CHEMICAL NATURE, MOLECULAR STRUCTURE, AND FORMATION MECHANISM OF BIOCHAR: MOLECULAR DYNAMICS STUDIES AND EXPERIMENTAL APPROACH

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Optimizing the pyrolysis process for biochar production requires a comprehensive understanding of how operational parameters influence the molecular structure of biochar. Moreover, to maximize the yield of biofuels in subsequent processes, it is crucial to focus on converting the carbon present in biomass to biochar, as biofuels contain approximately 80% carbon on a mass basis. The challenge of carbon conversion efficiency can be addressed by unraveling the theoretical formation mechanism of biochar during the pyrolysis process and identifying pathways to remove oxygen from biomass in the form of H_2O instead of CO and CO_2. Such knowledge can aid in enhancing the reactivity and conversion efficiency of biochar in subsequent processes. Furthermore, an accurate understanding of the molecular structures of biochar is critical to optimize the pyrolysis process for biochar production. Nevertheless, the complex nature of the large systems that make up biochar presents a significant challenge for molecular modeling and formation mechanism studies. Complexity is due to the multilevel character of biomass pyrolysis, the multiple reaction steps that occur in the process, the solid-gas interaction, and the multiscale of the phenomena involved in the process.

Most of the molecular models developed in the last decades were for diverse coal ranks. The selection of molecules to represent the characterization data in these molecular models has been a manual and subjective process, which is prone to investigator bias and heavily reliant on trial and error. As a result, many of the existing molecular models and methodologies found in the literature may not capture the full structural diversity and functionality of coal, and thus, may not provide accurate predictions of biochar's molecular structure. Hence, it is imperative to devise a sophisticated modeling approach that surpasses the oversimplification of the molecular depiction to evade models that are shallow and do not align with experimental observations. Consequently, in this work, a high-level modeling approach that comprehends biochar's chemical nature beyond average characterization values avoids researcher bias and provides molecular structures of biochar samples that are comparable and realistic has been developed. Furthermore, this approach provides a theoretical formation mechanism of biochar through a molecular dynamics approach using reactive force fields. Fig -1 illustrates an overview of the methodology followed.

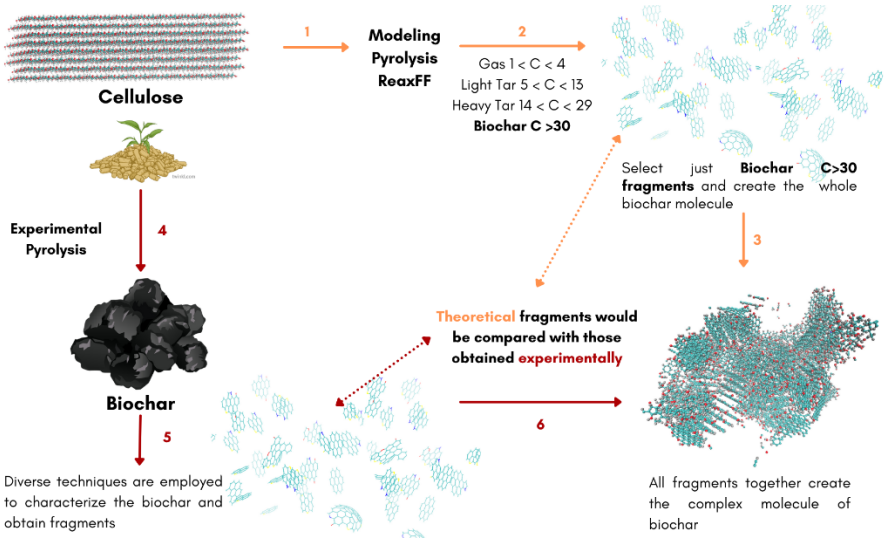

Figure 1 – Sketch of the theoretical and experimental pathway to obtain the molecular structure of biochar.