Supplementary Materials

for

Enhanced 2,4,6-Tribromophenol Degradation via Slow-Release S(IV) in Fe(II)-Activated $CaSO_3$ Advanced Oxidation Process

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Text S1. 1,10-phenanthroline spectrophotometry for determination of Fe species.

10% hydroxylamine hydrochloride, 0.5% 1,10-phenanthroline were prepared with ultrapure water. Buffer solution was prepared by mixing 40 g ammonium acetate and 50 mL acetic acid, then obtained mixture was diluted to 100 mL. For the determination of Fe_{tot}, 0.1 mL 1,10-phenanthroline solution, 1 mL buffer solution and 0.2 mL hydroxylamine hydrochloride solution were added to a 10 mL colorimetric tube, then 5 mL sample solution was added and measured at λ = 510 nm. For the determination of Fe(II), all experimental procedures were largely identical but with no addition of hydroxylamine hydrochloride solution.

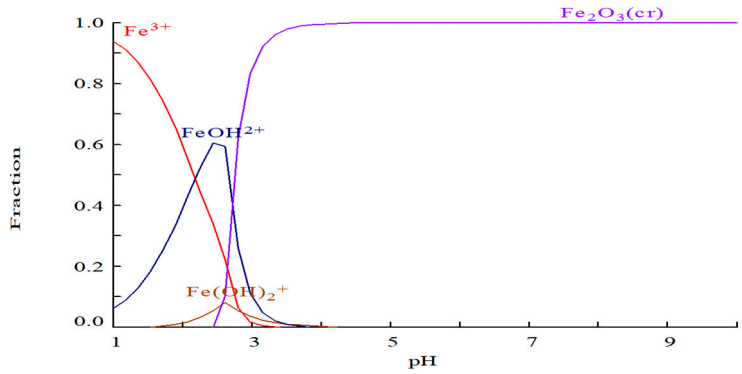


Figure S1. Distribution curves of Fe(III) under different solution pH

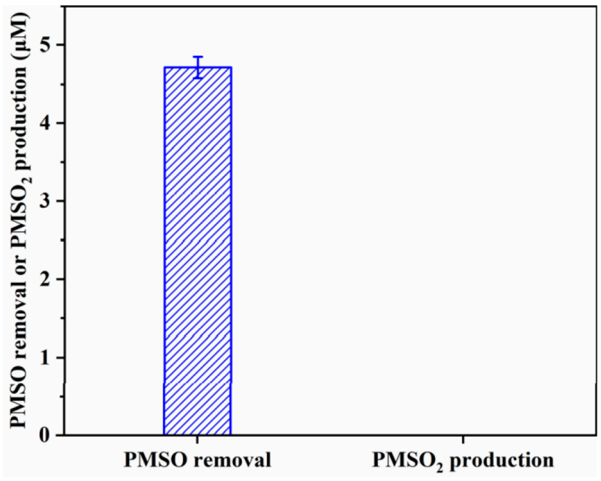


Figure S2. PMSO probe experiments in the Fe(II)/$CaSO_3$ system.

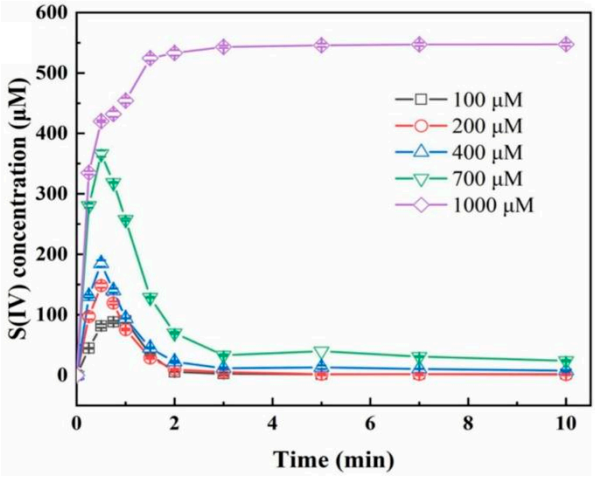


Figure S3. Variation of S(IV) concentration with different initial $CaSO_3$ dosage.

