Supporting Document

Antimony (V) Adsorption at the Hematite–Water Interface: A Macroscopic and In Situ ATR-FTIR study

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Table S1. Hematite and suspension parameters used in the triple-layer surface complexation modeling of antimony adsorption.

Parameter (Unit)	**Value**
S_A, specific surface ($m^2\ g^{-1}$)	24†
n_s, ≡FeOH total site density (nm^{-2})	1.0‡
S_T, total site concentration ($mmol\ L^{-1}$)	0.782‡
C_1, inner-Helmholtz capacitance ($F\ m^{-2}$)	0.97§
C_2, outer-Helmholtz capacitance ($F\ m^{-2}$)	0.2§
a, suspension density ($g\ L^{-1}$)	2
Background electrolyte (M KCl)	0.001 and 0.01

†Elzinga and Kretzschmar (2013).

‡Current study. Site density value was computed using $n_s = (S_T A_N)/(10^{18} a S_A)$, where A_N is the Avogadro constant.

§Sahai and Sverjensky (1997a).

Table S2. Aqueous speciation and proton and counter-ion adsorption reactions used in the triple-layer surface complexation modeling of antimony adsorption by hematite.

Reaction	log K or log K^{int}†	Reference
Aqueous Speciation		
$Sb(OH)_5^0 + H_2O = Sb(OH)_6^- + H^+$	−2.85	Accornero et al. (2008)
$H_2O = H^+ + OH^-$	−14.00	Martell et al. (2004)
Proton and Counter-Ion Adsorption		
$\equiv FeOH^0 + H^+ = FeOH_2^+$	5.70	Sahai and Sverjensky (1997a)
$\equiv FeOH^0 = FeO^- + H^+$	−11.30	Sahai and Sverjensky (1997a)
$\equiv FeOH^0 + H^+ + Cl^- = FeOH_2^+ - Cl^-$	8.51	Sahai and Sverjensky (1997b)
$\equiv FeOH^0 + K^+ = FeO^- - K^+ + H^+$	−8.68	Sahai and Sverjensky (1997b)

†Common logarithm of the aqueous speciation or the intrinsic surface complexation equilibrium constants (25 °C).

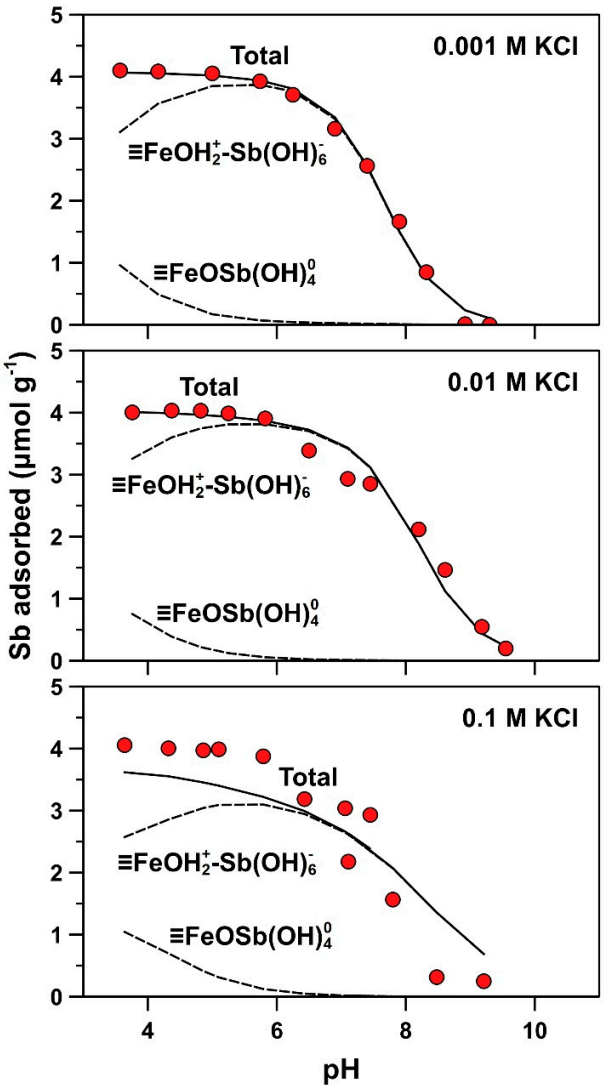

Figure S1. The surface speciation of adsorbed Sb into inner-sphere [$\equiv FeOSb(OH)_4^0$] and outer-sphere [$\equiv FeOH_2^+ - Sb(OH)_6^-$] complexes (Model I) on hematite predicted by the TLM as a function of pH in 0.001, 0.01, and 0.1 M KCl ionic media.

