

Supplementary Information

Oxidation and reduction performance of 1,1,1-trichloroethane in aqueous solution by means of a combination of persulfate and zero-valent iron

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Fig. S1 Schematic diagram of the head-to-bottom rotation drum.

Fig. S2 TCA Control tests for volatilization, persulfate and Fe^{2+} alone after 12 h (Conditions: $[\text{TCA}]_0 = 0.15 \text{ mM}$, $[\text{persulfate}]_0 = 9.0 \text{ mM}$, $[\text{Fe}^{2+}]_0 = 8.9 \text{ mM}$; Note: the pH values of 2.5, 5, 7 were chosen as the pH during persulfate-ZVI system varied from 2.8 to 5.9).

Fig. S3 Comparison of TCA degradation performance between persulfate- Fe^{2+} and persulfate-ZVI system (Conditions: $[\text{TCA}]_0 = 0.15 \text{ mM}$, $[\text{Fe}^{2+}]_0 = 8.9 \text{ mM}$, $[\text{ZVI}]_0 = 0.05 \text{ g}$, $[\text{persulfate}]_0 = 9.0 \text{ mM}$, $20 \text{ }^\circ\text{C}$).

Fig. S4 The solution pH variation in the persulfate-ZVI system (Conditions: $[\text{TCA}]_0 = 0.15 \text{ mM}$, $[\text{persulfate}]_0 = 9.0 \text{ mM}$, $[\text{ZVI}]_0 = 0.05 \text{ g}$, $20 \text{ }^\circ\text{C}$).

Fig. S5 Effect of Fe^{2+} on TCA degradation in the presence of ZVI alone (Conditions: $[\text{TCA}]_0 = 0.15 \text{ mM}$, $[\text{Fe}^{2+}]_0 = 8.9 \text{ mM}$, $[\text{ZVI}]_0 = 0.05 \text{ g}$, $20 \text{ }^\circ\text{C}$).

Text S1 Analytical methods for TCA and the intermediates.

(1) Operating conditions for TCA analysis by a GC

Parameters	Conditions
Injection port	240 °C, split ratio: 20/1
Capillary column	DB–VRX, 60 m × 320 μm i.d. × 1.4-μm
Oven	Isothermal at 75 °C
Carrier gas	Nitrogen (>99.999%), 5 mL/min
Detector	Electron capture detector, 260 °C

(2) Operating conditions for the volatile intermediates by an automatic purge and trap (P&T) coupled to a GC/MS

1 mL of aqueous sample was removed into a 42 mL volatile organic analysis (VOA) vial, and then the vial was fully filled by water for analysis.

	Parameters	Conditions
P&T conditions	Sample volume	5 mL
	Gas flow	40 mL min ⁻¹
	Purge cycle	11 min at ambient temperature
	Desorb cycle	4 min at 180 °C
	Bake cycle	210 °C
GC/MS conditions	Injection port	230 °C, split ratio: 15/1
	Carrier gas	Helium, 1.2 mL/min
	Capillary column	DB–VRX, 60 m×320 μm i.d.×1.4-μm
	Oven program	40 °C (2min) 250 °C at 20 °C min ⁻¹ (3min)
	Interface temperature	200 °C
	Ion source temperature	250 °C
	Mass range	TIM mode, <i>m/z</i> : 35-275

(3) GC/MS conditions for the carboxylic acid intermediates

Parameters	Conditions
Injection port	200 °C, split ratio: 5/1
Solvent delay	8 min
Capillary column	DB-VRX, 60 m × 320 μm i.d. × 1.4-μm
Carrier gas	Helium, 1.5 mL/min
Oven program	35 °C (10min) 65 °C at 2 °C min ⁻¹ (5min) 280 °C at 20 °C min ⁻¹ (3min)
Interface temperature	200 °C
Ion source temperature	250 °C
Mass range	TIM mode, <i>m/z</i> : 35-150

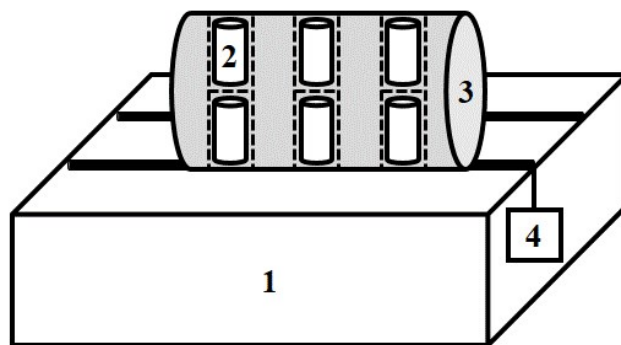


Fig. S1 Schematic diagram of the head-to-bottom rotation drum.