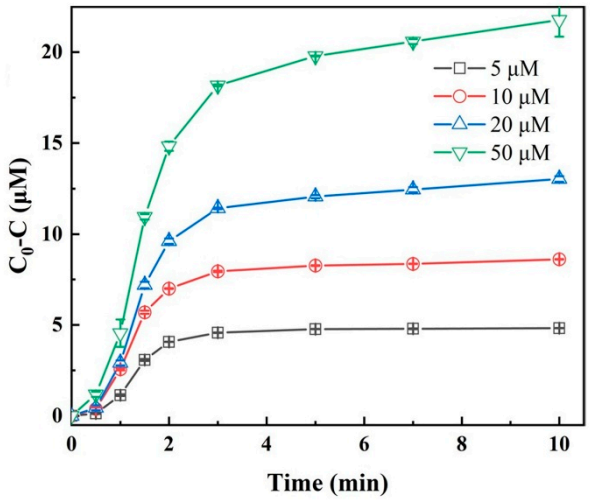


Figure S4. Absolute amount of degraded TBP during reaction with different initial TBP dosage.

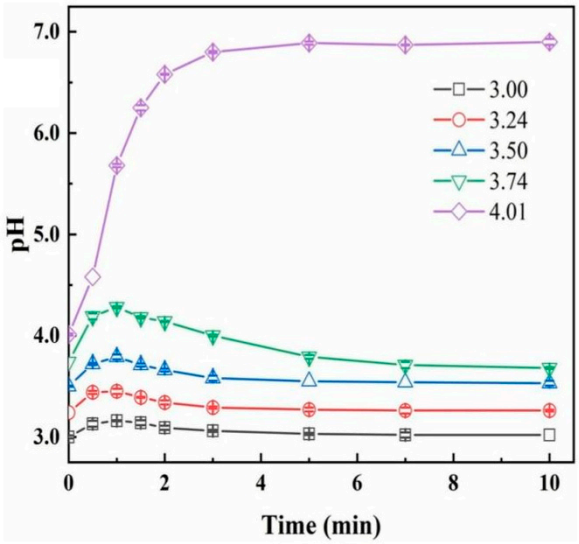


Figure S5. Variation of solution pH during reaction with different initial pH values.

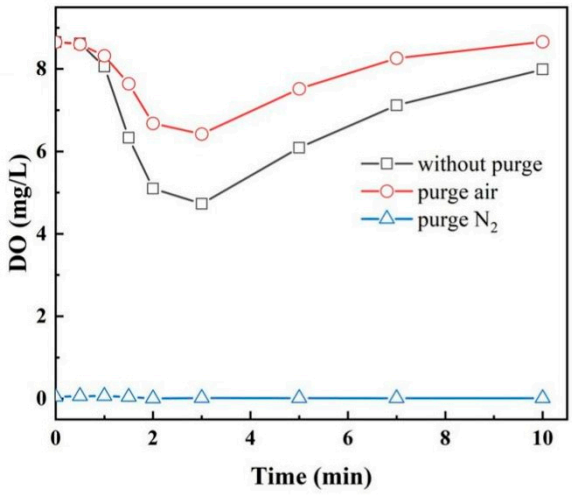


Figure S6. Variation of dissolved oxygen during reaction.

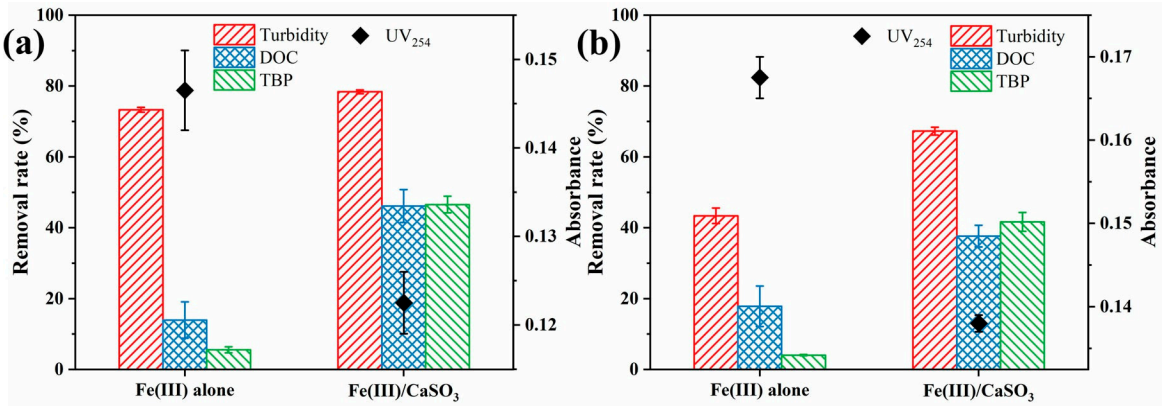


Figure S7 Removal of turbidity, DOC, TBP, and UV254 by the coagulation with Fe(III) alone and Fe(III)/CaSO3: (a) lake water; (b) secondary sedimentation tank effluent. Experimental conditions: [TBP] = 10 μM, [Fe(III)] (lake water) = 50 μM, [Fe(III)](secondary sedimentation tank effluent) = 100 μM, [$CaSO_3$] = 400 μM, initial pH = 3.5, temperature = 25 °C

