Supplemental Information

In-situ Activation of Persulfate by Iron Filings and Degradation of 1,4-dioxane

Hua Zhong [a], Mark L Brusseau [*,a,b], Yake Wang [a], Ni Yan [b], Lauren Quig [c], Gwynn R Johnson [c]

[a] Soil, Water, and Environmental Science Department

School of Earth and Environmental Sciences

University of Arizona

Tucson, AZ 85721

[b] Hydrology and Water Resources Department

School of Earth and Environmental Sciences

University of Arizona

Tucson, AZ 85721

[c] Civil & Environmental Engineering

Maseeh College of Engineering & Computer Science

Portland State University

Portland, OR 97201

Water Research

2015

[*]Corresponding author, Brusseau@email.arizona.edu

Table 1S. ICP-MS-based Metal concentrations in bulk solution after contact of 5 mM persulfate solution or pure water with iron filings at a liquid/solid ratio of 10:1 (v/w). The flask reactor was shaken at 200 rpm, 30±1°C. The metals with concentration lower than 0.01 mg/L are not included.

Analyte	1 h contact	24 h contact	24 h contact with water
Metals measured by ICP-MS method (mg/L)			
Na	195.84	186.56	1.52
Fe	168.26	115.97	0.14
Mn	5.96	9.53	0.01
Ca	0.61	0.69	0.05
Ni	0.51	0.05	0.00
K	0.50	0.65	0.29
Mg	0.30	0.44	0.03
Ba	0.03	0.02	0.00
Co	0.02	0.01	0.00
Zn	0.01	0.01	0.00
Mo	0.00	0.03	0.00
Cu	0.00	0.01	0.00
Sulfur and iron species measured by spectrophotometric method (mg/L)			
Fe^{2+}	111.74	82.77	0.12
Fe^{3+}	102.45	55.38	-0.04
Total Fe	214.19	138.15	0.08
pH	4.70	5.28	6.42

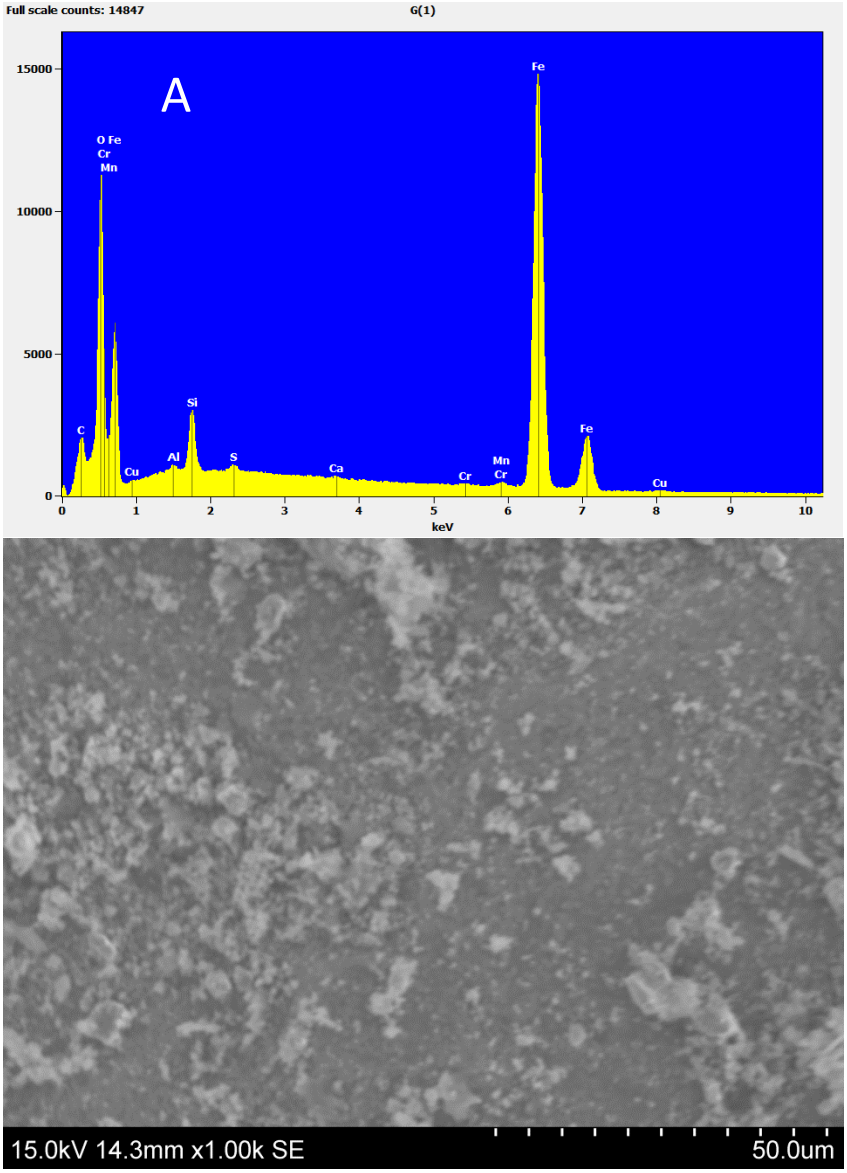


Figure S1. (A) SEM-EDS spectroscopy and the image of scanned area for iron filing sample.

