Supporting Information

Predicting Cr(VI) adsorption on soils: the role of the competition of soil organic matter

Zhenqing Shi,[a,*] Shimeng Peng,[a] Xiaofeng Lin,[a] Yuzhen Liang,[a] Suen-Zone Lee,[b] Herbert E. Allen[c]

[a] School of Environment and Energy, South China University of Technology, Guangzhou, Guangdong 510006, PR China

[b] Chia Nan University of Pharmacy and Science, Tainan City 71710, Taiwan

[c] Department of Civil and Environmental Engineering, University of Delaware, Newark, DE 19716, USA

*Corresponding author:

Zhenqing Shi; Tel: +86 20 39380503; e-mail: zqshi@scut.edu.cn

Table S1. Surface complexation reactions for SOC modeling[1]

Reaction	(Δz_0, Δz_1, Δz_2)[a]	log *K*
$2HFA + Fe^{3+} + H_2O = FA_2FeOH + 3H^+$	(-0.2, 0, 0.2)	-4.6
$2HFA + Fe^{3+} = FA_2Fe^+ + 2H^+$	(-0.2, 0, 1.2)	-1.68
$HFA + Ca^{2+} = FACa^{2+} + H^+$	(-0.5, 0, 1.5)	-2.2
$2HFA + Ca^{2+} = FA2Ca + 2H^+$	(-0.75, 0, 0.75)	-11.3
$HFA + Mg^{2+} = FAMg^+ + H^+$	(-0.5, 0, 1.5)	-2.5
$2HFA + Al^{3+} = FA_2Al^+ + 2H^+$	(0.2, 0, 1.2)	-4.06
$2HFA + Al^{3+} + H_2O = FA_2AlOH + 3H^+$	(-0.2, 0, 0.2)	-9.45

[a] Δz_0, Δz_1, Δz_2 represent the *o*-, *b*-, *d*-planes, respectively.

Table S2. Surface complexation reactions for ferrihydrite modeling[2-4]

Reaction	(Δz_0, Δz_1, Δz_2)[a]	log *K*
$FeOH^{1/2-} + H^+ = FeOH_2^{1/2+}$	(1, 0, 0)	8.1
$FeOH^{1/2-} + Na^+ = FeOHNa^{1/2+}$	(0, 0, 1)	-0.6
$FeOH^{1/2-} + Ca^{2+} = FeOHCa^{3/2+}$	(0.32, 1.68, 0)	3.17
$2FeOH^{1/2-} + 2H^+ + CrO_4^{2-} = (FeO)_2CrO_2^-$	(1, -1, 0)	19.35
$FeOH^{1/2-} + H^+ + RO^- = FeOR^{1/2-} + H_2O$	(0.5, -0.5, 0)	25
$FeOH^{1/2-} + H^+ + NO_3^- = FeOH_2NO_3^{1/2-}$	(1, -1, 0)	7.42

[a] Δz_0, Δz_1, Δz_2 represent the *o*-, *b*-, *d*-planes, respectively.

Table S3. Surface complexation reactions for goethite modeling[5]

Reaction	(Δz_0, Δz_1, Δz_2)[a]	log *K*
$FeOH^{1/2-} + H^+ = FeOH_2^{1/2+}$	(1, 0, 0)	9.2
$FeOH^{1/2-} + Na^+ = FeOHNa^{1/2+}$	(0, 0, 1)	-1
$FeOH^{1/2-} + Ca^{2+} = FeOHCa^{3/2+}$	(0.2, 1.8, 0)	3.55
$2FeOH^{1/2-} + 2H^+ + CrO_4^{2-} = (FeO)_2CrO_2^-$	(0.4, -0.4, 0)[b]	17.1
$FeOH^{1/2-} + H^+ + CrO_4^{2-} = FeOCrO_3^-$	(0.2, -1.2, 0) [b]	8.0
$FeOH^{1/2-} + H^+ + RO^- = FeOR^{1/2-} + H_2O$	(0.5, -0.5, 0)	25
$FeOH^{1/2-} + H^+ + NO_3^- = FeOH_2\ NO_3^{-1/2-}$	(1, -1, 0)	8.2

[a] Δz_0, Δz_1, Δz_2 represent the *o*-, *b*-, *d*-planes, respectively.

Table S4. Additional model parameters of metal oxides used in the study[2, 5]

Metal oxides	Specific surface area (m^2 g^{-1})	Site no. 1 (site nm^{-2})	Inner capacitance (F m^{-2})	Outer capacitance (F m^{-2})
Ferrihydrite[a]	750	4	1.3	5
Goethite[b]	50	2.7	1.02	5

[a] Δz_0, Δz_1, Δz_2 represent the *o*-, *b*-, *d*-planes, respectively.

