Modelling of tri-valent metal binding to humic substances using the NICA-Donnan model

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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 succesfully modelled with WHAM Models VI and VII and the NICA-Donnan (N-D) model. Fits of the N-D model for divalent metal binding to both fulvic- (FA) and humic acid (HA) using the present defaut parameters are good with R^2>0.90 and RMSE generally below 0.20. The N-D fits for some of the trivalent metals, however, seem to be less accurate with R^2 of 0.60 or lower for Al, Cm and Am. A larger uncertainty in the data for these elements, may explain the poorer fits to some extent. Here we analyse the modelling of Al, Cr and Eu using published data in combination with new measurements of metal binding to HS.
The analysis shows that a revised modelling of the electrostatic effects, the inclusion of binding of hydrolysed metal species and/or the incusion of dimeric metal species strongly improve the fits of trivalen metal binding to humic substances with the NICA-Donann model. But the effects of the three evaluated aspects varies amongst the metals which might be due to the pH at which the first hydroxy species become important .