. Jones, F. J. W. Mosselmans, and A. V Chadwick, "of the Mary Rose The preservation of waterlogged archaeological wooden finds , such as,"Mater. Today, vol. 14, no. 7–8, pp. 354–358, 2011.

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Student Poster Award

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Session Classification: Poster +

Track Classification: (MS7) Mathematical and numerical methods for multi-scale multi-physics, non-linear coupled processes