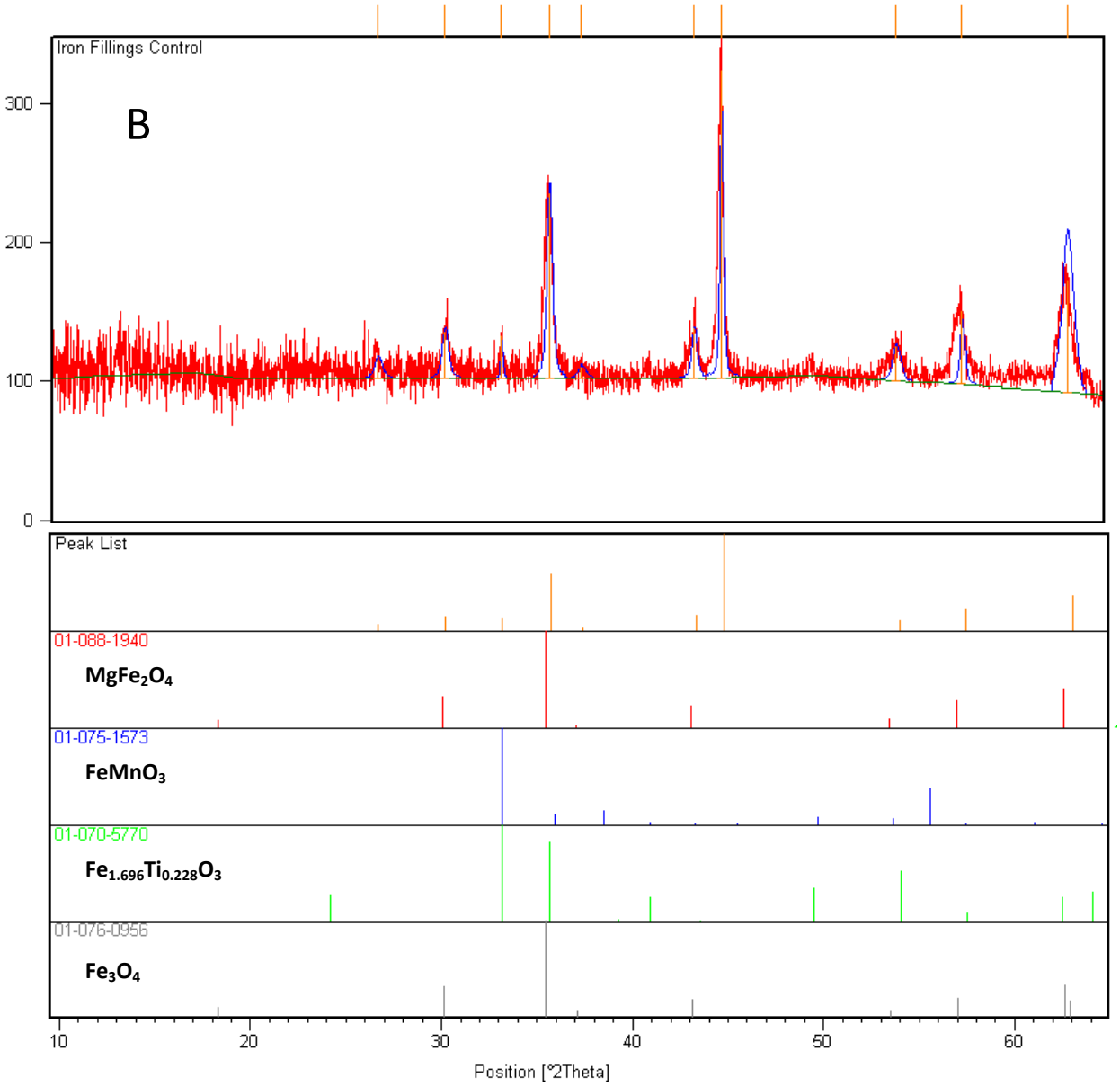


Figure S1. (B) XRD spectroscopy and identified minerals for iron filing sample.

