

Supporting Information

Reduction of PCE and TCE by Magnetite Revisited

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Analytical methods for chlorinated ethenes and reduction products

PCE and TCE were quantified with GC-ECD after a liquid-liquid extraction of 0.25 to 1 mL of sample containing both the aqueous and solid phases added to 2 mL of hexanes. The ECD column was a Supelco Equity-5 (0.25 mm diameter x 30 m length, 0.5 μm film thickness). The carrier gas was nitrogen at a constant total flow velocities of 1.0 mL/min and a 10:1 inlet split ratio. The detector make-up gas was 95% Argon: 5% methane with flow of 30 mL/min. The oven was programmed for an initial hold of 1 min at 45 $^{\circ}\text{C}$, then 10 $^{\circ}\text{C}/\text{min}$ to 200 $^{\circ}\text{C}$. The ECD method detection limits are 0.05 $\mu\text{moles}/\text{L}$ PCE and 0.02 $\mu\text{moles}/\text{L}$ TCE for ($n = 15$).

The daughter products ethane, ethylene, acetylene, the dichloroethenes, and vinyl chloride were detected using a GC-FID. The column used was an Agilent GS-GasPro column (0.320 mm diameter x 30 m length). The carrier gas was nitrogen at a constant total flow of 1.4 mL/min and 7.5:1 inlet split ratio. The detector air flow was 450 mL/min, hydrogen flow 40 mL/min, and make-up gas type was nitrogen and a combined flow rate of 35 mL/min. The oven was set for an isothermal run of 4.5 min at 70 $^{\circ}\text{C}$. The C_2 gas analysis was done with 100 μL headspace injections into the column. The detection limits for the FID method are 1.35 $\mu\text{moles}/\text{L}$ ethane, 1.36 $\mu\text{moles}/\text{L}$ ethylene and 1.34 $\mu\text{moles}/\text{L}$ acetylene for ($n = 10$). Products with carbon number $>\text{C}_2$ were not analyzed in this study. We used Henry's law and the specific dimensionless coefficient H^{cc} to calculate dissolved C_2 gases and headspace PCE and TCE.¹ The averaged values for the H^{cc} are as follows: PCE = 1.54, TCE = 2.447, Ethane = 0.0471, and Ethylene = 0.146 and Acetylene = 1.016.¹

Calculation of k_{field} and $t_{1/2\text{-field}}$

In order to estimate field rates for PCE and TCE reduction, we have calculated a k_{field} value (in yr^{-1}) following a scheme used in Wiedemeier et al.² In that study, the authors used magnetic susceptibility data to calculate the amount of magnetite in their field samples. They used a value for the magnetic susceptibility of their field sediments of $4 \times 10^{-8} \text{ m}^3/\text{kg}$. They then used this value to derive the amount of magnetite per kg of aquifer material based on the magnetic susceptibility of magnetite ($1.117 \times 10^{-3} \text{ m}^3/\text{kg}$), the density of magnetite ($5,170 \text{ kg}/\text{m}^3$), and the bulk density of an aquifer sediment ($1,700 \text{ kg}/\text{m}^3$). Based on this calculation, estimated magnetite concentrations were $\sim 0.1 \text{ g magnetite}/\text{kg sediment}$. The maximum magnetic susceptibility that they report in their paper is $\sim 1 \times 10^{-6} \text{ m}^3/\text{kg}$. Based on their magnetic susceptibility data, one could expect masses of magnetite from 0.1 g to 10 g/kg.

Using this value, we calculated the in-aquifer 1st order decay constant (k_{aquifer}) based on our rate constant for PCE and TCE degradation:

For example, the average k_{SA} for our pH ~ 8.0 , 5 g/L magnetite, $\sim 10 \text{ mM Fe(II)}$ experiments is:
 $k_{\text{SA}} = k_{\text{obs}}/\text{SA} = 1.9 \times 10^{-8} \text{ s}^{-1}/(5 \text{ g/L} \cdot 60 \text{ m}^2/\text{g}) \cdot 3.1536 \times 10^7 \text{ s/year} = 2.0 \times 10^{-3} \text{ L m}^{-2} \text{ yr}^{-1}$

Assuming $\rho_{\text{bulk}} = 1700 \text{ kg}/\text{m}^3$, effective porosity: $\eta_e = 0.2$, that the aquifer magnetite specific surface area is consistent with that used in our study ($\text{SSA} \sim 60 \text{ m}^2/\text{g}$), and 1 g magnetite/kg sediment (m_{mag}):

$$k_{field} = \frac{m_{mag} \cdot \rho_{bulk} \cdot SSA_{mag} \cdot k_{SA}}{\eta_e} \times \frac{1m^3}{1000 L}$$

$$k_{field} = 1 \frac{\text{g magnetite}}{\text{kg sediment}} \times 1,700 \frac{\text{kg sediment}}{\text{m}^3} \times 60 \frac{\text{m}^2}{\text{g}} \times \frac{1}{0.2} \frac{\text{m}^3 \text{ sediment}}{\text{m}^3 \text{ groundwater}} \times 2.0 \times 10^{-3} \frac{\text{L}}{\text{m}^2 \cdot \text{yr}} \times \frac{1m^3}{1000 L} = 1.0 \text{ yr}^{-1}$$

We estimate $k_{field} = 1.0 \text{ yr}^{-1}$. Which gives a half-life of $\ln(2)/1 = 0.69$ year.

