

Isotherm equations for heavy metal sorption on soils accounting for aqueous complex formation

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Heavy metal sorption to soil have been studied for decades and have been described with sorption isotherm equations. As the solid and solution phase of soils are very heterogeneous, empirical treatment of partitioning between solid and soil solution is still being used and related to soil properties. Here, we present a simple extension of isotherm equations to account for heavy metal complex formation in solution. As heavy metals are commonly analyzed using ICP spectroscopy, the total metal concentration - the sum of all metal species - in solution is being detected. Hence, sorption isotherms describe the concentration of the metal sorbed to solid phase as a function of the sum of metal species including the aqueous complex. We derive a simple algebraic expression for the partitioning for a free metal species and a metal complex. Combining the expression with existing isotherm equations yields a new family of equation that quantifies the effect of aqueous complex formation on the apparent sorption behavior. The new isotherm equations are typically sigmoidal and fall in the S-class or subgroup 4 of L-class and H-class of the Giles classification. Based on data found in the literature, we apply the new equations based Langmuir, Freundlich and Langmuir-Freundlich equations to heavy metal sorption on various soils. We furthermore successfully described the sorption behavior of Cd on soil in the presence of EDTA concentrations ranging from 0 to 600 mg/L based on the experiments by You et al. [1]. The equations have the advantage, that the additional two parameters are directly related to the total amount of the complexing agent and the affinity. The equations are in particular useful to describe isotherms with concave shapes at low concentrations.

[1] You, Xueji, et al. Environmental Science and Pollution Research 27 (2020): 41623-41638.