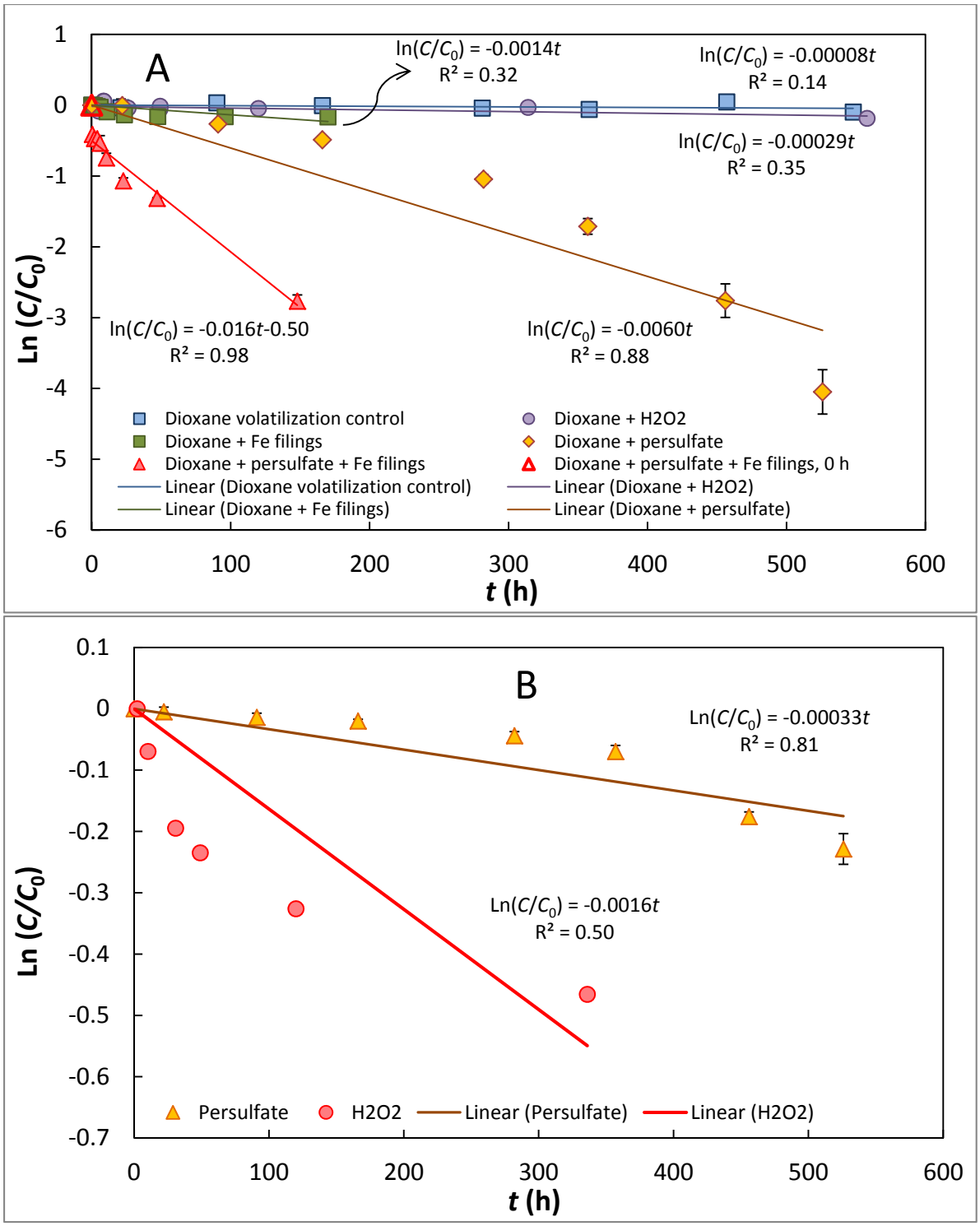


Figure S2. (A) Degradation of dioxane and (B) oxidant decomposition in batch reaction system. The initial dioxane concentration is approximately 0.5 mM. The persulfate or H_2O_2 concentration is approximately 5 mM.