Table S1. PCE/TCE with Magnetite alone

[C] ₀ (μM) ^a	pH	Mass loading (g/L)	Stoichiometry			% loss ^b	% Products ^b	% C recovery ^b	Duration (days) ^b
			x _{ms}	x _d	x _{XRD}				
PCE									
~50 ^c	7.5	5	0.50	0.55 ± 0.02	0.53	7.0	0	88	139
~50 ^c	7.5	5	0.50	0.55 ± 0.02	0.53	7.0	0	97	139
~50 ^c	7.5	5	0.50	0.55 ± 0.02	0.53	6.9	0	101	105
~50 ^c	7.5	5	0.50	0.55 ± 0.02	0.53	6.87	0	96	105
~50 ^c	7.5	5	0.50	0.55 ± 0.02	0.53	6.87	0	106	105
TCE									
48	7.0	10	0.46	0.5 ± 0.02	n.d. ^d	-10.7	0	111	91
52	7.5	5	0.50	0.55 ± 0.02	0.53	9.9	0	93	56
45	7.5	20	0.46	0.5 ± 0.02	n.d.	-6.3	0	106	140
49	8.0	10	0.45	0.5 ± 0.02	n.d.	-7.8	0	111	91
56 ^e	8.0	5	0.50	n.d. ^d	0.52	-2.3 ^e	0	102 ^e	142 ^e
PCE Control^e									
55	7.5	0	-	-	-	30	0	70	172
TCE Control^e									
55	7.5	0	-	-	-	29	0	71	135

^a [C]₀ is the initial concentration of the analyte spiked within reactor.

^b % products, % analyte loss, and % C recovery are evaluated at the final reported time point.

^c ~50 is the nominal concentration of PCE or TCE added. Calculations in ^b are based on nominal concentrations.

^d n.d. measurement not determined.

^e Averages of triplicate reactors.

TABLE S2. PCE/TCE Magnetite + aqueous Fe(II) reactors with products.

