# Rare Earth Element binding to humic substances: a modelling approach

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The biogeochemical cycle of Rare Earth Elements (REEs), being scandium, yttrium and the lanthanide group, is being affected by their increased use in the production of high-tech and communication devices and in medicical applications. Due to its increase used enrichment of certain REEs has been detected in natural waters.

No regulatory thresholds for REE concentrations and emissions into the environment are set as present knowledge on the environmental behaviour and effects of REEs is scarce. The fate and behaviour of REEs in the environment is largely determined by their binding to reactive components, of which organic matter, metal oxides, and clays are considered important. The use of thermodynamic models which predict the partitioning and speciation of trace metals in terrestrial and aquatic systems is of key importance. Ion binding models have allowed to understand the environmental cycling of trace elements in which humic substances (HS, humic and fulvic acids) are the most reactive fractions of natural organic matter, presenting a high affinity for metal ions. However, their reactivity is difficult to study due to their colloidal nature, associated with a heterogeneous affinity distribution. The NICA-Donnan model (NDM) is one of the most used models for ion binding to HS however, at present there are no NDM parameters for REEs binding to HS except Eu.

Here we obtain generic ND parameters for all 14 stable lanthanides based on published data on their binding to HS. The geochemical speciation program ORCHESTRA in combination with the patrameter optmimization software PEST were used to fit the experimental data with the NDM. The newly derived model parameters are evaluated with published experimental data on REE binding to HS in competition with other metals and were used to predict the solid solution partitioning in soils using a multi-surface model and compared with previously obtained experimental data, thus allowing a better understanding of the environmental cycling of these elements.