Supporting Information

Adsorption capacity of the corrosion products of nanoscale zerovalent iron towards emerging contaminants

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14 pages: 11 Figures and 2 Tables

Supporting Information

Table S1. Mass balance in different reaction systems

Reaction systems	NA initial concentration (μM)	NA desorbed concentration (μM)
NZVI(0.2 $g \cdot L^{-1}$)	10	10.10
NZVI(0.2 $g \cdot L^{-1}$)+H_2O_2(0.5 mM)		10.04
NZVI(0.2 $g \cdot L^{-1}$)+H_2O_2(1 mM)		9.89
NZVI(0.2 $g \cdot L^{-1}$)+H_2O_2(2 mM)		9.88
NZVI(0.2 $g \cdot L^{-1}$)+H_2O_2(5 mM)		9.94
NZVI(0.2 $g \cdot L^{-1}$)+H_2O_2(10 mM)		9.92

Supporting Information

Table S2. Summary of the surface complexation model and parameters for the oxidized NZVI product.

Parameters	Value*
Site density (nm^{-2})	1.50
Capacitance ($F\ m^{-2}$)	2.10
$\equiv FeOH_2^+ \leftrightharpoons \equiv FeOH + H^+$; pK_{a1}	5.19
$\equiv FeOH \leftrightharpoons \equiv FeO^- + H+$;pK_{a2}	-7.82
log ^{S}K of oxidized NZVI	25.5

** W. Cheng, R. Marsac and K. Hanna, Influence of Magnetite Stoichiometry on the Binding of Emerging Organic Contaminants, Environ. Sci. Technol., 2018, 52, 467-473.*