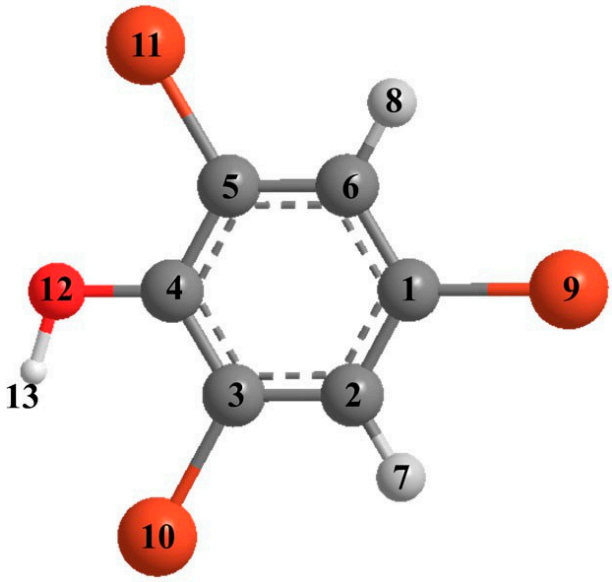


Figure S8. Optimized molecular structure of TBP.

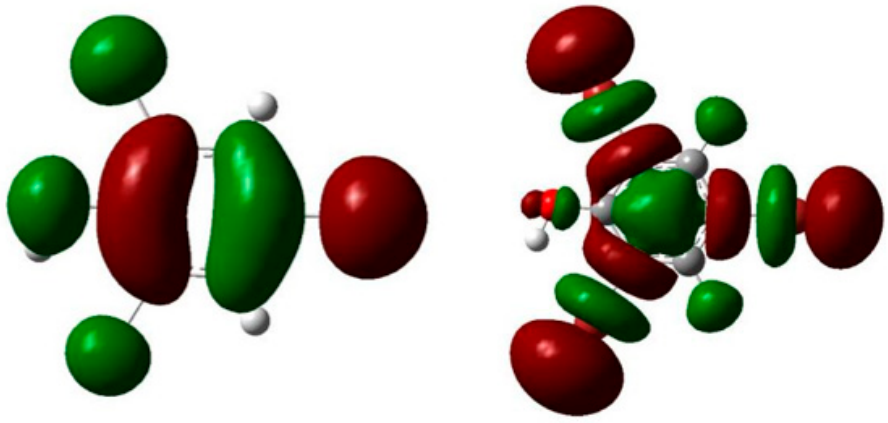


Figure S9. Molecular orbital analysis of HOMO and LUMO in TBP.

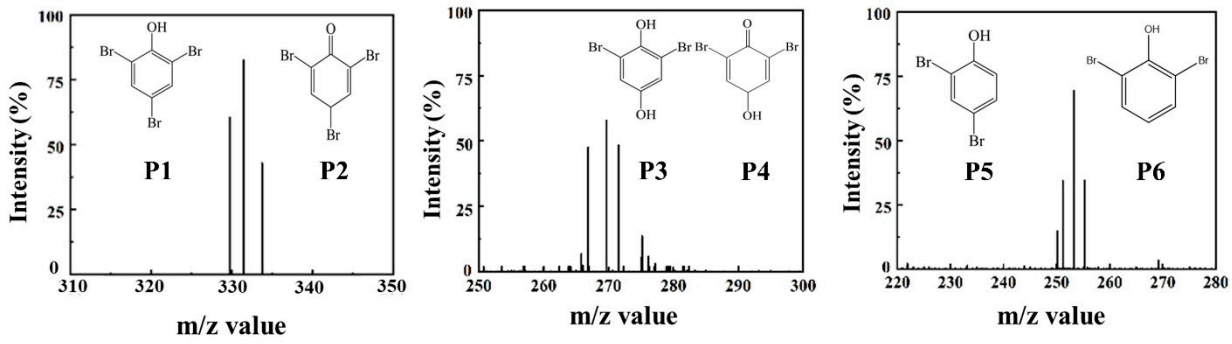


Figure S10. LC-MS/MS spectra of TBP degradation products in the Fe(II)/$CaSO_3$ system.