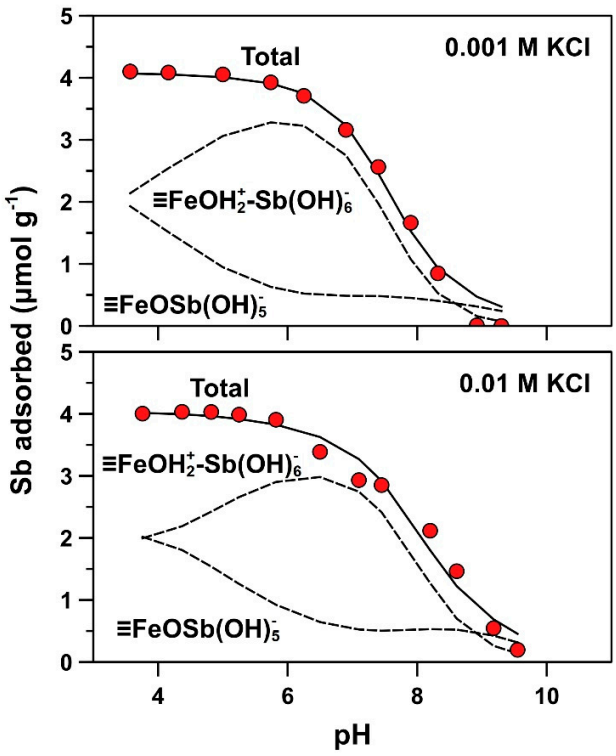

Figure S2. The surface speciation of adsorbed Sb into inner-sphere [≡FeOSb(OH)$_5^-$] and outer-sphere [≡FeOH$_2^+$–Sb(OH)$_6^-$] complexes on hematite (Model II) predicted by the TLM as a function of pH in 0.001 and 0.01 M KCl ionic media.

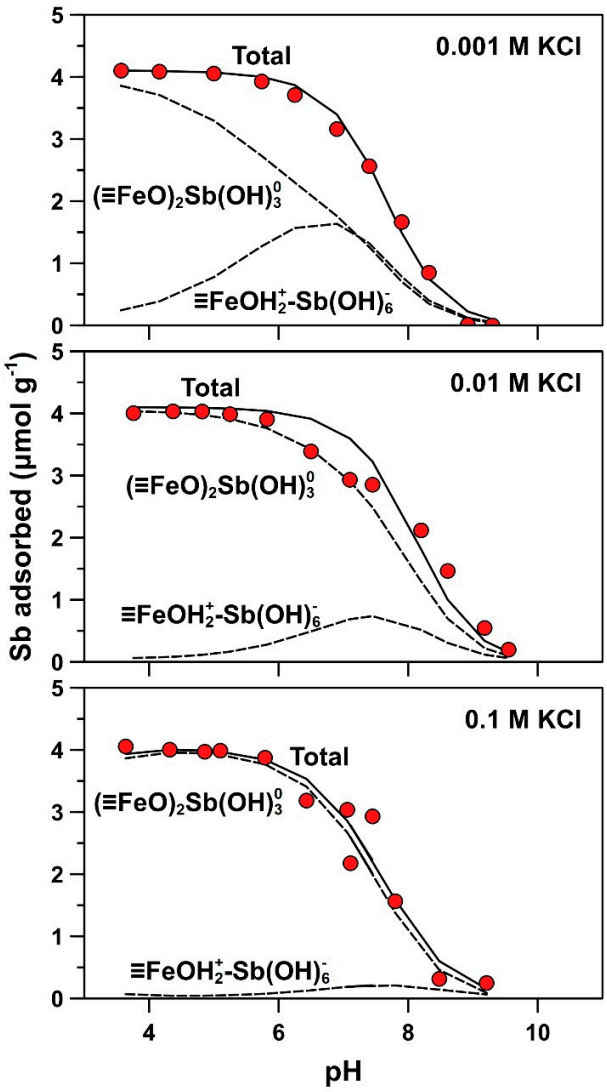

Figure S3. The surface speciation of adsorbed Sb into inner-sphere bidentate [$(\equiv FeO)_2Sb(OH)_3^0$] and outer-sphere [$\equiv FeOH_2^+ - Sb(OH)_6^-$] complexes (Model III) on hematite predicted by the TLM as a function of pH in 0.001, 0.01, and 0.1 M KCl ionic media.