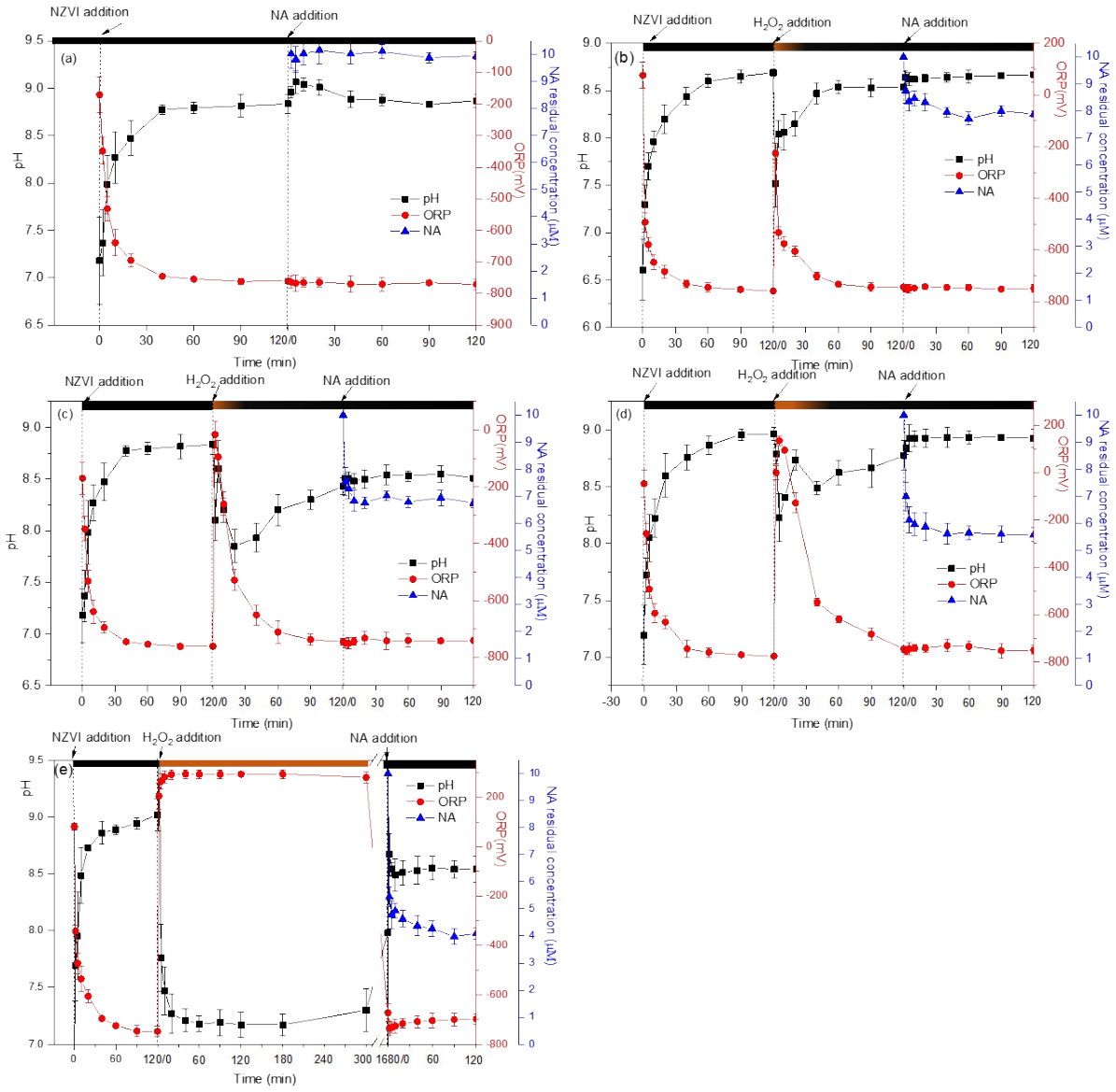

Figure S1. Variations in pH, ORP, color and NA concentration during NZVI oxidation and adsorption process at different H_2O_2 concentration (a) 0 mM; (b) 0.5 mM; (c) 1 mM; (d) 2 mM; (e) 10 mM. Experimental conditions: [NZVI] = 0.2 g·L^{-1} $[NA]_{initial}$ = 10 μM , 20 ±1 °C.

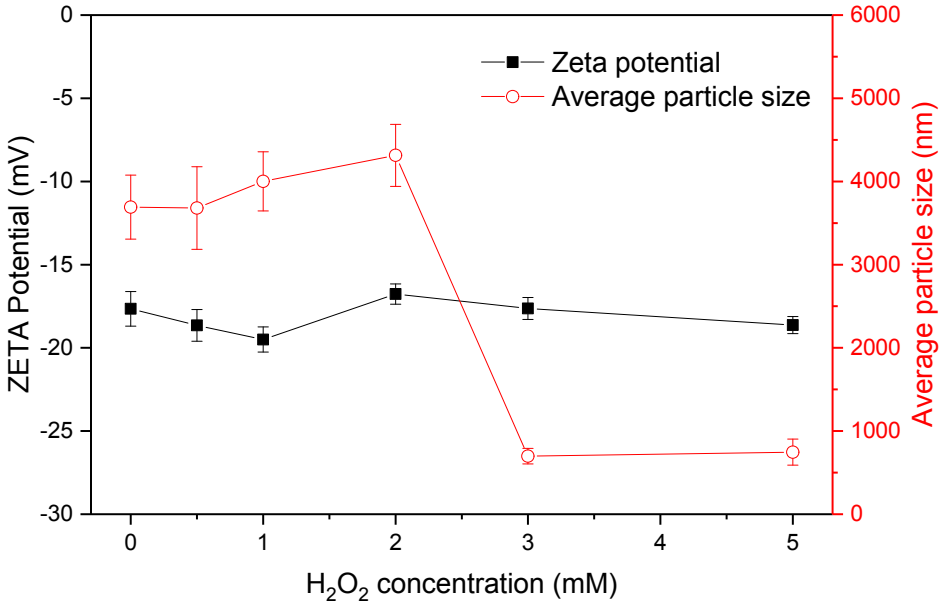

Figure S2. Zeta potential and average particle size of oxidized NZVI at different H_2O_2 concentrations No dissolved Fe(II) concentration was detected under the experimental conditions of this study. Experimental conditions: [NZVI] = 0.2 $g \cdot L^{-1}$, [H_2O_2] = 5 mM, I = 1 mM. pH 9.0 ± 0.2, 20 ±1 °C.