[CE] ₀ ^a μM	pH	Solids loading (g/L)	[Fe(II)] ₀ mM ^b	Saturation Index ^c	[Fe(II)] _f mM ^b	Stoichiometry		% loss ^f	% products ^f	% C recovery ^f	Duration (days)	<i>k</i> _{obs} s ⁻¹	<i>k</i> _{SA} L m ⁻² d ⁻¹	<i>k</i> _{field} ^h yr ⁻¹	<i>t</i> _{1/2 field} years
						<i>x</i> _d ^d	<i>x</i> _{xrd} ^e								
PCE															
53.7	7.9	5	32.9	0.66	29.7	0.52 ± 0.03	0.50	28	6	78	125	6.1 × 10 ⁻⁹	1.8 × 10 ⁻⁶	0.33	2.1
54.0	8.0	5	0.93	-0.72	n.d. ^g	0.54 ± 0.03	0.51	18	3	85	140	2.9 × 10 ⁻⁹	8.4 × 10 ⁻⁷	0.16	4.5
50.1	8.5	5	32.0	1.81	3.60	0.52 ± 0.03	0.50	40	16	76	125	1.7 × 10 ⁻⁸	4.9 × 10 ⁻⁶	0.91	0.76
55.3	8.6	5	7.58	1.30	1.61	0.52 ± 0.03	0.50	41	13	72	125	1.3 × 10 ⁻⁸	3.7 × 10 ⁻⁶	0.70	0.99
53.1	9.0	5	0.86	1.24	n.d.	0.54 ± 0.03	0.51	32	12	80	140	1.0 × 10 ⁻⁸	2.9 × 10 ⁻⁶	0.54	1.3
53.3	9.3	5	7.71	2.71	0.71	0.52 ± 0.03	0.50	32	10	77	125	9.6 × 10 ⁻⁹	2.8 × 10 ⁻⁶	0.52	1.3
45.8	9.4	5	31.4	3.64	3.86	0.52 ± 0.03	0.50	41	15	74	125	1.6 × 10 ⁻⁸	4.6 × 10 ⁻⁶	0.86	0.81
TCE															
55.3	8.0	5	0.82	-0.80	n.d.	0.54 ± 0.03	0.51	28	11	83	139	9.6 × 10 ⁻⁹	2.8 × 10 ⁻⁶	0.97	0.72
50.8	8.0	5	8.23	0.30	4.85	0.53 ± 0.01	0.48	24	24	99	167	1.8 × 10 ⁻⁸	5.2 × 10 ⁻⁶	1.3	0.52
51.6	8.0	5	8.54	0.31	4.23	0.53 ± 0.01	0.48	27	28	101	167	2.1 × 10 ⁻⁸	6.1 × 10 ⁻⁶	1.1	0.62
51.1	7.9	5	9.19	0.15	4.13	0.53 ± 0.01	0.48	26	18	93	167	1.4 × 10 ⁻⁸	4.0 × 10 ⁻⁶	1.2	0.59
49.7	8.0	5	9.19	0.26	5.09	0.53 ± 0.01	0.48	14	24	110	167	1.8 × 10 ⁻⁸	5.2 × 10 ⁻⁶	0.80	0.86
51.1	8.0	5	9.24	0.29	4.34	0.53 ± 0.01	0.48	31	30	99	167	2.5 × 10 ⁻⁸	7.2 × 10 ⁻⁶	0.86	0.81
49.7	8.0	5	9.24	0.27	5.2	0.53 ± 0.01	0.48	29	26	97	167	2.1 × 10 ⁻⁸	6.0 × 10 ⁻⁶	0.75	0.92
50.1	8.0	5	9.42	0.27	5.23	0.53 ± 0.01	0.48	28	30	102	167	2.2 × 10 ⁻⁸	6.3 × 10 ⁻⁶	0.86	0.81
49.8	8.0	5	9.49	0.28	5.48	0.53 ± 0.01	0.48	25	24	99	167	1.5 × 10 ⁻⁸	4.3 × 10 ⁻⁶	2.8	0.25
49.3	8.0	5	9.50	0.28	5.36	0.53 ± 0.01	0.48	22	24	102	167	1.6 × 10 ⁻⁸	4.6 × 10 ⁻⁶	0.97	0.72
50.5	8.0	5	9.52	0.28	4.98	0.53 ± 0.01	0.48	25	19	94	167	1.4 × 10 ⁻⁸	4.0 × 10 ⁻⁶	0.070	9.9
51.1	8.0	5	9.52	0.29	4.18	0.53 ± 0.01	0.48	24	20	97	167	1.6 × 10 ⁻⁸	4.6 × 10 ⁻⁶	0.31	2.3
54	8.0	5	10.0	0.30	n.d.	0.48 ± 0.03	0.56	75	46	71	168	5.2 × 10 ⁻⁸	1.5 × 10 ⁻⁵	0.091	7.6
51.2	8.0	5	10.69	0.41	4.57	0.53 ± 0.01	0.48	27	26	99	167	1.8 × 10 ⁻⁸	5.2 × 10 ⁻⁶	0.49	1.4
61.2	8.0	5	11.2	0.35	n.d.	0.48 ± 0.03	0.56	10	5	94	287	1.3 × 10 ⁻⁹	3.7 × 10 ⁻⁷	0.11	6.2
49.5	7.9	5	31.2	0.64	19.56	0.48 ± 0.03	0.45	-0.8	3	103	69	5.7 × 10 ⁻⁹	1.6 × 10 ⁻⁶	0.19	3.7
69.3	8.4	5	13.1	1.22	n.d.	0.48 ± 0.03	0.56	22	5	83	287	1.7 × 10 ⁻⁹	4.9 × 10 ⁻⁷	0.14	5.0
53.9	8.5	5	0.67	0.13	n.d.	0.54 ± 0.03	0.51	25	11	85	139	9.1 × 10 ⁻⁹	2.6 × 10 ⁻⁶	0.21	3.2
51.1	8.5	5	7.55	1.18	4.18	0.48 ± 0.03	0.45	5	2	97	125	2.1 × 10 ⁻⁹	6.0 × 10 ⁻⁷	0.97	0.72
51.5	8.6	5	32.9	1.94	3.50	0.48 ± 0.03	0.45	4.5	4	99	125	3.5 × 10 ⁻⁹	1.0 × 10 ⁻⁶	1.3	0.52
54.2	9.0	5	7.83	2.24	0.58	0.48 ± 0.03	0.45	13	3	90	125	2.6 × 10 ⁻⁹	7.5 × 10 ⁻⁷	1.1	0.62
52.2	9.1	5	30.9	3.07	1.87	0.48 ± 0.03	0.45	11	4	93	125	4.0 × 10 ⁻⁹	1.2 × 10 ⁻⁶	1.2	0.59

^a [CE]₀ = Initial chloroethylene concentration

^b [Fe(II)]_{0,f} = initial or final Fe(II) concentration, respectively

^c Saturation index = log(IAP/K_{sp}). The ion activity product (IAP) was determined with initial Fe(II) concentration and pH for each experiment. K_{sp} = [Fe²⁺] [OH]² = 5 × 10⁻¹⁵.