(1) Holder, (2) reaction vial (fixed by compartments), (3) the rotation drum, (4) motor.

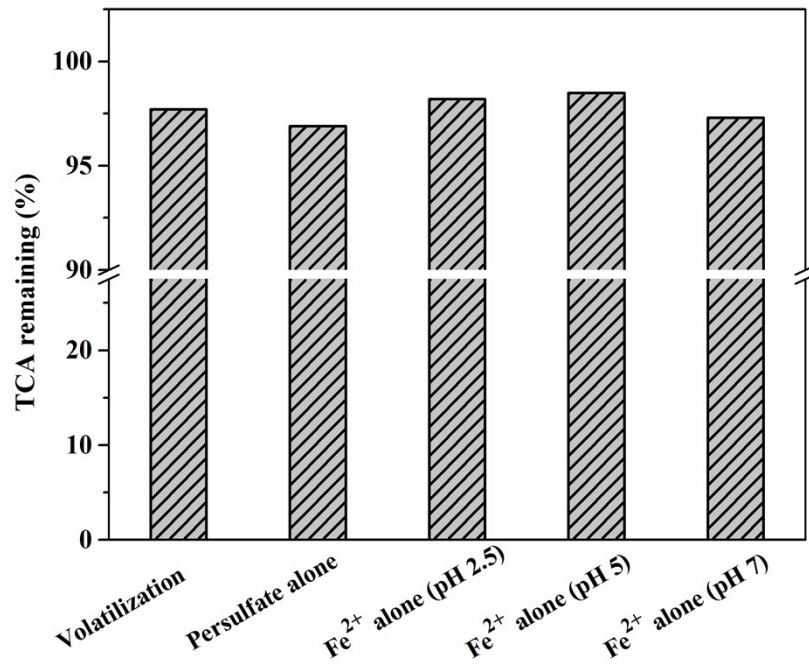


Fig. S2 TCA Control tests for volatilization, persulfate and Fe²⁺ alone after 12 h ([TCA]₀ = 0.15 mM, [persulfate]₀ = 9.0 mM, [Fe²⁺]₀ = 8.9 mM; Note: the pH values of 2.5, 5, 7 were chosen as the pH variation during persulfate-ZVI system was from 2.8 to 5.9)

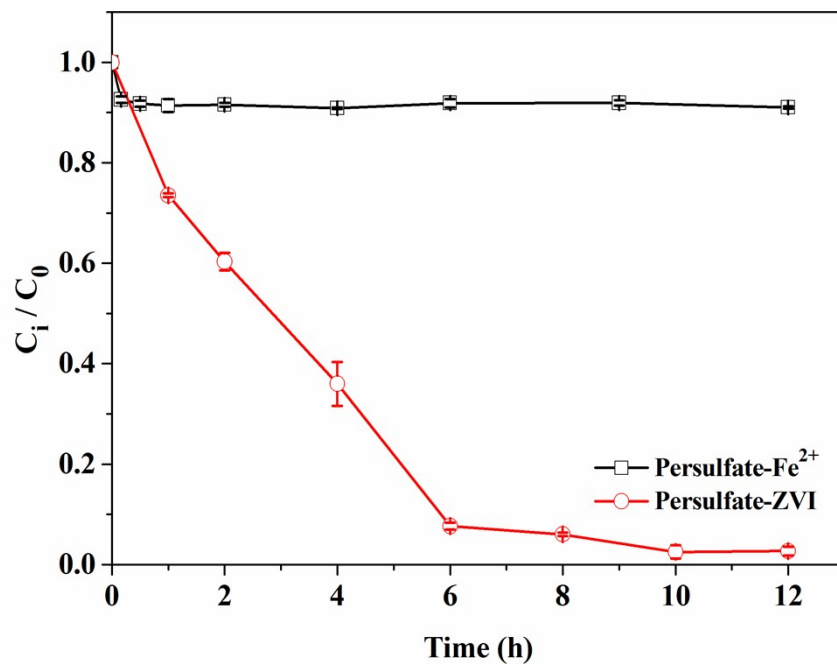


Fig. S3 Comparison of TCA degradation performance between persulfate- Fe^{2+} and persulfate-ZVI system (Conditions: $[TCA]_0 = 0.15$ mM, $[Fe^{2+}]_0 = 500$ mg L^{-1} , $[ZVI]_0 = 0.05$ g, $[persulfate]_0 = 9.0$ mM, 20 °C).