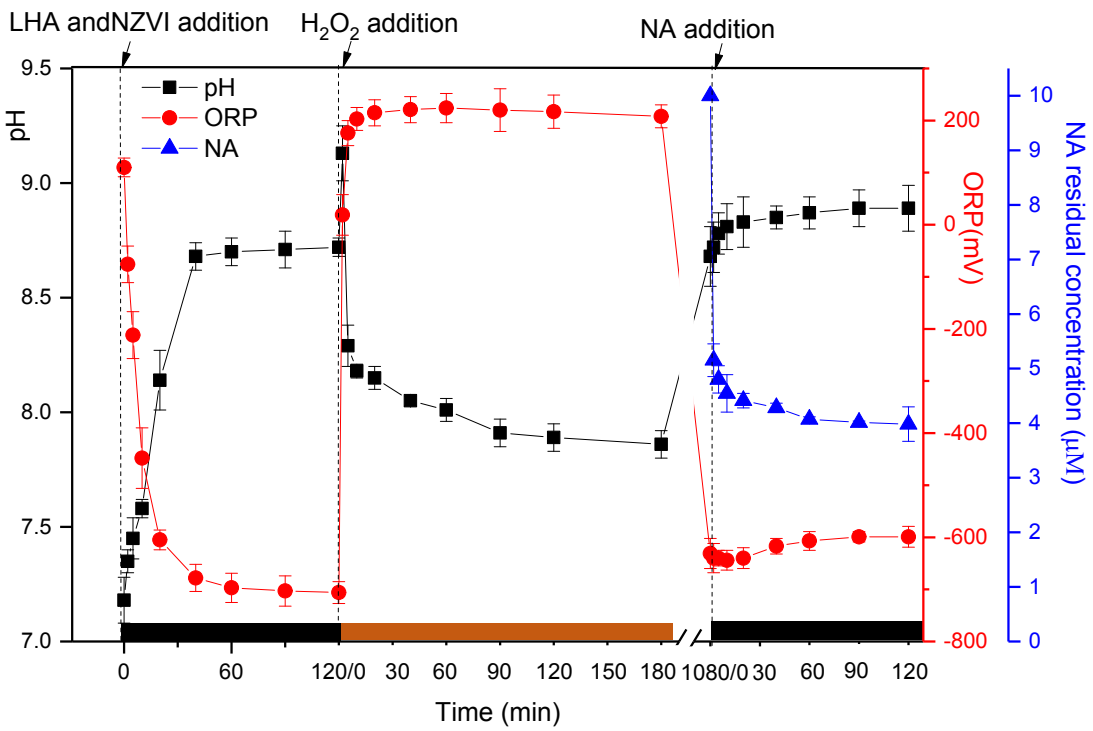

Figure S3. Variations in pH, ORP and NA concentration during NZVI oxidation and adsorption process at 2 mM H_2O_2 concentration with the presence of LHA. Experimental conditions: [LHA] = 5 mg·L^{-1}, [NZVI] = 0.2 g·L^{-1}, [H_2O_2] =2 mM, $[NA]_{initial}$ = 10 μM, 20 ±1 °C.