^d *x*_d = Magnetite Fe(II)/Fe(III) ratio from dissolution

^e *x*_{xrd} = Magnetite Fe(II)/Fe(III) ratio from x-ray diffraction.

^f % PCE or TCE loss, % Products and % Carbon recovery are taken from the final reported time point.

^g (n.d.) indicates not determined.

^h *k*_{aquifer} calculated with the assumptions: sediment magnetite content = 1 g/kg, ρ_{bulk} = 1700 kg/m³, effective porosity: η_e = 0.2, that the aquifer magnetite specific surface area is 60 m²/g.

TABLE S3. PCE/TCE with Magnetite + aqueous Fe(II) reactors without products.

[C] ₀ ^a (μM)	pH	Mass loading (g/L)	[Fe(II)] ₀ ^b (mM)	Saturation Index ^c	Stoichiometry		% loss ^f	% products ^f	% C recovery ^f	Duration (day)
					x_d ^d	x_{xrd} ^e				
PCE										
51.7	7.5	5	0.88	-1.7	0.54 ± 0.03	0.51	26	0	74	140
~50	7.5	5	2.7	-1.3	0.55 ± 0.02	0.53	10	0	90	78
~50	7.5	5	4.6	-1.0	0.39 ± 0.03	0.54	2.8	0	97	78
65	7.5	17	10.0	-0.70	0.50 ± 0.06	n.d. ^g	-24.5	0	125	91
~70	7.5	17	25.0	-0.30	0.50 ± 0.06	n.d.	-14.5	0	115	91
48.9	8.0	5	7.47	0.21	0.52 ± 0.03	0.5	6.4	0	96	125
TCE										
22 ^h	6.1	147	201 ^h	-2.0	0.43	n.d.	3.8	0	96	104
51	7.5	20	10.0	-0.70	0.50 ± 0.06	n.d.	4.0	0	96	128
50.5	7.5	20	25.0	-0.30	0.50 ± 0.06	n.d.	-2.0	0	102	128
55.2	8.1	5	8.11	0.45	0.48 ± 0.03	0.45	6	0	94	195
55.9	7.5	5	0.92	-1.7	0.54 ± 0.03	0.51	26	0	74	139

* The magnetite Fe₃O₄ mineral used in the reactor was freshly precipitated and not freeze dried.

^a [C]₀ = Initial chloroethylene concentration

^b [Fe(II)]₀ = initial Fe(II) concentration, respectively

^c Saturation index = log(IAP/K_{sp}). The ion activity product (**IAP**) was determined with initial Fe(II) concentration and pH for each experiment. $K_{sp} = [Fe^{2+}] [OH^-]^2 = 5 \times 10^{-15}$.³

^d x_d = Magnetite Fe(II)/Fe(III) ratio from dissolution

^e x_{xrd} = Magnetite Fe(II)/Fe(III) ratio from x-ray diffraction.

^f % **PCE or TCE loss**, % **Products** and % **Carbon recovery** are taken from the final reported time point.

^g (**n.d.**) indicates not determined.

^h 22 g of a mixture of freeze dried magnetite with the stoichiometry determined by a weighted average.



Figure S1. Photographs of reactors containing 5 g/L magnetite reacted with low Fe(II) (~1 mM, left) and high Fe(II) (~10 mM, right). The solids on the right contain white $\text{Fe}(\text{OH})_2(\text{s})$. Conditions: 10 mM MOPS buffer at pH 8.0, and 50 μM TCE.

