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Linear lignin as a potential consolidant for archaeological wood treatment: a hybrid Monte Carlo and molecular dynamics study

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Lignin is one of the abundant polymers found in wood cell wall composite acting as the cohesive matrix that surrounds the wood holocellulose and provides increased hydrophobicity and chemical stability to the composite. Due to its less susceptibility to biological attack and high compatibility with holocellulose, synthesized lignin-like oligomers have been considered as potential consolidation material for archaeological wood [1]. In addition, and cellulose mixtures have attracted increased attention for the production of novel material, biofuels and, chemicals. Due to the highly heterogeneous structure of lignin and complications of its extraction in experimental approaches, relatively little evidence exists on lignin and cellulose interaction and its response to water adsorption on molecular level. In the present study, atomistic modeling is employed to investigate hygromechanical properties of lignocellulose mixtures and to inform the role of lignin as a consolidation agent in wood composite. Mixtures of amorphous cellulose with uncondensed coniferyl and sinapyl lignin are prepared by employing an iterative hybrid all-atom molecular dynamics and grand canonical Monte-Carlo (GCMC) simulation [2] as a model representing wood holocellulose and lignin matrix, hydrated in a range relative humidity from fully dry to saturation pressure. The hybrid GCMC/MD technique provides an excellent tool to capture the highly coupled nature of sorption-induced swelling in the lignocellulose mixture by enabling us to capture the sorption by applying relative humidity in GCMC and allowing the resultant swelling during relaxation in the MD stage of the simulation. The presented model, methodology and the choice of simulation parameters such as system size are validated through comparison with available simulation and experimental data. By applying the mechanical tests to hydrated samples role of lignin in adsorption-induced mechanical softening in wood polymer is also studied. The sorption isotherms, swelling curves and mechanical data reveal reduced moisture adsorption and swelling together with mechanical softening as the lignin content increase signifying the effect of the polymer interaction, which is further characterized by measuring porosity pore size distribution, hydrogen bonding network and cohesive energy calculation. Rule of mixture is introduced as an analysis tool to reveal the role of polymer interphase [3]. The underlying molecular mechanism describing the lignocellulose Hygromechanical response is compared to what we learned in our recent studies regarding molecular phenomena involved in polyethylene glycol consolidation of wood in order to unravel molecular characteristics of an inspired wood cell wall consolidant.

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References

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Participation

Unsure

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