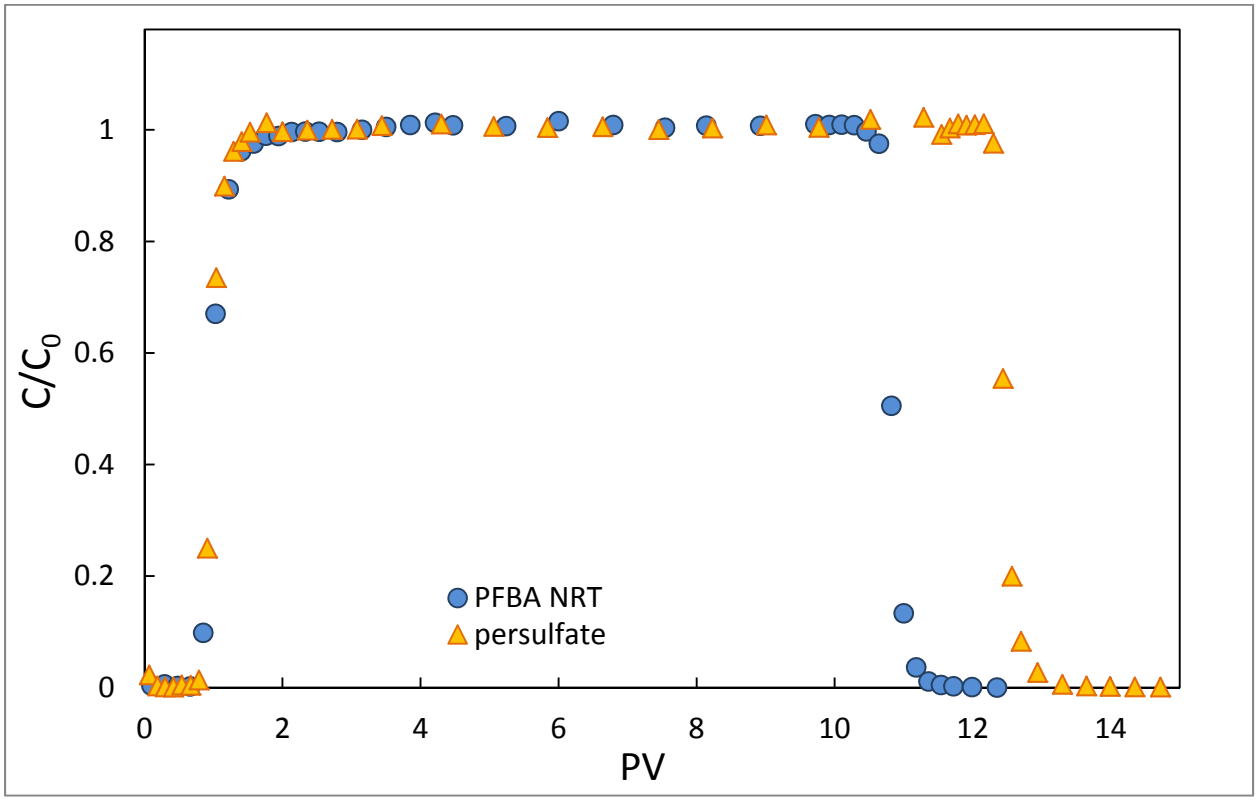


Figure S3. Breakthrough curves of non-reactive tracer pentafluorobenzoate (PFBA NRT) and persulfate in sand-packed column.

