PEST-ORCHESTRA: A tool for optimizing model parameters for humic substances reactivity

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Humic substances are a complex mixture of macromolecules that have a high affinity for metal ions and can affect their mobility and bioavailability in the environment. Due to the high heterogeneity of humic substances, their reactivity is difficult to determine, and several models exist to describe their acid-base properties and their complexation to metal ions. Among the various speciation model platforms, the software ORCHESTRA[1] has the advantages to be independent of the operating system and free. Furthermore, it is very flexible, since model its model definitions are in text format and thereby accessible and can be modified by users for extensions and modifications. However, until now, no method is available to optimize model parameters using ORCHESTRA. Here we describe the coupling of the PEST parameter optimization software (http://pesthomepage.org/) with the ORCHESTRA speciation software, and validate this method as a way to describe humic substances reactivity within the framework of the NICA-Donnan model[2], by comparing results with literature data.

The optimization procedure has been applied to obtain optimum NICA-Donnan parameters for the binding of protons and metal ions to Laurentian fulvic acid (LFA). An unconstrained fit gave us proton-binding parameters in good agreement with the results obtained by Milne *et al.*[3] on the same dataset using the ECOSAT-FIT software. This allow us to validate our approach. A more constrained procedure to determine proton-binding parameters is also proposed, adapted from Lenoir *et al.*[4]. This method is also applied to optimization of metal-binding (Pb, Cd, Zn) parameters for the same LFA.

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