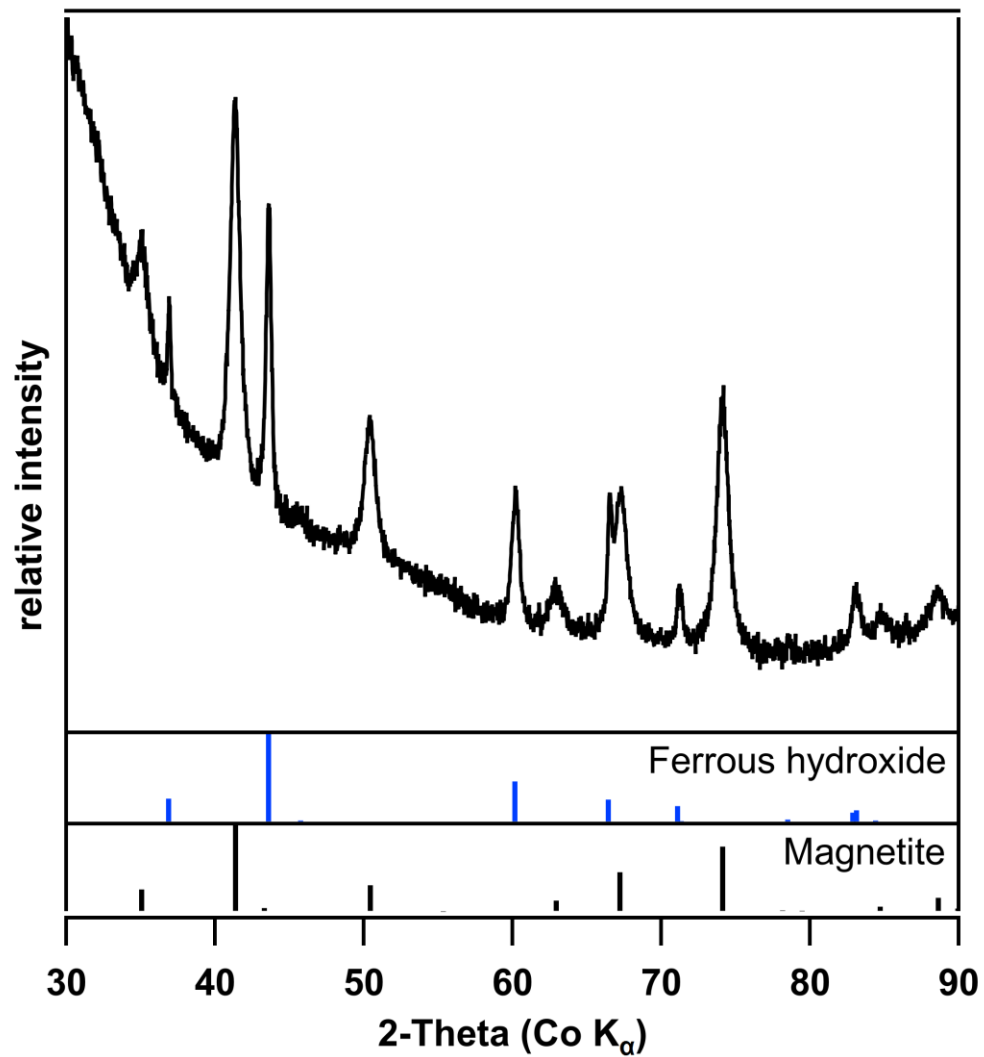


Figure S2. X-ray diffraction pattern of a TCE reactor with magnetite and Fe(II) where 30.0% products were observed after 167 days. Blue bars indicate ferrous hydroxide and black bars indicate magnetite. The background at $2\theta < 60^\circ$ is from the Kapton film used to seal the sample from air. Experimental conditions: 51 μ M TCE, 10 mM MOPs/NaCl, 9.2 mM Fe(II), pH 8.0.

