Size matters: On the search of understanding surface complexation by nano oxide materials

TJISSE HIEMSTRA[1]

[1]Department of Soil Quality
Wageningen University The Netherlands

Availability and mobility of ions in the environment is strongly influenced by the presence of reactive surfaces. No solid exists without surfaces. Ion reactivity in nature is highly determined by the presence of nano oxide materials, having an extremely high surface to mass ratio. Little is needed to create a high binding capacity.

Surface complexation modeling (SCM) is a powerful tool to relate processes at the molecular scale of interfaces to solution conditions in the environment. The challenge is to translate the variety of observed surface complexes to corresponding ion concentrations in the aqueous phase because these concentrations ultimately determine the fate of contaminants and (micro-) nutrients in the environment.

Well-defined crystalline metal (hydr) oxides often possess various crystal faces with different ion binding properties and therefore, these have been used to unravel the mechanisms of ion binding thereby using a range of spectroscopic methodologies. This information has contributed to the development of mechanistic surface complexation models, especially the Charge Distribution (CD) and multisite ion complexation (MUSIC) model.

At the nanoscale, particles may no longer have well-defined surfaces and particularly these materials often form the backbone of ion reactivity in nature. Ferrihydrite (Fh) is the most stable Fe (hydr)oxide at the nanoscale. The smallest particles have more Fe at the surface than in the core and may bind large quantities of AsO_4, PO_4 & Natural Organic Matter.

In the present contribution, an overview will be given of surface complexation phenomena in relation to SCM. Recent progress [1] in understanding the surface and mineral structure of ferrihydrite [3] will also be discussed and its meaning for ion binding. Comparison will be made with goethite. In addition, the surface Gibbs free energy of Fh will be highlighted as a major driver for the behavior of this nanomaterial [2]. Ion binding will influence this thermodynamic property as will be discussed in relation to Fh formation and its relative stability.

References

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