Title: Mechanisms of emerging contaminants removal by novel neem chip biochar

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Abstract: Emerging contaminants (ECs) play a vital role in water pollution. The treatment methods used for the removal are expensive and complex. It is therefore highly needed to develop cost-effective materials for the effective removal of ECs. This study comprehensively investigated the potential of biochar material pyrolyzed at different temperatures in removing mancozeb, a potential EC, reported to significantly pollute water sources in Sri Lanka. Detailed isotherm, kinetics, thermodynamics and rate-limiting factor analysis were performed for biochar with high adsorptive capacity along with FTIR and XRD characterization. Results revealed that biochar pyrolyzed at 900 ◦C exposed higher adsorptive performance of 187.68 mg/g. Moreover, a detailed isotherm study exhibited that the adsorption of mancozeb to biochar is multilayer in nature. The pseudo second-order equation is well fitted to explain the adsorption rate of mancozeb. In addition, the thermodynamic analysis explains that the adsorption is spontaneous and endothermic. The XRD information well explains the carbon network development with an increase in pyrolysis temperature. At higher pyrolysis temperatures, the constricted carbon network was formed. FTIR analysis expresses that the functional groups are degraded at higher pyrolysis temperature. The rate-limiting analysis indicates that the removal rate of mancozeb by biochar derived from neem chips pyrolyzed at 900 ◦C initially induced by mass diffusion followed by intraparticle diffusion. The innovative finding of the use of biochar produced from neem chip for the removal of mancozeb makes an opening to the development of noval strategies for the effective removal of ECs at the commercial level.