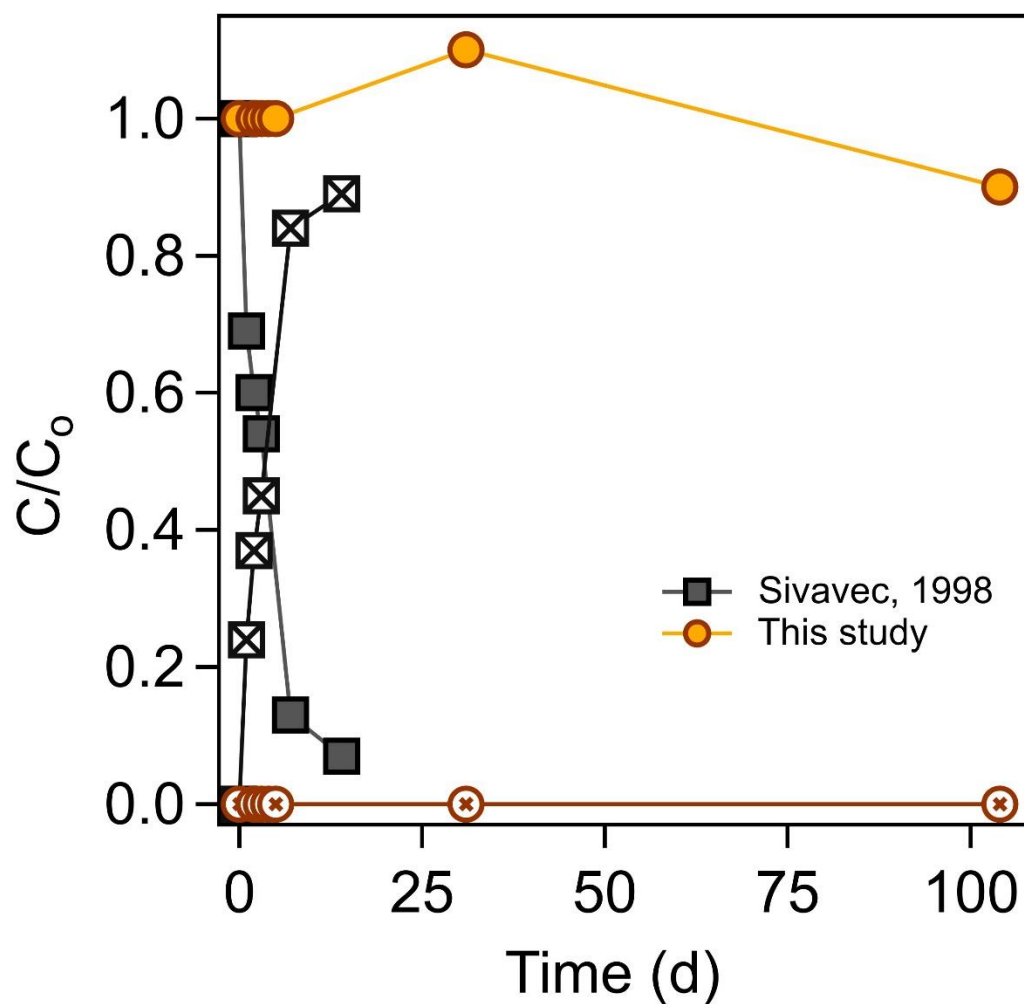


Figure S3. TCE reduction (or lack thereof) as reported in the Sivavec patent⁴ and our attempt to reproduce the data under similar conditions. **Sivavec:**⁴ 7.0 μM TCE, 217 g/L Fe_3O_4 (s), 200 mM Fe(II), pH 6.0. **This study:** 22 μM TCE, 147 g/L Fe_3O_4 (s), 201 ± 12 mM Fe(II), 10 mM MOPs/NaCl, pH 6.1

Table S4. PCE/TCE with aqueous Fe(II) alone and no products

[C] ₀ ^a (μM)	pH	[Fe(II)] ₀ ^b (mM)	Saturation Index ^c	[Fe(II)] _f ^b (mM)	% loss ^d	% products ^d	% C recovery ^d	Duration (day)
PCE								
58.2	7.0	0.3	-3.0	0.16	20	0	80	138
55.2	7.0	1.03	-2.7	1.08	29.6	0	82	134
53.3	7.0	7.79	-1.8	7.52	19.1	0	81	117
50.2	7.0	27.41	-1.3	n.d. ^e	16	0	84	140
56.1	7.5	1.03	-1.6	1.06	20.4	0	70.4	134
51.2	7.5	7.52	-0.78	7.17	17.7	0	82	117
49.2	7.5	13.52	-0.52	n.d.	13	0	87	140
50.3	7.5	27.32	-0.28	n.d.	14	0	78	140
56.3	7.6	0.21	-2.3	0.21	26.1	0	74	138
57.2	8.0	1.03	-0.62	1.04	16.4	0	80	134
57	8.1	0.2	-1.2	0.18	21.9	0	78	138
53.6	8.5	1.01	0.35	1.02	16.4	0	84	134
59.1	8.6	0.23	-0.22	0.2	8.5	0	92	138
51.4	8.6	7.67	1.3	1.56	15.9	0	84	117
57	9.1	0.28	0.93	0.14	19	0	81	138
52.7	9.1	1.07	1.4	0.37	15.6	0	85	134
55.7	9.2	7.58	2.5	1.15	25.2	0	75	117
TCE								
49.4	7.0	6.71	-1.9	8.08	1	0	99	117
54.1	7.0	26.54	-1.3	n.d.	21	0	79	140
51.9	7.1	0.34	-3.0	0.33	1	0	99	138
53.3	7.1	1.06	-2.5	1.02	4.1	0	96	134
53.5	7.5	1.04	-1.6	1.08	4.1	0	96	134
52.6	7.5	13.13	-0.59	n.d.	14	0	86	140
56.9	7.5	28.16	-0.25	n.d.	16	0	84	140
53	7.6	0.23	-2.2	0.2	2.4	0	98	138
51.1	7.6	7.59	-0.70	7.64	1	0	99	117
51.7	8.0	1.01	-0.71	1.06	2.2	0	98	134
66.3	8.0	9.84	0.29	n.d.	23.5	0	77	75
152.9	8.0	9.9	0.30	n.d.	-36.6	0	33.2	75
~50 ^f	8.0	10.27	0.31	n.d.	2.3	0	98	75
~50 ^f	8.0	11.54	0.36	n.d.	3.1	0	97	75
79.9	8.0	11.64	0.37	n.d.	35	0	65	75
~50 ^f	8.0	11.79	0.37	n.d.	6.3	0	94	75
52.5	8.1	0.2	-1.2	0.24	11.1	0	89	138
53.5	8.1	7.71	0.21	6.27	5.5	0	95	117
53.8	8.5	0.16	-0.43	0.25	4.5	0	96	138
52.7	8.5	1.03	0.35	1	2.7	0	97	134
52.8	8.5	7.48	1.2	1.99	6.5	0	94	117
52.1	9.0	0.21	0.55	0.16	1.1	0	99	138
53.9	9.1	1.04	1.4	0.46	6.3	0	94	134
52	9.1	7.23	2.3	0.88	2.7	0	97	117

^a [C]₀ = Initial chloroethylene concentration

^b [Fe(II)]_{0,t} = initial or final Fe(II) concentration, respectively

^c Saturation index = log(IAP/K_{sp}). The ion activity product (IAP) was determined with initial Fe(II) concentration and pH for each experiment. $K_{sp} = [Fe^{2+}][OH^-]^2 = 5 \times 10^{-15.3}$

^d % PCE or TCE loss, % Products and % Carbon recovery are taken from the final reported time point.