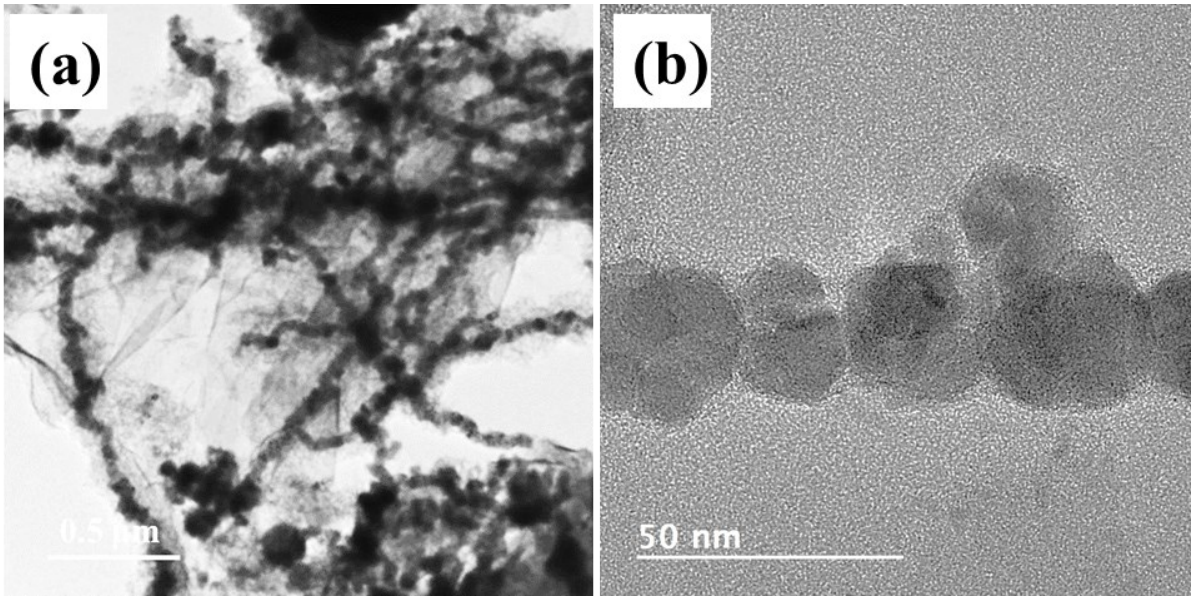

Figure S4. (a) Chain-like structures of oxidized NZVI; (b) constitution units of nano chain. Experimental conditions: [NZVI]= 0.2 $g \cdot L^{-1}$, $[H_2O_2]$ = 5 mM, 18h oxidation time, , 20 ±1 °C.

