

LCD Model for Humics Adsorption to Oxides

Liping Weng and Willem H. van Riemsdijk

Department of Soil Quality, Wageningen University, P.O. Box 8005, 6700 EC, Wageningen, The Netherlands

Humic acid and fulvic acid are important reactive components in natural organic matter. Humic materials can adsorb strongly to mineral surfaces such as iron (hydr)oxides. The adsorption of humics plays an important role in controlling the solubility of natural organic matter, the surface characteristics of soil particles, and the speciation of many elements in the environment.

The adsorption of humics is due to mainly chemical and electrostatic interactions. The adsorption is dependent on the nature of the humics (humic acid or fulvic acid), solution chemistry (pH, salt level, presence of other small ions), and the characteristics of the oxides (pzc, surface area). Mechanistic models are useful tools to better understand the mechanisms and factors influencing the adsorption. However, to model the adsorption of particles is difficult, especially for the particles with variable charge. For humics, it is even more complicated by the chemical heterogeneity of the material.

The LCD (Ligand and Charge Distribution) is a model concept that was recently developed to describe organic molecule adsorption to oxides. The LCD model makes use of the advanced models for ion binding to oxides (i.e. CD-MUSIC model) and to humics (i.e. NICA model). The average chemical state of humics in both the solution phase and the adsorption phase is calculated with the NICA model by taking into account the competition of the small ions (e.g. protons) with the surface sites. The equilibrium phase distribution of humics is calculated in the LCD based on a thermodynamic relationship (SPADE model) that was derived from the free energy change of the humics upon adsorption.

Fulvic acid differs from humic acid in solubility, molecular size and charge density. The adsorption of fulvic and humic acid to goethite shows both similarities and differences in terms of adsorption magnitude, salt dependency and pH dependency. The LCD model was applied to describe the adsorption of fulvic and humic acid. Promising results have been achieved. The simulation exercise is helpful to understand the complex adsorption process of the humics at the surface of oxides.