Contribution ID: **8** Type: **Oral**

Insights into cellulose solvation in organosolv mixtures: a molecular dynamics and quantum mechanics study

The use of multicomponent solvents has provided remarkable results in biomass fractionation processes of several levels of severity. Despite all invested efforts, no fractionation method is currently capable of achieving lignocellulose deconstruction in an economically viable commercial scale process. Understanding the factors that drive to the interaction of biomass with different solvents is the key to successful fractionation. Understanding the mutual organization between organic solvents and water in multi-component systems and their specific interactions with the wood polymers can be achieved by means of computational methods, which can provide detailed information at the molecular level. Our results on the atomistic understanding of preferential interactions of water-organics solvent components with cellulose have been obtained from molecular dynamics simulations in conjunction with density functional theory (DFT) approaches, including ab-initio molecular dynamics. Structure and dynamics of cellulose-solvent interfaces were characterized by torsion angles of cellulose backbone and hydroxymethyl chains, H-bonding, interaction energies, and pair correlation functions (RDF) at several water-organosolv concentrations. Structure analysis shows that chain deformation of solvated cellulose by conformational transition of the hydroxymethyl chain evolves in the order Water>Ethanol>Isopropanol>Acetontrile. The center-of-mass RDFs revealed a saturation-like behavior of some concentrated mixtures, displaying a solvent phase separation at the cellulose interface. Furthermore, analysis of the site-to-site RDFs shows a preferential orientation of solvent molecules toward specific oxygens of the glucose monomer. This preferential solvent-O(cellulose) binding vary with the nature of the organic solvent and the water content. Non-linearity of interactions between mixed solvents and cellulose is in good agreement with experimental swelling data [1].

1. J. Bossu, N. Le Moigne, S. Corn, P. Trens, F. Di Renzo, *Wood Sci. Technol.* 52 (2018), 987-1008.

Preferred topic

Conformation of polymers in solvents

Primary authors: AGUILERA-SEGURA, Sonia M. (Institut Charles Gerhardt Montpellier, UMR 5253 UM-CNRS-ENSCM); Dr MINEVA, Tzonka (Institut Charles Gerhardt Montpellier, UMR 5253 UM-CNRS-ENSCM); Dr DI RENZO, Francesco (Institut Charles Gerhardt Montpellier, UMR 5253 UM-CNRS-ENSCM); Dr BOSSU, Julie (Institut Charles Gerhardt Montpellier, UMR 5253 UM-CNRS-ENSCM)

Presenter: AGUILERA-SEGURA, Sonia M. (Institut Charles Gerhardt Montpellier, UMR 5253 UM-CNRS-ENSCM)