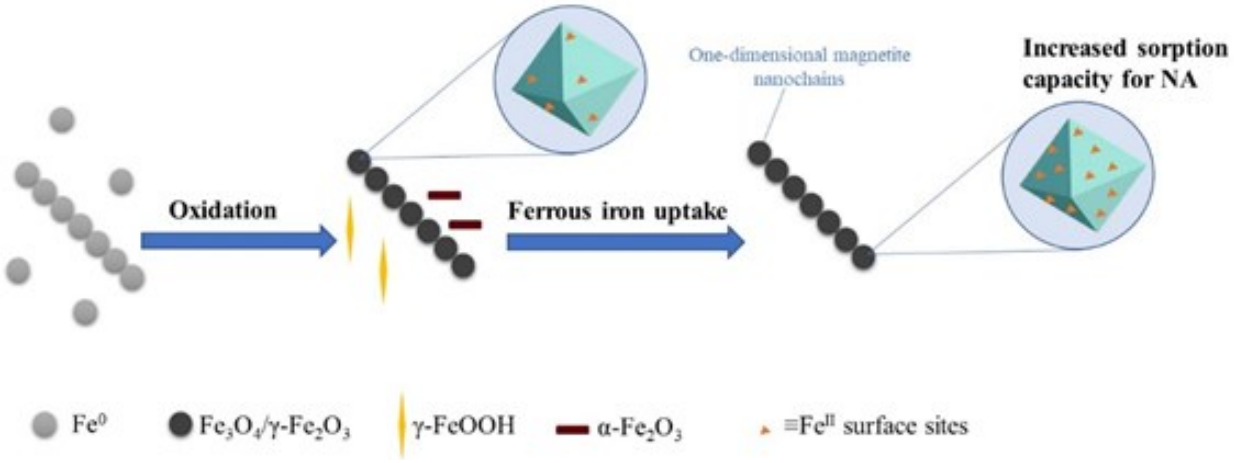

Figure S5. Schematic illustrating the oxidation process of NZVI by H_2O_2

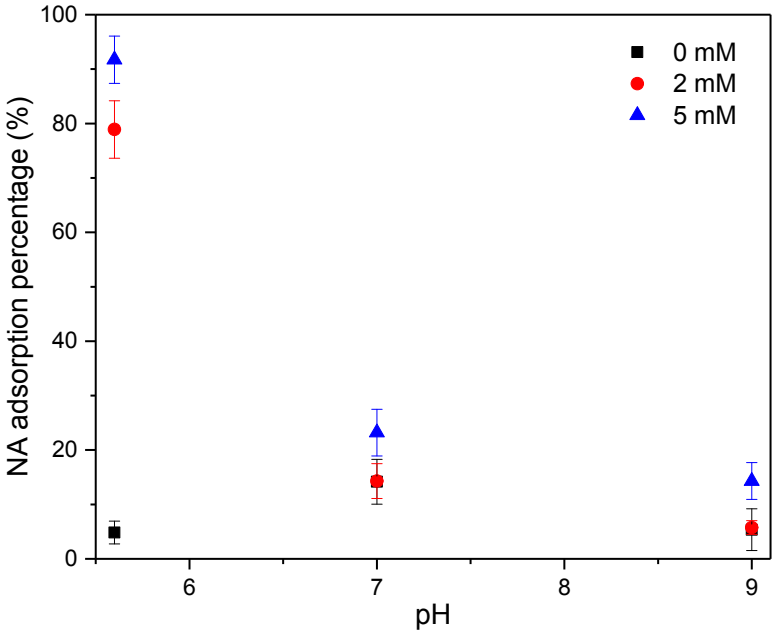

Figure S6. NA removal by the oxidized NZVI particles at two H_2O_2 concentrations in buffered systems. Experimental conditions: [NZVI]= 0.2 $g \cdot L^{-1}$, [MES]=10 mM, [HEPES]=10 mM, [TRIZMA]=10 mM, $[NA]_{initial}$= 10 μM, 20 ±1 °C.

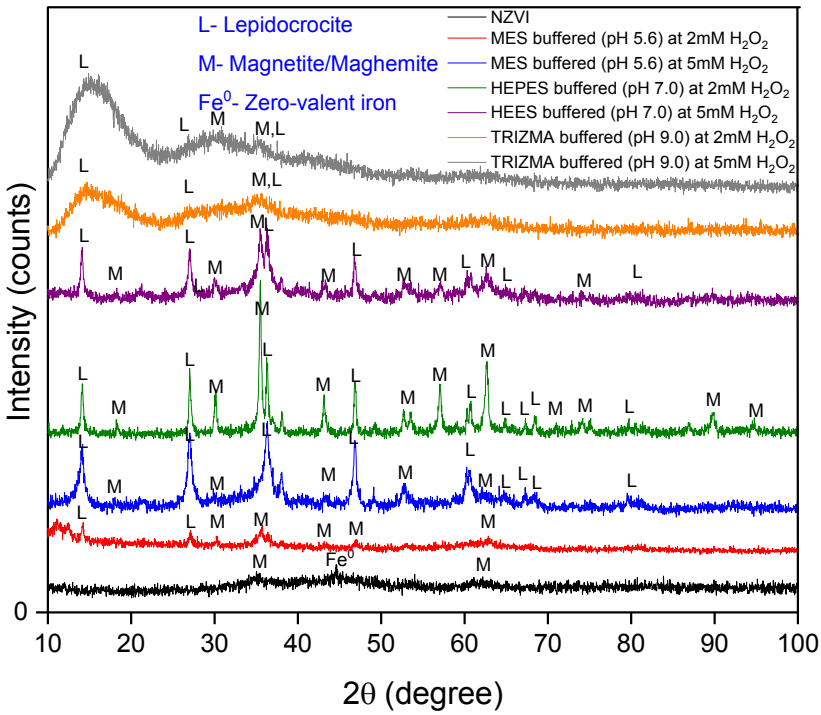

Figure S7. XRD patterns of NZVI oxidation products in buffered systems at two H_2O_2 concentrations. Experimental conditions: [NZVI]= 0.2 g·L^{-1}, [MES]=10 mM, [HEPES]=10 mM, [TRIZMA]=10 mM, $[NA]_{initial}$= 10 μM, 20 ±1 °C.