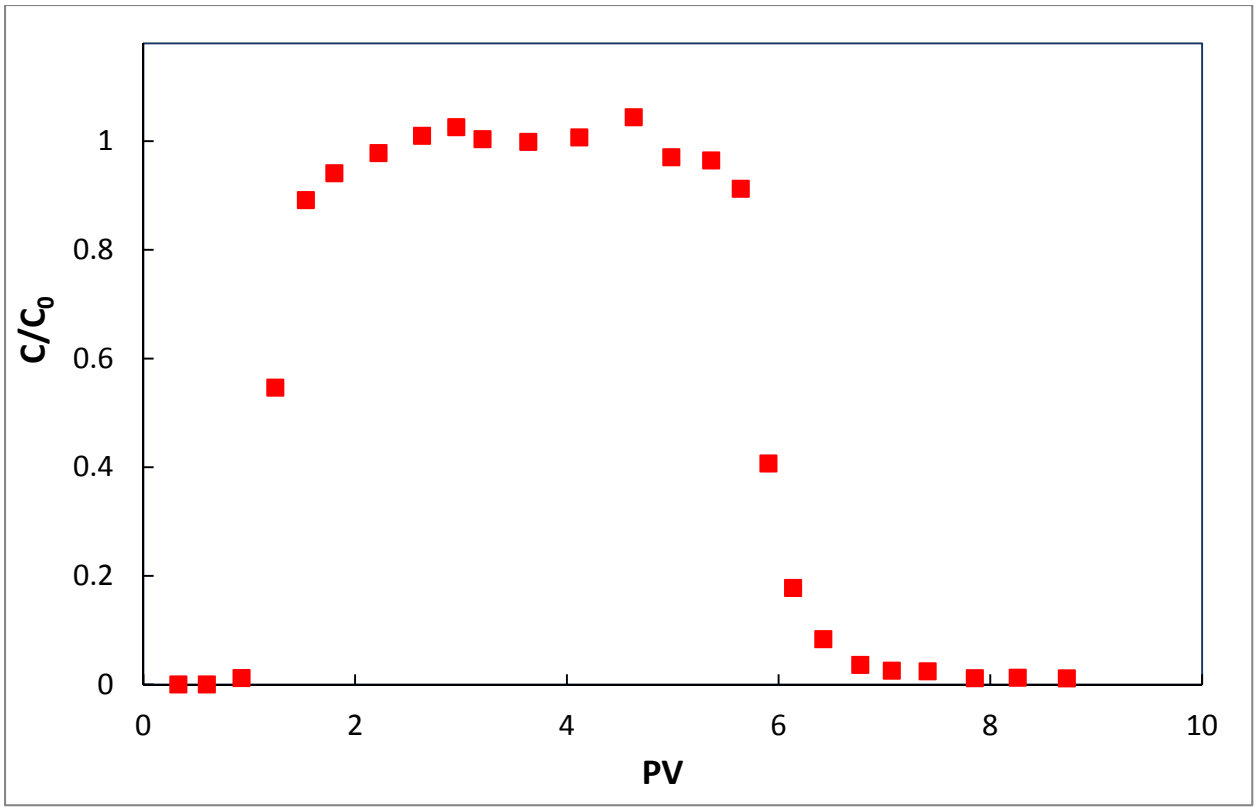
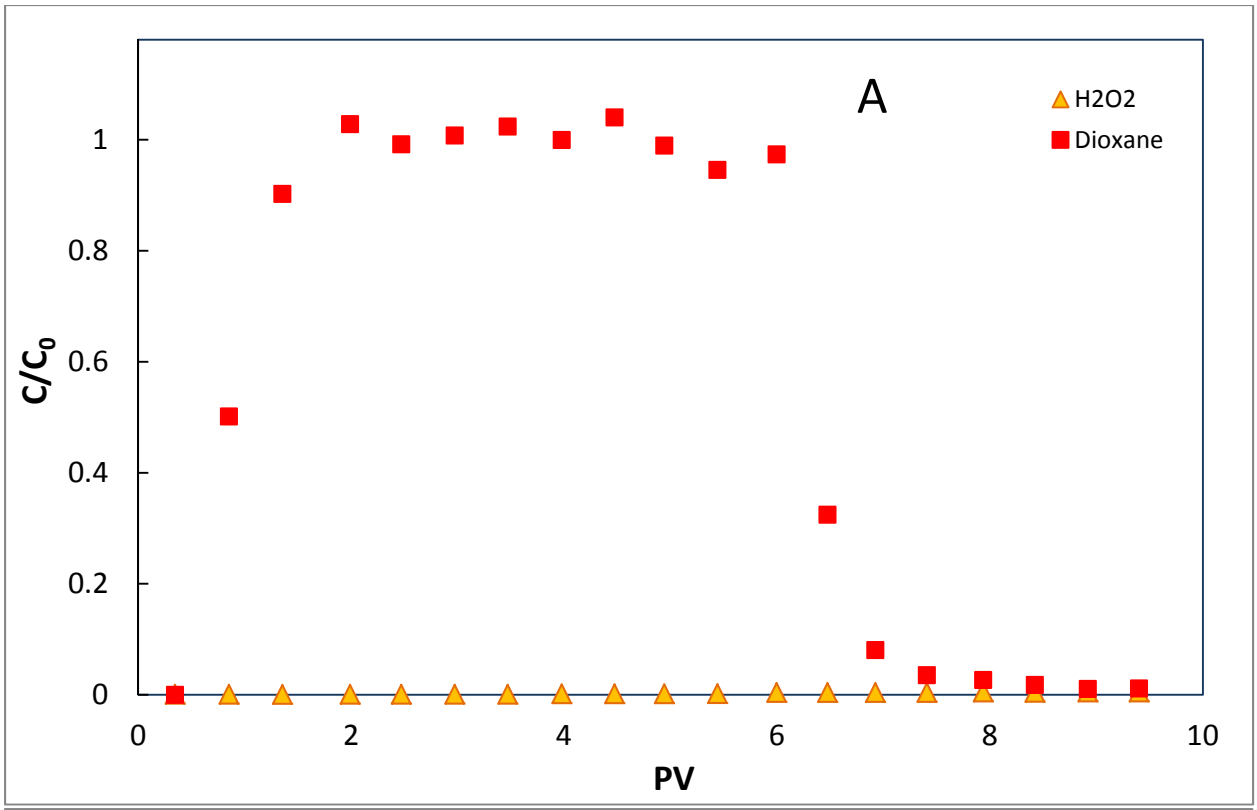
