ELUCIDATING PYROLYSIS OIL OLIGIMERIC CHEMICAL STRUCTURES: EXPERIMENTAL STUDIES AND DENSITY FUNCTIONAL THEORY CALCULATIONS

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More than 40 wt. % of the mass of pyrolysis oils derived from lignocellulosic materials if formed by oligomeric molecules. These oligomeric molecules are obtained from the thermal degradation of cellulose, hemicellulose, and lignin and are removed from the reacting environment via evaporation and thermal ejection. Cellulose and Hemicellulose are typically soluble in Combination reactions in the liquid intermediate or the vapor phase and form small quantities of oligomeric molecules. Hundreds of peer-reviewed studies have been published on the characterization of bio-oil water soluble and insoluble. More recently, ICR-MS studies allowed a preliminary assignment of tentative chemical formulas to several sugar and lignin-derived oligomers. Durante the conference, we will discuss dimer, trimer, and tetramer structures based on chemical balances of cellulose dehydration and fragmentation reactions Lignin demethylation reaction after the homolytic cleavage for a hardwood model lignin in the pyrolysis process. Different configurations of oligomers were evaluated by varying the positions of the G and S units in the hardwood model lignin through DFT calculations. Likewise, we calculated cellulose dehydration and fragmentation reaction products. The PIs are working to build a database with bio-oil compounds and a methodology to build surrogated bio-oils to develop mathematical models to describe the behavior of bio-oil refineries.