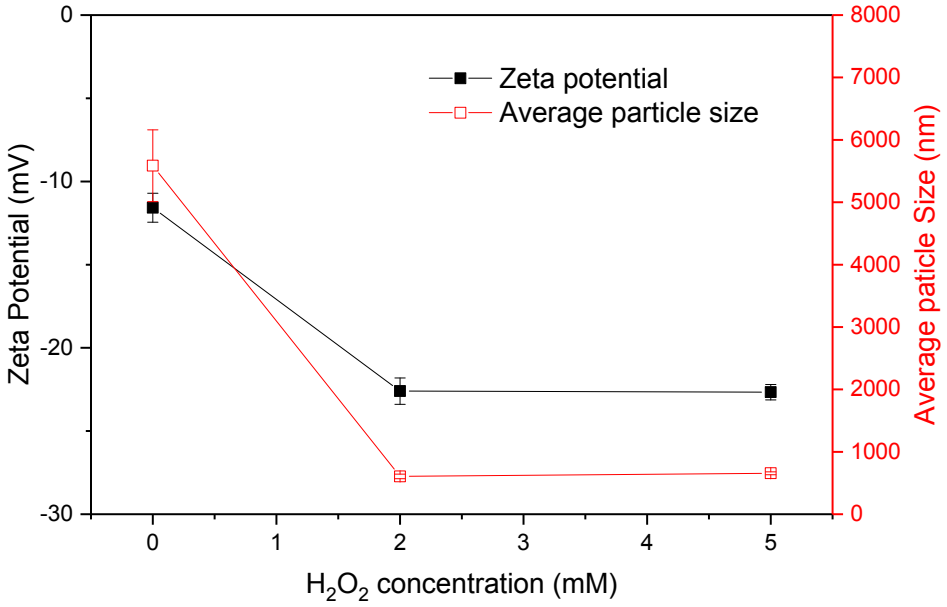

Figure S8. Zeta potential and average particle size of oxidized NZVI in TRIZMA buffered system (pH 9) at two H_2O_2 concentrations. Experimental conditions: [NZVI] =0.2 g/L, [TRIZMA]=10 mM.

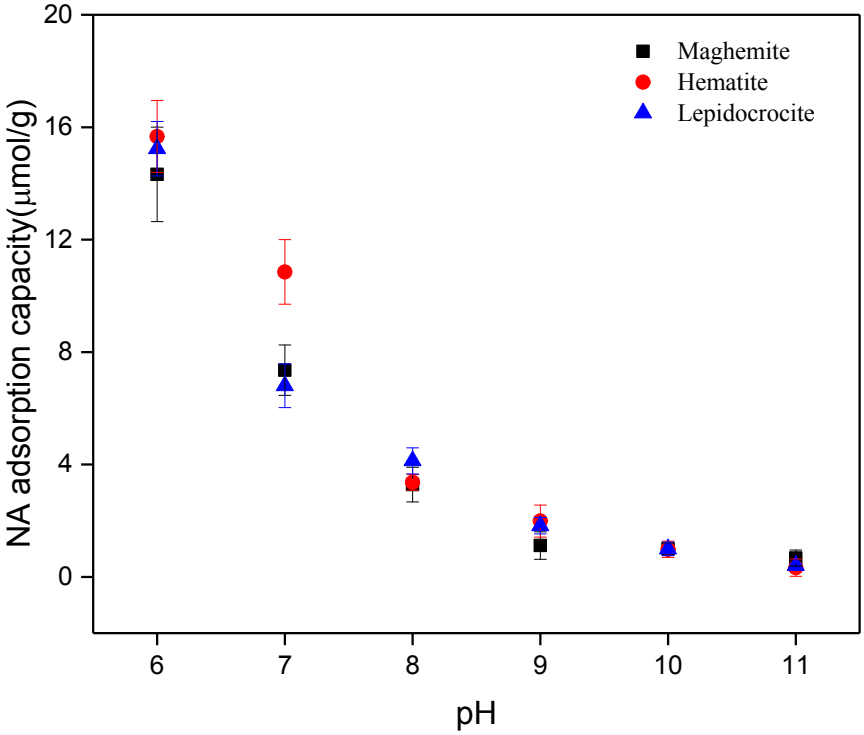

Figure S9. NA adsorption versus pH onto three ferric oxyhydroxides. Experimental conditions: [Maghemite] = 0.2 g·L^{-1}, [Hematite] = 0.2 g·L^{-1}, [Lepidocrocite] = 0.2 g·L^{-1} $[NA]_{initial}$ = 10 μM, 20 ±1 °C.