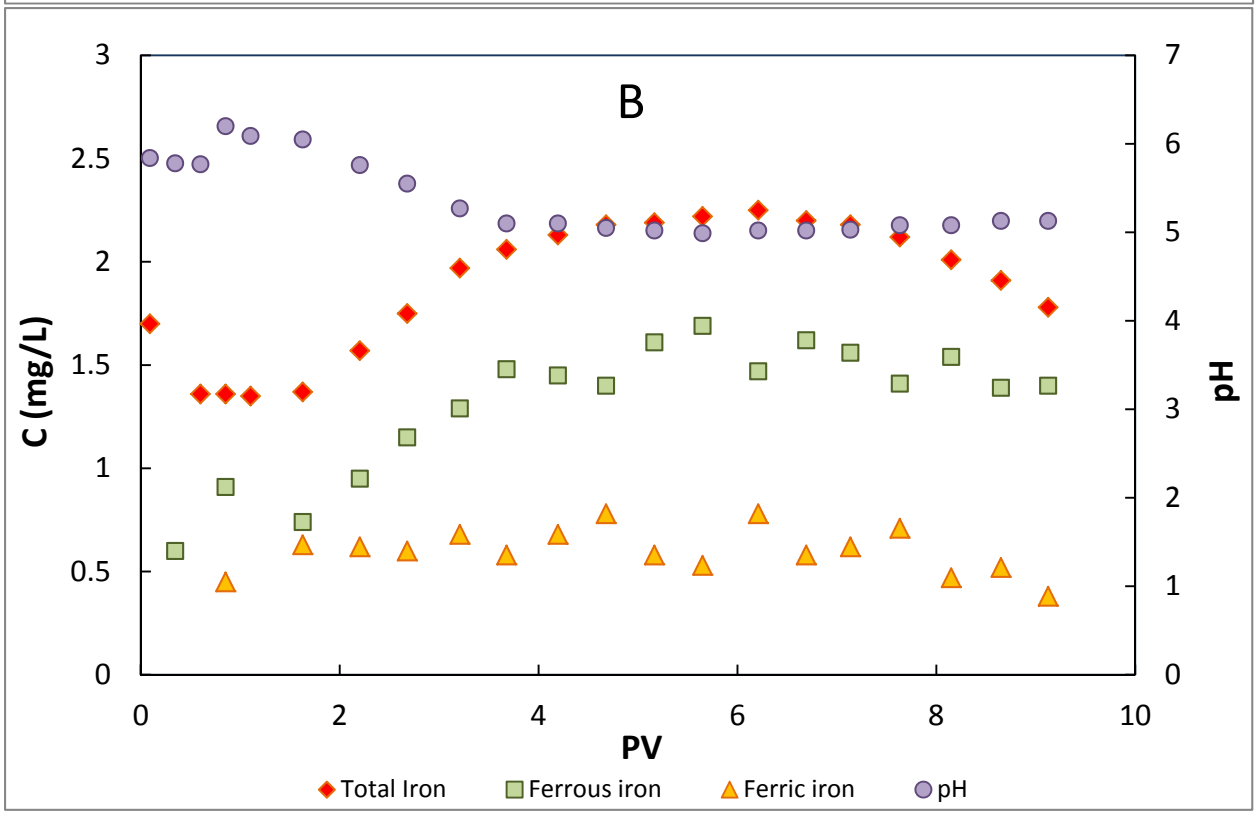