^e (n.d.) indicates not determined.

^f First time point determined was not at time zero, and thus the [C]₀ is reported as a nominal concentration.

Table S5. PCE/TCE with aqueous Fe(II) alone, with products

[C] ₀ ^a (μM)	pH	[Fe(II)] ₀ ^b (mM)	Saturation Index ^c	[Fe(II)] _f ^b (mM)	% loss ^d	% products ^d	% C recovery ^d	Duration (day)	<i>k</i> _{obs} (s ⁻¹)
PCE									
50.2	8.0	31.7	0.80	1.99	27.6	2.7	75	193	1.7 × 10 ⁻⁹
54.0	8.1	36.80	1.1	33.99	23.3	1.1	77	156	8.5 × 10 ⁻¹⁰
52.7	8.5	~13.34	1.4	n.d. ^e	14	1.0	86	140	1.3 × 10 ⁻⁸
54.0	8.6	28.52	1.9	1.39	39.0	0.3	61	188	1.8 × 10 ⁻¹⁰
51.2	9.0	~13.34	2.4	n.d.	19	1.0	74	140	1.8 × 10 ⁻⁸
44.4	9.0	28.00	2.7	0.63	11.9	2.0	90	188	4.8 × 10 ⁻¹⁰
TCE									
196.9	8.0	31.62	0.80	9.39	-21.5	3.8	125	193	2.3 × 10 ⁻⁹
58.9	8.0	31.98	0.81	15.19	26.6	9	82	193	5.6 × 10 ⁻⁹
52.6	8.1	35.66	0.95	33.9	7	8	100.6	156	2.5 × 10 ⁻⁹
50.2	8.5	28.26	1.8	1.73	5	7.2	102	193	4.3 × 10 ⁻⁹
50.9	8.5	29.21	1.8	1.57	-7.9	1.2	109	193	6.6 × 10 ⁻¹⁰
56.2	8.5	~13.34	1.4	n.d.	29	6	75	140	3.0 × 10 ⁻⁹
51	8.9	28.55	2.6	0.46	7.4	9	102	193	5.7 × 10 ⁻⁹
55.6	9.0	~13.34	2.4	n.d.	24	7	83	140	5.7 × 10 ⁻⁹
51.5	9.2	28.08	3.1	0.33	23.3	13	90	193	7.7 × 10 ⁻⁹

^a [C]₀ = Initial chloroethylene concentration

^b [Fe(II)]₀ = initial Fe(II) concentration

^c Saturation index = log(IAP/K_{sp}). The ion activity product (IAP) was determined with initial Fe(II) concentration and pH for each experiment. K_{sp} = [Fe²⁺] [OH⁻]² = 5 × 10^{-15.3}

^d % PCE or TCE loss, % Products and % Carbon recovery are taken from the final reported time point. Negative loss numbers indicate higher measured TCE concentrations at the final time point than the initial time point.

^e n.d. = not determined.