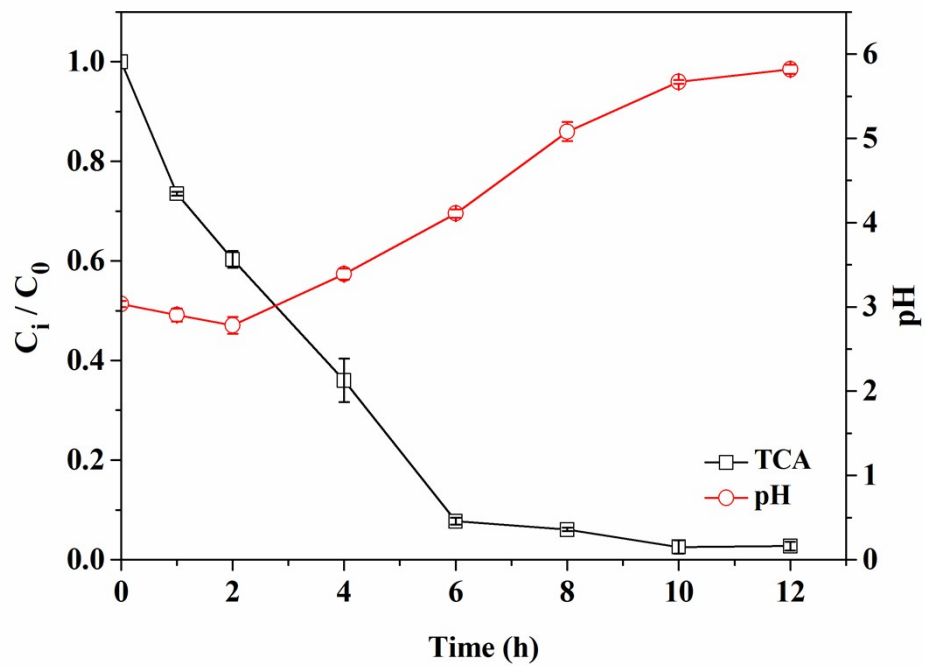


Fig. S4 The solution pH variation in the persulfate-ZVI system (Conditions: $[TCA]_0 = 0.15$ mM, $[persulfate]_0 = 9.0$ mM, $[ZVI]_0 = 0.05$ g, 20 °C).

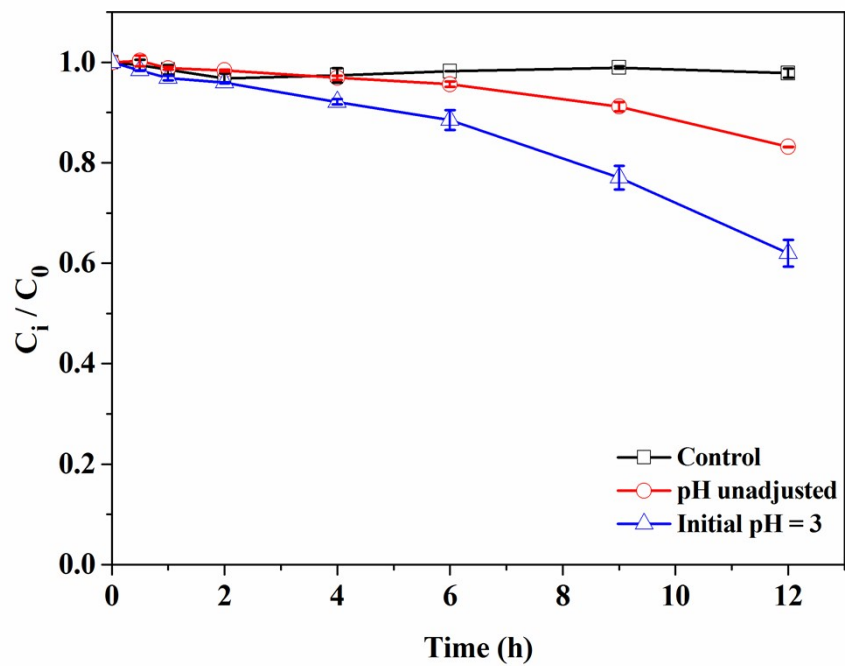


Fig. S5 Effect of Fe^{2+} on TCA degradation in the presence of ZVI alone (Conditions: $[\text{TCA}]_0 = 0.15 \text{ mM}$, $[\text{Fe}^{2+}]_0 = 500 \text{ mg L}^{-1}$, $[\text{ZVI}]_0 = 0.05 \text{ g}$, $20 \text{ }^\circ\text{C}$).