World Academy of Science, Engineering and Technology
International Journal of Environmental and Ecological Engineering
Vol:17, No:06, 2023

Effect of Halloysite on Heavy Metals Fate during Solid Waste Pyrolysis: A Combinatorial Experimental/Computational Study

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Abstract : In this study, the low-cost halloysite (Hal) was utilized for the first time to enhance the solid-phase enrichment and stability of heavy metals (HMs) during solid waste pyrolysis through experimental and theoretical methods, and compared with kaolinite (Kao). Experimental results demonstrated that Hal was superior to Kao in improving the solid-phase enrichment of HMs. Adding Hal reduced the proportion of HMs in the unstable fraction (F1+F2), consequently lowering the environmental risk of biochar and the extractable state of HMs. Through Grand canonical Monte Carlo and Density Functional Theory (DFT) simulations, the adsorption amounts and adsorption mechanisms of Cd/Pb compound on Hal/Kao surfaces were analyzed. The adsorption amounts of HMs by Hal were significantly higher than Kao and decreased with increasing temperature, and the difference in adsorption performance caused by structural bending was negligible. The DFT results indicated that Cd/Pb monomers were stabilized by establishing covalent bonds with OH or reactive O atoms on the Al-(0 0 1) surface, whereas the covalent bonds with ionic bonding properties formed between Cl atoms and unsaturated Al atoms played a crucial role in stabilizing HM chlorides. This study highlights the potential of Hal in stabilizing HMs during pyrolysis without requiring any modifications.

Keywords : heavy metals, halloysite, density functional theory, grand canonical Monte Carlo
Conference Title : ICECC 2023 : International Conference on Environment and Climate Change
Conference Location : Rome, Italy
Conference Dates : June 05-06, 2023