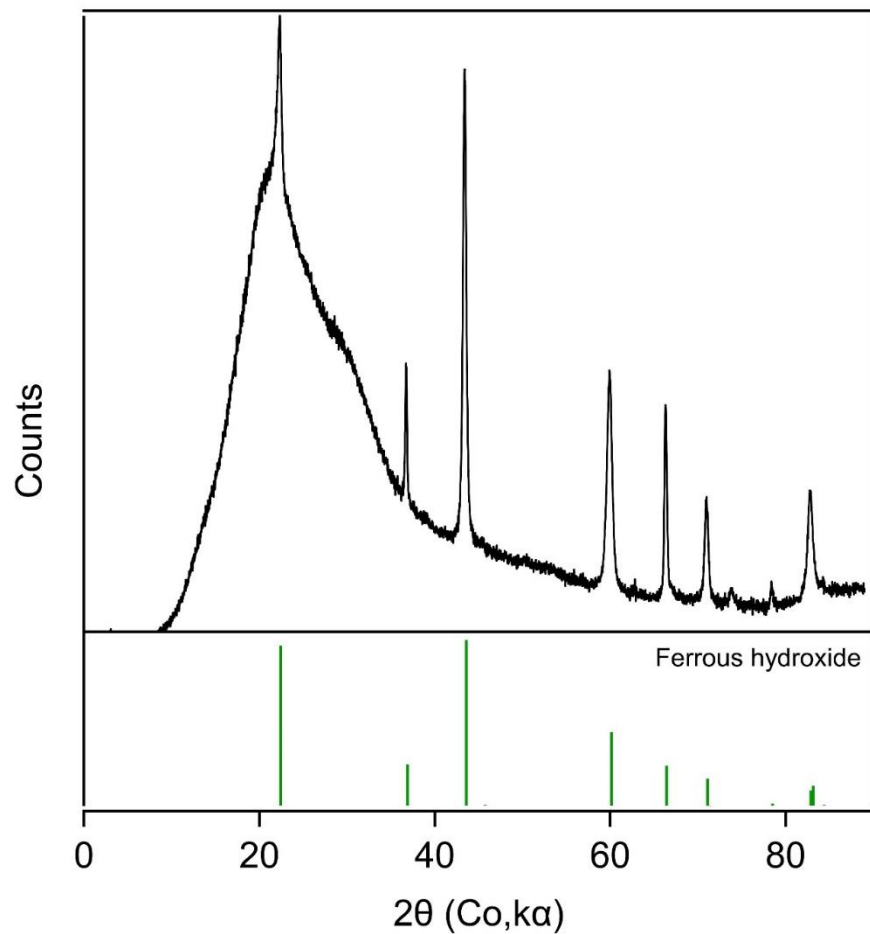


Figure S4. X-ray diffraction pattern of a TCE reactor with Fe(II) alone after 193 days where 9.0% products were observed. Light green bars indicate ferrous hydroxide. The background before 60° 2θ is due to Kapton film used to seal the sample from air. Experimental conditions: 60 μM TCE, 10 mM MOPs/NaCl, 32 mM Fe(II), pH 8.0.

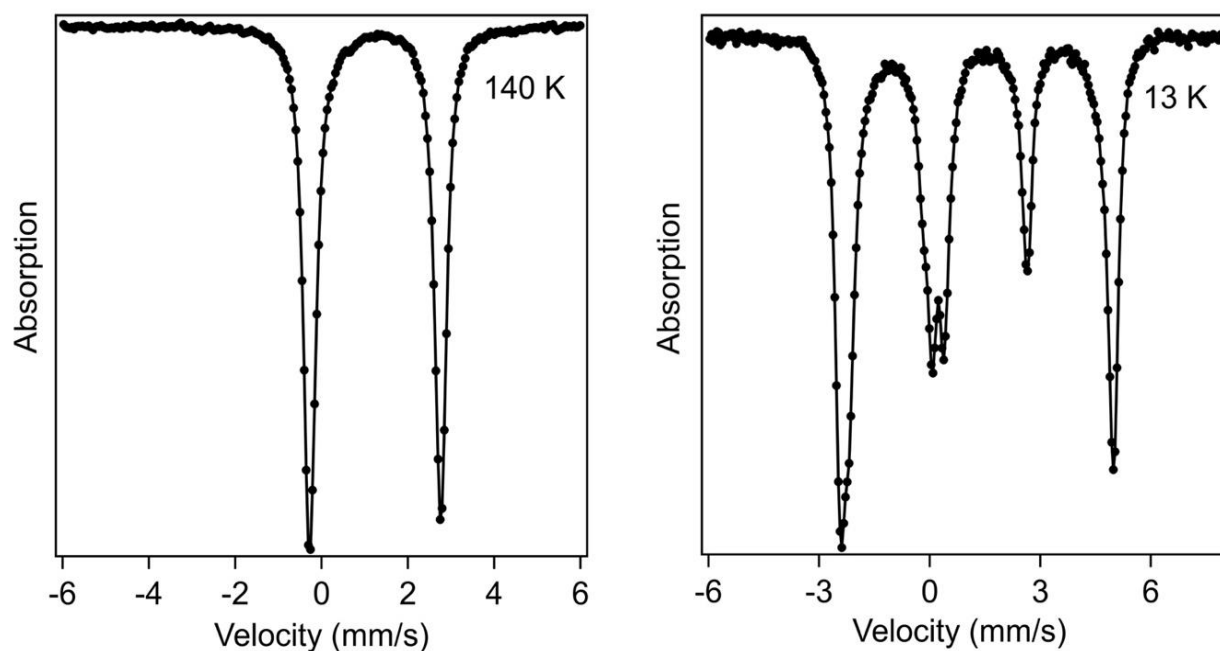


Figure S5. Mössbauer spectrum of the white precipitate in Fe(II) alone reactors after reacting with 60 μ M TCE, 10 mM MOPs/NaCl, pH 8.0 for 193 days where 9.0% products were observed. Note: 32 mM Fe(II) was the initial concentration of dissolved iron added.

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