Figure S4. Breakthrough curve of dioxane in the iron-filing-packed column in the absence of oxidants. Influent dioxane concentration is approximately 0.5 mM. Pore-water velocity is 3.0 cm/h.


A
H2O2
Dioxane
C/C0
PV
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10


B
C (mg/L)
pH
PV
Total Iron
Ferrous iron
Ferric iron
pH
0
0.5
1
1.5
2
2.5
3
0
1
2
3
4
5
6
7
0
2
4
6
8
10

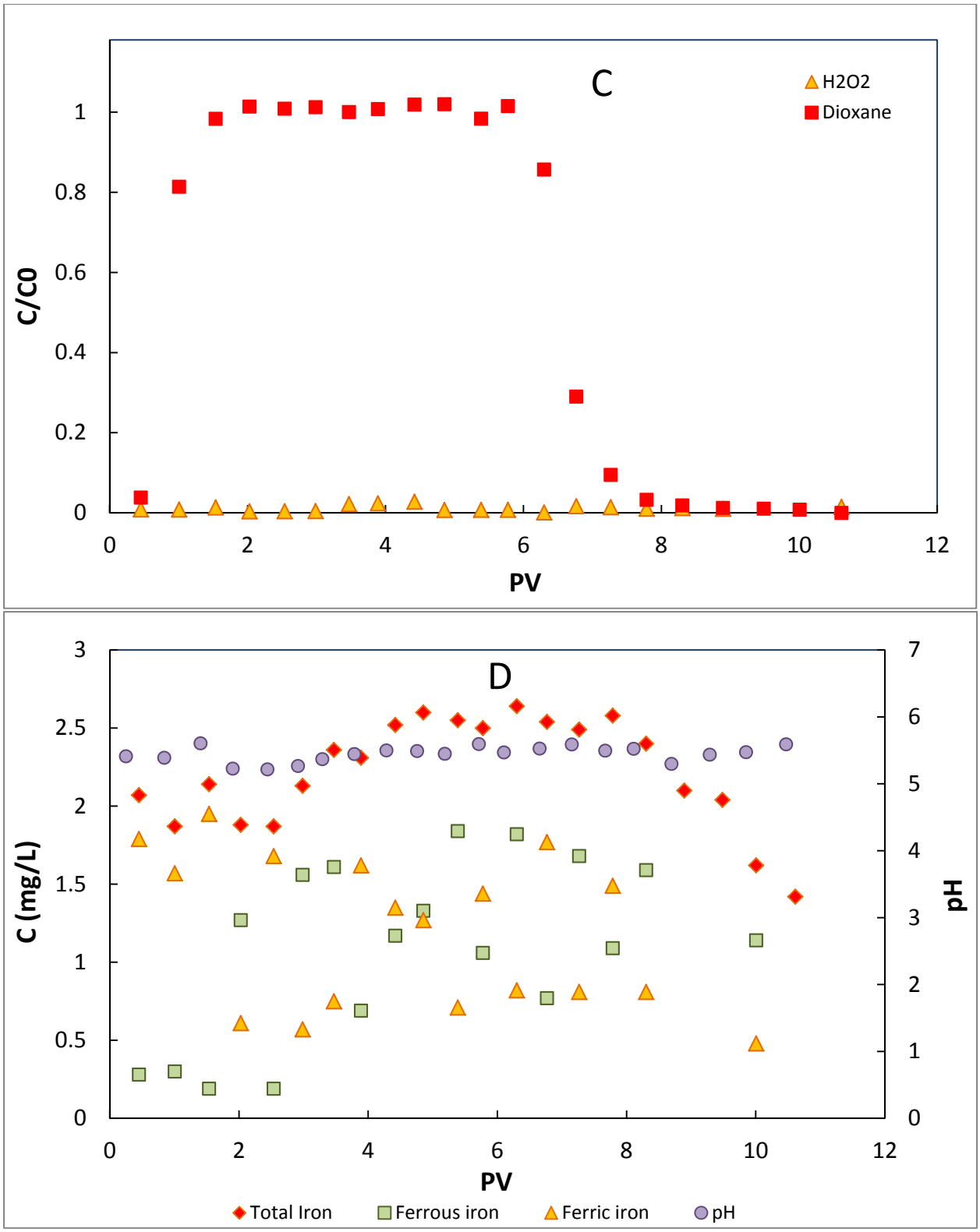


Figure S5. Degradation of dioxane by H_2O_2 in iron-filing-packed column and the related solution chemistry. Influent H_2O_2 and dioxane concentrations are 5 mM and 0.5 mM, respectively. (A) Breakthrough curves of H_2O_2 and dioxane at the pore-water velocity of 31 cm/h. (B) Concentration of

iron species and pH in the effluent at the pore-water velocity of 31 cm/h. (C) Breakthrough curves of H_2O_2 and dioxane at the pore-water velocity of 3.0 cm/h. (D) Concentration of iron species and pH in the effluent at the pore-water velocity of 3.0 cm/h.

