Interactions Between Ionic Liquids and Cellulose Fibers Monitored by Molecular Dynamics

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Introduction: In Brazil, fuel ethanol production is mainly achieved by fermentation of sugar cane followed by bagasse, its lignocellulosic residual biomass. The cellulose fiber is a highly ordered polymer of glucose monomers linked by β 1-4 linkages and organized into chains aligned in planes, forming overlapping sheets. Intra- and inter-chain hydrogen bonds assist in fiber's stabilization and hampers the access of cellulases to cleave it into smaller polymers. The use of ionic liquids (IL) as solvents is proposed to bypass the recalcitrance problem. IL were reported to quickly dissolve crystalline cellulose fibers and wood chips. Reconstituted cellulose precipitate in an amorphous structure, with chains more accessible to cellulases. **Objectives:** In this work, simulations were performed, ILs and a cellulose fiber, aiming to set an atomic point of view over the deconstruction problem, and IL's effect over biomass. **Materials and Methods:** ILs were parametrized to the CHARMM 36. Molecular dynamics simulations were performed for both ILs boxes and ILs plus cellulose fibers respectively at 10 ns at 298 K and 50 ns at 313 K , both in the NPT ensemble, 1 atm and PME electrostatics. Ionic Liquids parameters were tested by calculating the box average density and comparing with published results. For cellulose fiber's system, the ILs effect was measured by RMSD, the fibers's torsion angle and average number of hydrogen bonds. We also used simulations in water boxes as a negative control for simulations. **Results and Discussion:** Results from the parametrization shows that the calculated parameters are in good agreement with those measured experimentally. Now we are aiming to understand how fibers in ILs have significantly higher RMSD values than those on water. Also, fibers in IL have smaller torsion angles than those on water. **Conclusions:** We suggest that cellulose in IL are more prone to break due to less flexible structure and higher glucose residues mobility.

Keywords: Biofuels, Cellulose, Molecular Dynamics