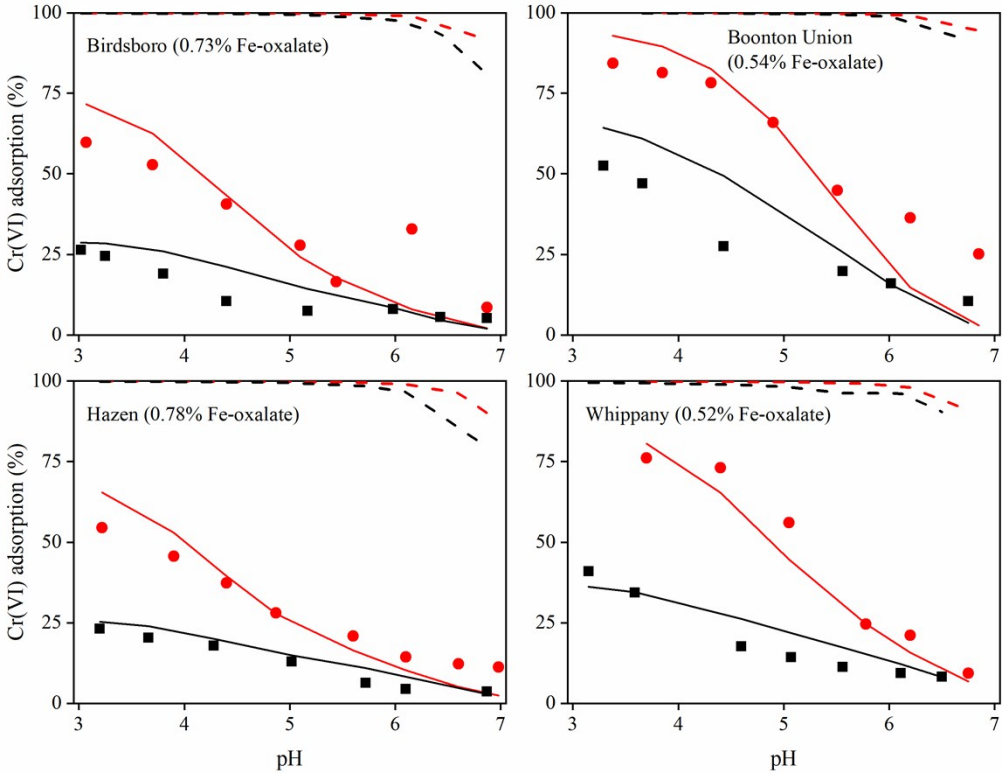

Fig. S1. Modeling adsorption edges for Cr(VI) adsorption on 14 soils at two initial Cr(VI) concentrations. Symbols are experimental data and solid lines are model fits presented in Fig. 1. Dashed lines are model calculations without considering RO^- competition. The soil names and Fe concentrations extracted by oxalate are indicated in the figure. Black squares and red circles represent the initial Cr(VI) concentrations of 0.01 mM and 0.1 mM, respectively.

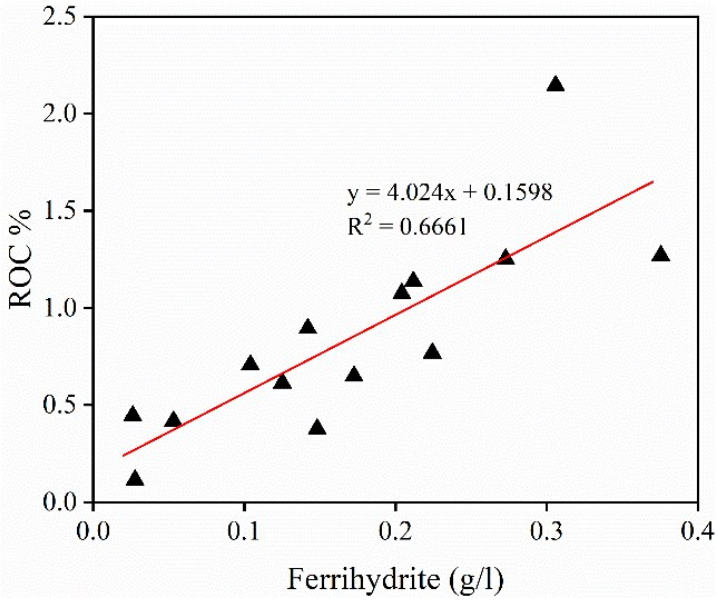

Fig. S2. The relationships between the reactive organic carbon (ROC) concentrations and the concentrations of ferrihydrite in soils.

Reference

1 J. P. Gustafsson, Visual MINTEQ ver. 3.1. Available at http://vminteq.lwr.kth.se/download/ [Verified 20 March 2018], 2018.

2 J. P. Gustafsson, Arsenate adsorption to soils: Modelling the competition from humic substances, *Geoderma*, 2006, **136**, 320-330.

3 C. Tiberg and J. P. Gustafsson, Phosphate effects on cadmium(II) sorption to ferrihydrite, *J. Colloid Interface Sci.*, 2016, **471**, 103-111.

4 C. Tiberg, C. Sjöstedt, I. Persson and J. P. Gustafsson, Phosphate effects on copper(II) and lead(II) sorption to ferrihydrite, *Geochim. Cosmochim. Acta*, 2013, **120**, 140-157.

5 R. Weerasooriya and H. J. Tobschall, Mechanistic modeling of chromate adsorption onto goethite, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2000, **162**, 167-175.