MOLECULAR DYNAMICS SIMULATION OF REALISTIC BIOCHAR MODELS WITH CONTROLLED POROSITY

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Biochar is an amorphous carbon-rich material with numerous properties and functionality generated from biomass pyrolysis. Biochar surface functional groups and porous structures have proven applications in treating flue gases and organic and inorganic pollutants in soil and water/wastewater, energy storage and carbon capture. The wide availability of biomass sources has increased interest in biochar as a sustainable and environmentally friendly material. The properties and porous structures of biochar vary depending on the type of biomass and high heat treatment temperature (HHT). Biochars produced at HHT between 400°C – 800°C generally have lower H/C and O/C ratios, higher porosities, larger pore sizes and higher surface areas as temperature increases. While experimental studies have demonstrated the influence of biochar macroscopic properties on processes, there is little knowledge of the governing role porous structure and functional groups play on these processes at the atomistic scale. Having insights on these processes at the nanoscales is extremely important for the optimisation of biochar for application, especially in the adsorption of gases. Atomistic simulations methods have shown the potential to generate such amorphous materials. However, most models reported are either all carbon atoms or graphitic sheets that are very dense or with simplistic slit pores that ignore the importance of heteroatoms such as O, N, S and pore morphologies observed in experiments. Hence, developing realistic models with these properties are necessary to understand their role in the governing adsorption mechanisms that will aid in guiding the design and optimisation of biochar materials for target applications. In this work, molecular dynamics simulations in the isobaric ensemble was used to generate realistic biochar models that account for experimentally determined H/C, O/C, N/C, aromaticity, micropore size range, micropore volumes and true densities of biochars. A pore generation approach was developed called virtual atoms that consist of Lennard-Jones spheres with varying van der Waals radius and softness. Its interaction via a soft-core potential with the biochar matrix allows the creation of pores with rough surfaces while changing the van der Waals radius parameters gives control to the pore-size distribution. We focused on microporosity, creating average pore sizes of 0.5 - 2 nm in diameter and pore volumes of 0.05 – 1 cm3/g that align with experimentally observed gas adsorption studies of amorphous porous biochars. Realistic biochar models developed with surface functionalities, micropore size distribution and pore morphologies will aid study adsorption processes in confined micropores at the atomistic scale and shed light on governing processes not observed experimentally.