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Revisiting the NICA-Donnan model and its parameterisation for metal binding to humic substances.

Jan E. Groenenberg[1,2]

[1]Soil Chemistry and Chemical Soil Quality, Wageningen University and Research, The Netherlands
[2] LIEC: Laboratoire Interdisciplinaire des Environnements Continentaux
UMR 7360 CNRS-Université de Lorraine
France

e-mail: bertjan.groenenberg@wur.nl

The bio-availability and fate of metals in the environment is largely determined by their binding to particulate and dissolved organic matter. The humic fraction therein is considered the most important fraction with respect to metal binding. The binding of various metals to humic substances (HS) has been successfully modelled with WHAM Models VI and VII [1] and the NICA-Donnan (N-D) model [2]. Since the publication of the generic N-D model parameters for proton and metal binding by Milne in 2001-2003 [3] various new experimental data on metal binding to humic substances have become available which may be used to derive more reliable model parameters for those metals already included. Furthermore the upcoming interest in the environmental behaviour trace metals of emerging concern including the technological critical elements (TCEs) demand for an update of the N-D model parameters.

Together with the update it is timely to critically review the model and the way it is parameterised. A closer look at the parameters derived by Milne et al. shows weaker model fits for some metals, especially some trivalent metals compared to the divalent metals. There is criticism on the non-uniqueness of the model parameters derived for the N-D model which is partly due to the problem inherent to any electrostatic model that it is impossible to find a unique mathematical solution to vary the local electrostatic potential at the binding sites [4]. Furthermore the electrostatic Donnan model and its present parameterisation results in physically unrealistic Donnan volumes particularly for the fulvic acid [4].

The alternative optimisation procedure as proposed by Lenoir et al. [5] may help to overcome the criticized points to some extent. Furthermore the use of structural relations between model parameters as used by Tipping et al. [1] may help to come to a more coherent set of model parameters for metal binding. Here we will derive an extended set of model parameters for metal binding and evaluate the consequences in terms of model fit and robustness using an alternative procedure as a first step to come to a revised parameterisation of the NICA-Donnan model

References

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