

**Title:** Effect of Thermodynamics on Mancozeb Adsorption by Neem Chip Biochar

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**Abstract:** Emerging contaminants (ECs) create threats to the well-being of all living organisms globally. Among ECs, fungicides could be easily leached into the water bodies to create water pollution. In Sri Lanka, the use of mancozeb in crop farming has climbed due to increased demand for food. There is a need for the effective removal of mancozeb from water using low-cost adsorbents. Therefore, an attempt was made to understand the thermodynamic effect to add new knowledge to the adsorptive mechanism of mancozeb adsorption by neem chip biochar. Biochar materials were prepared from neem chips at four different pyrolysis temperatures (300, 500, 700 and 900 °C) using muffle furnace. An adsorptive experiment was done using pH of 5, initial concentration of 200 mg/L, dosage of 1 g/L and the temperature of 25 °C. The biochar with best adsorptive performance (mg/g) was selected for detailed thermodynamic study at temperatures, 25, 30 and 40 °C using Van't Hoff equation. Results revealed that the biochar pyrolyzed at 900 °C (NBC 900) expressed the highest mancozeb removal percentage of 93.84 and the adsorptive performance 187.68 mg/g compared to other biochars pyrolyzed at 300, 500 and 700 °C. The change in Gibb's free energy ( $\Delta G^\circ$ ) values at 25, 30 and 40 °C is -11.005 kJ/mol, -13.544 kJ/mol and -18.622 kJ/mol respectively. Based on this thermodynamic outcome, it can be concluded that the adsorption process of mancozeb by NBC 900 is spontaneous in nature. Positive enthalpy change ( $\Delta H^\circ$ ) indicates that the adsorption process is endothermic and positive entropy change ( $\Delta S^\circ$ ) indicates that the affinity of biochar on mancozeb adsorption is strong. Hence, this information is highly useful to study the effect of temperature on the removal of mancozeb by NBC 900 from the aqueous phase and helps understand affinity of biochar toward mancozeb adsorption for better design of adsorption systems.