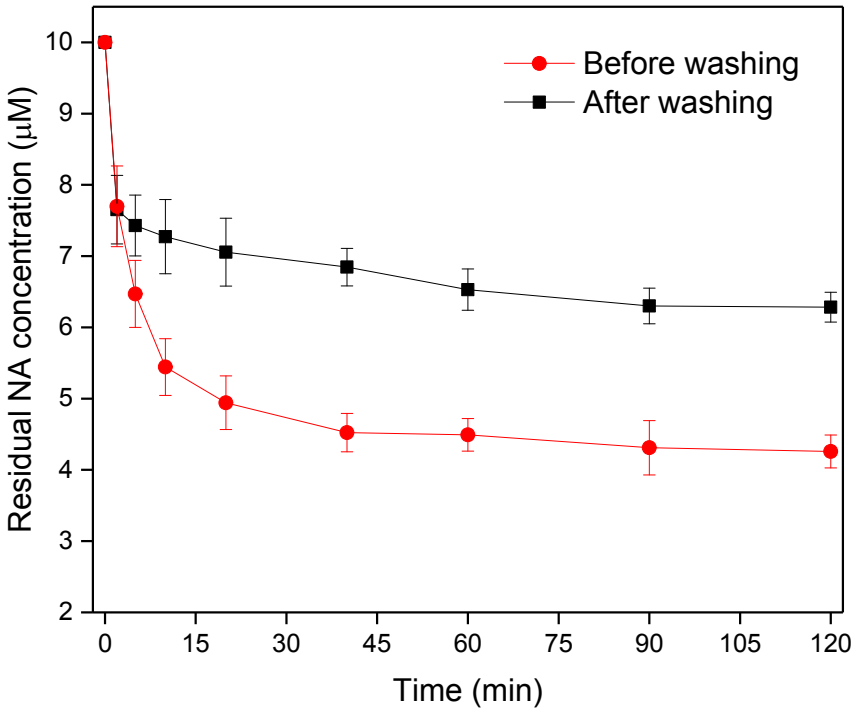

Figure S10. Adsorption kinetics of NA by oxidized NZVI at 5 mM of H_2O_2 before and after surface washing with DDIW. No dissolved Fe(II) concentration was detected under the experimental conditions of this study (*i.e.* pH 9). Experimental conditions: [NZVI]= 0.2 $g \cdot L^{-1}$, $[H_2O_2]$= 5 μM, $[NA]_{initial}$= 10 μM, pH 9.0 ± 0.2, 20 ±1 °C.

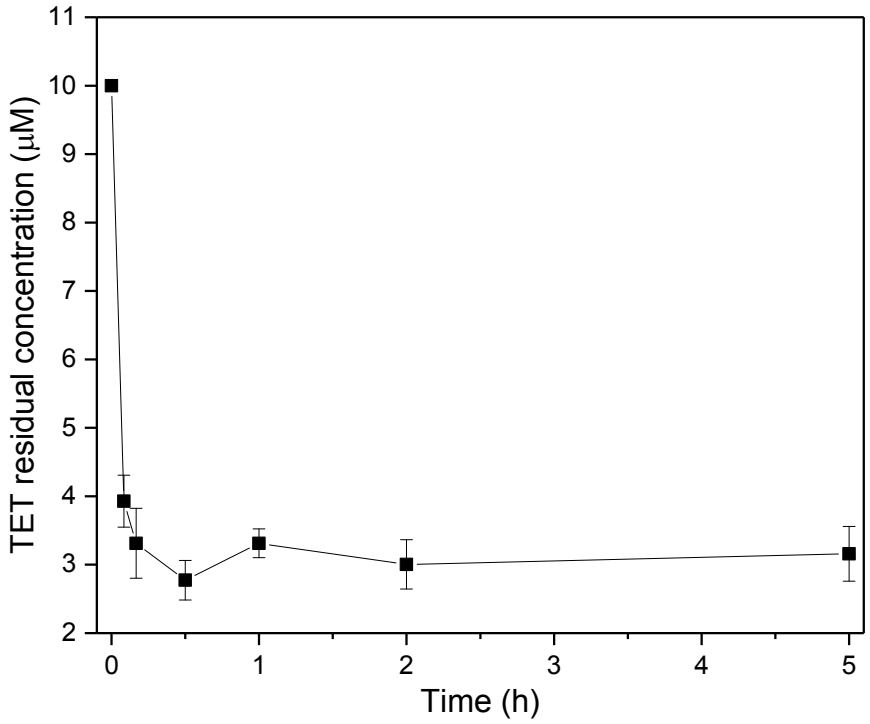

Figure S11. TET removal kinetics by the oxidized NZVI product at 5 mM H_2O_2. Experimental conditions: [NZVI]= 0.2 g·L^{-1}, [H_2O_2]=5 mM, [TET]$_{initial}$= 10 μM, pH 9.0 ± 0.2, 20 ±1 °C.