

## Surface complexation modeling of nickel (II) and vanadium (V) adsorption on biochar

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Biochars are proven to be effective in the removal of inorganic contaminants from water<sup>1</sup>. Although extensive modeling study of metal adsorption at the surface of biochars has been performed using empirical approaches, few studies have employed surface complexation modelling (SCM)<sup>4</sup>. Employing SCM to biochar-containing systems will contribute to a mechanistic understanding of the adsorption of metals at their surface.

In this study, specific surface area, pore volume, pore diameter and elemental composition of two biochars produced from wheat straw and sewage sludge were determined. Potentiometric titrations along with Boehm titrations were carried out to measure the proton ( $H^+$ ) reactivity of biochars. Equilibrium constants and site concentrations were calculated using Fiteql 4.0<sup>3</sup>. Ni(II) and V(V) adsorption experiments were carried out as a function of pH, ionic strength and sorbent-to-Ni and -V ratios. The adsorption data along with  $pK_a$  and biochar surface functional group concentrations were used to calculate the metal binding stability constants. Three different SCM approaches including the non-electrostatic model (NEM), diffuse double layer model (DDLDM) and triple layer model (TLM) were tested. Preliminary results show that biochars have substantial proton reactivity, and uptake significant amount of  $Ni^{+2}$ . Thus, SCM may be an effective method of predicting metal removal to biochars from water with elevated concentrations of heavy metals.

[1] Ahmad *et al.* (2014) *Chemosphere*, **99**: 19-33. [2] Borrok *et al.* (2005) *Am. J. Sci.*, **305(6-8)**: 826-853. [3] Herbelin and Westall (1999) Rept. 99-01, Dept. Chem., Oregon State Univ. [4] Vitanaga *et al.* (2015) *J. Environ. Manage.*, **151**: 443-449.