Cellulose is the main component of plant cell walls. Its structure is constituted by polymerization of glucose molecules linked by β-1,4 bonds forming a highly recalcitrant polysaccharide, resistant to acidic, alkaline and enzymatic hydrolysis. Ionic liquids (IL) like 1-Ethyl-3-methylimidazolium acetate (EMIM-Ac) are capable to dissolve lignocellulose biomass, and are known as “green solvents” for their ability to be recovered and recycled. IL have many practical advantages over other solvents such as low volatility, high temperature stability and the ability to be tailored to meet specific physicochemical goals. In this work we investigated how EMIM-Ac disrupts the structure and dissolve cellulose fibers through molecular dynamics (MD). Aiming to understand this mechanism and guide the design of new IL combinations, optimized to deconstruct the crystalline fibers and recover amorphous cellulose. EMIM-Ac parameters were generated from the CHARMM General Force Field, and the partial atomic charges were assigned from the HF-631G* optimized geometry, by Restrained ElectroStatic Potential (RESP). Systems were built with Packmol using a DP20 cellulose in water or EMIM-Ac. Each system had its energy minimized with the conjugated gradients with 10K steps. Molecular dynamics simulations were performed for 50ns, in the NPT ensemble at 323 K, 1 atm and PME electrostatics. The systems where compared with each other in terms of RMSD and the fiber torsional angle. It was found that the fiber in EMIM-Ac had a significantly higher RMSD than the one in water, meaning that the glucose residues in EMIM-Ac are more free to move in IL than in water. The torsional angle however was significantly higher on cellulose in water than in EMIM-Ac, meaning that it is more flexible on water. With these results we suggest that flexibility is important on cellulose structure and as IL restrain that flexibility the more rigid structure is more prone to break.

Keywords: Biofuels, Ionic Liquids, Molecular Dynamics, Green solvents

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