Supporting Information

Competitive and Synergistic Effects in pH Dependent Phosphate Adsorption in Soils: LCD Modeling

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Table SI-1. NICA-Donnan model parameters for FA. (parameters for Fe from Hiemstra *et al.* [24]; parameters for innersphere complex -≡$Fe_1OOCR^{-0.5}$ from Weng *et al.* [14]; all other parameters from Milne *et al*. [22, 23])

	carboxylic site	phenolic site
Q_{max} (mol/kg)	5.88	1.86
p	0.59	0.70
$\log\tilde{K}_{H}$	2.34	8.60
n_{H}	0.66	0.76
$\log\tilde{K}_{Ca}$	-2.17	-3.29
n_{Ca}	0.85	0.83
$\log\tilde{K}_{Al}$	-4.11	12.16
n_{Al}	0.42	0.31
$\log\tilde{K}_{Fe}$	2.70	8.30
n_{Fe}	0.36	0.23
$\log\tilde{K}_{in}$	-1.0	
n_{in}	0.66	
b	0.57	

Q_{max}: site density;

p: parameter for the intrinsic heterogeneity of the ligands;

$\tilde{K}_i$: mean affinity constant;

n_i: ion specific non-ideality parameter;

b: a constant used to calculate the Donnan volume;

subscript "$_{in}$" refers to the innersphere complex (≡$Fe_1OOCR^{-0.5}$).

Table SI-2. CD-MUSIC model parameters for goethite (all parameters are from Hiemstra *et al*. [10], except those for the innersphere complexes between surface sites and NOM, which are from Weng et al. [14])

basic parameters	PZC	site density (/nm^2)		capacitance (F/m^2)	
	9.0	≡FeOH$^{-0.5}$	≡Fe$_3$O$^{-0.5}$	C_1	C_2
		3.45	2.7	0.93	0.75

surface species	sites		charge distribution			ions	log*K*
	≡FeOH$^{-0.5}$	≡Fe$_3$O$^{-0.5}$	Δz_0	Δz_1	Δz_2		
≡FeOH$_2^{+0.5}$	1	0	1	0	0	1H$^+$	9.00
≡Fe$_3$OH$^{+0.5}$	0	1	1	0	0	1H$^+$	9.00
≡FeOH…Na$^{+0.5}$	1	0	0	1	0	1Na$^+$	-0.60
≡Fe$_3$O…Na$^{+0.5}$	0	1	0	1	0	1Na$^+$	-0.60
≡FeOH$_2$…Cl$^{-0.5}$	1	0	1	-1	0	1H$^+$, 1Cl$^-$	8.55
≡Fe$_3$OH…Cl$^{-0.5}$	0	1	1	-1	0	1H$^+$, 1Cl$^-$	8.55
≡FeOHCa$^{+1.5}$	1	0	0.31	1.69	0	1Ca^{2+}	3.23
≡FeOHCaOH$^{+0.5}$	1	0	0.31	0.69	0	-1H$^+$, 1Ca^{2+}	-6.42
≡FeOH…Ca$^{+1.5}$	1	0	0	2	0	1Ca^{2+}	1.8
≡Fe$_3$O…Ca$^{+1.5}$	1	0	0	2	0	1Ca^{2+}	1.8
≡(FeO)$_2$PO$_2^{-2.0}$	2	0	0.46	-1.46	0	2H$^+$, 1PO$_4^{3-}$	29.72
≡FeOPO$_2$OH$^{-1.5}$	1	0	0.28	-1.28	0	2H$^+$, 1PO$_4^{3-}$	27.63
≡Fe$_1$OOCR$^{-0.5}$	1	0	0.5	-0.5		1H$^+$, 1RCOO$^-$	-1.0*

Δz_0:charge attributed to 0-plane;

Δz_1: charge attributed to 1-plane;

Δz_2: charge attributed to 2-plane;

≡Fe$_1$OOCR$^{-0.5}$ refers to the innersphere complexes between surface sites and carboxylic groups and * the NICA $\log\tilde{K}_{in}$ for formation of this complex.

Figure SI-1. a. NOM and DOC (DOC measured at pH around 5).

b. NOM and P_PO_4 (P_PO_4 measured at pH around 4).

c. Net charge of NOM in soil 30 calculated by the model.