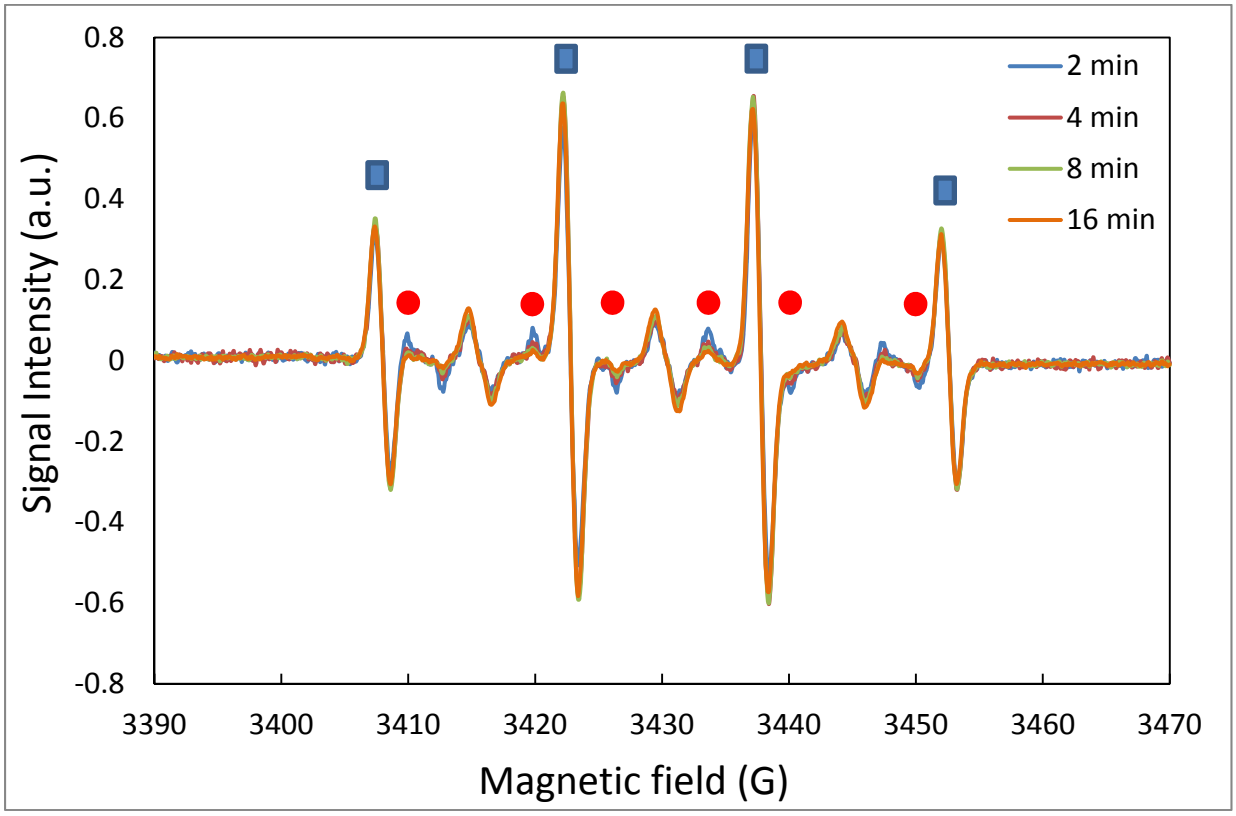


Figure S6 EPR spectra of persulfate solution over time. ■ DMPO-OH; ● DMPO-SO_4.

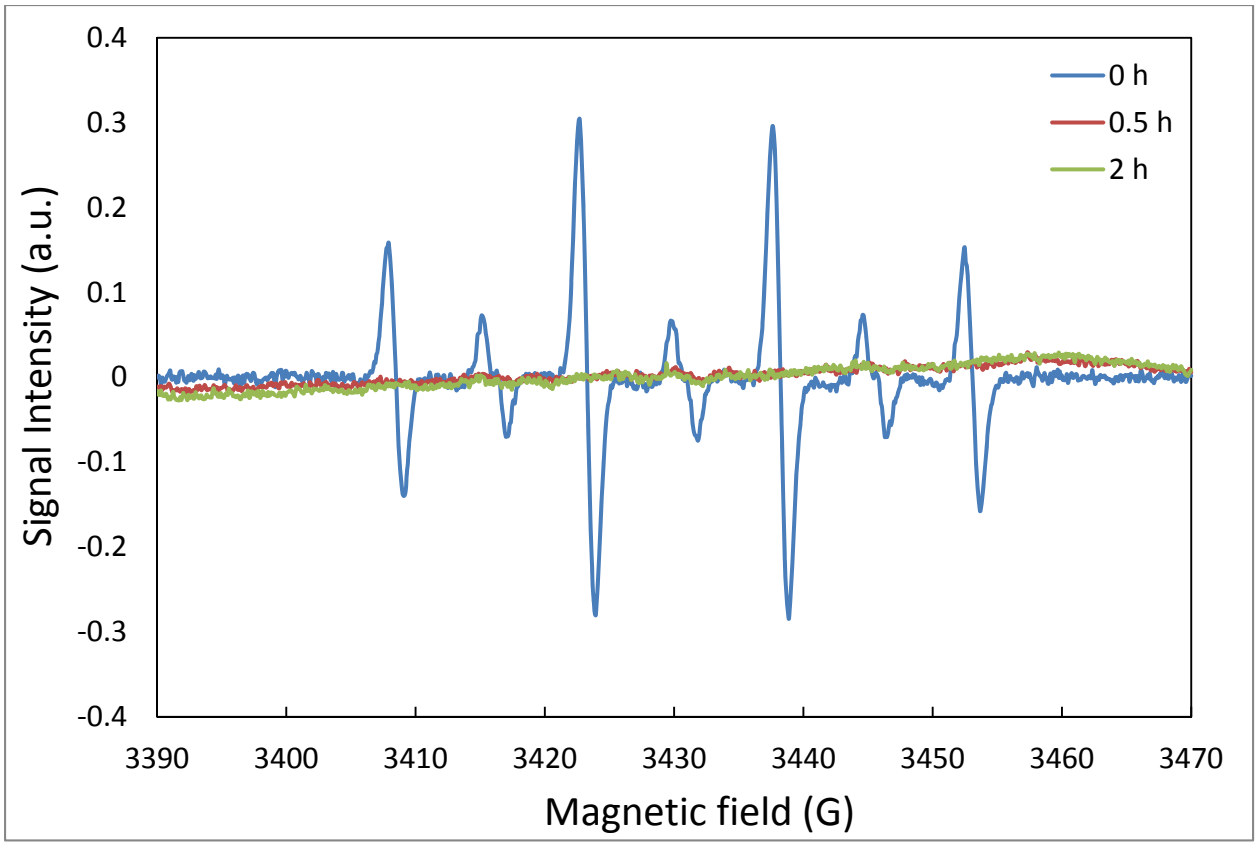


Figure S7. EPR spectra of the solution in persulfate-dioxane-iron filing batch reaction system.