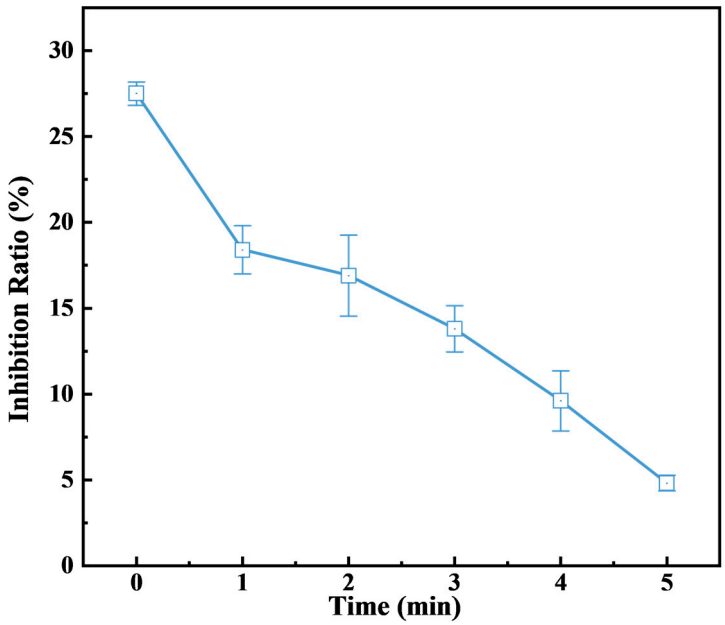
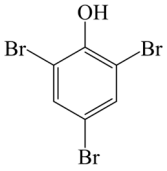
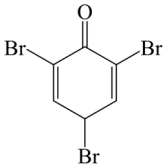
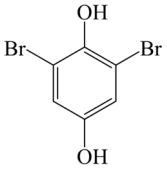
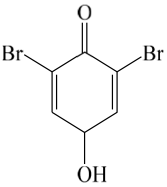
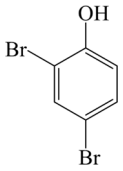


Figure S11. Luminescent bacteria toxicity test in the Fe(II)/$CaSO_3$ system.

Table S1. Natural bond orbital charges calculation in TBP molecular structure.

Atom		B3LYP			M06		
		N	N+1	N-1	N	N+1	N-1
C	1	-0.12992	-0.02953	-0.14568	-0.1372	-0.16753	-0.02802
C	2	-0.24874	-0.2044	-0.12154	-0.25435	-0.2801	-0.21749
C	3	-0.16714	-0.14223	-0.21551	-0.17501	-0.25158	-0.15777
C	4	0.29051	0.4137	0.12789	0.29783	0.25437	0.43499
C	5	-0.15478	-0.1176	-0.17124	-0.16271	-0.19892	-0.13167
C	6	-0.24812	-0.22313	-0.12415	-0.25363	-0.28688	-0.2363
H	7	0.28994	0.31698	0.11601	0.29922	0.25246	0.32585
H	8	0.28876	0.31567	0.11994	0.29788	0.26515	0.32454
Br	9	0.06899	0.2749	-0.1233	0.07397	-0.0682	0.27709
Br	10	0.08789	0.19666	-0.20597	0.09182	-0.22961	0.20566
Br	11	0.09154	0.22236	-0.14789	0.09658	-0.07632	0.22647
O	12	-0.70283	-0.57763	-0.37071	-0.71752	-0.74862	-0.58856
H	13	0.53392	0.55424	0.26217	0.54312	0.53579	0.5652

Table S2. Intermediate products in the Fe(II)/$CaSO_3$ system

Number	m/z	Molecular formula	Structural
P1	329.7714	$C_6H_3Br_3O$	
P2	329.7714	$C_6H_3Br_3O$	
P3	267.8558	$C_6H_4Br_2O_2$	
P4	267.8558	$C_6H_4Br_2O_2$	
P5	251.8608	$C_6H_4Br_2O$	
P6	251.8608	$C_6H_4Br_2O$	