0Supplementary Materials for

Atrazine degradation by aqueous ferrate(VI) activated with sulfite vs thiosulfate: Performance, products, and pathways

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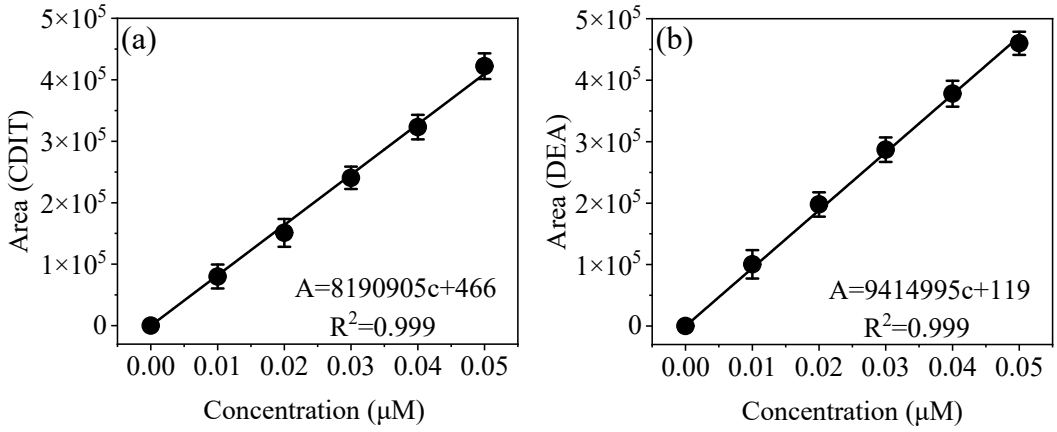


Fig. S1. The calibration curve of main oxidaion products CDIT (a) and DEA (b).

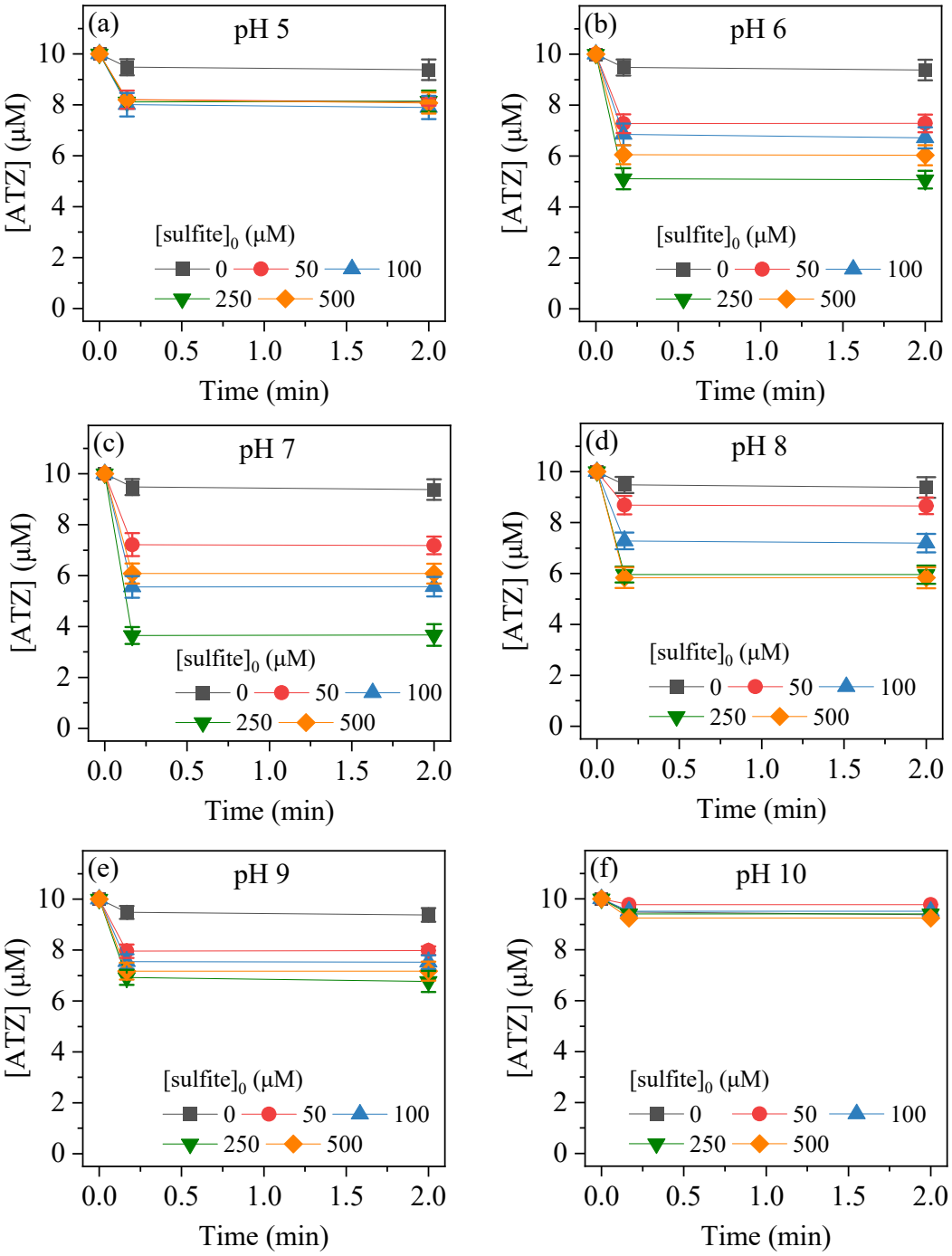


Fig. S2. The effects of pH and initial sulfite concentration on ATZ degradation in Fe(VI)/sulfite system. Experimental conditions: $[ATZ]_0$ = 10 μM, $[Fe(VI)]_0$ = 100 μM, $[sulfite]_0$ = 0~500 μM, and pH = 5~10.

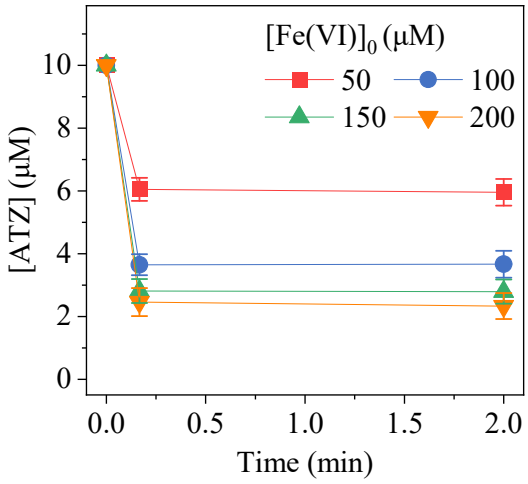


Fig. S3. The effects of initial Fe(VI) concentration on ATZ degradation in Fe(VI)/sulfite system. Experimental conditions: $[ATZ]_0$ = 10 μM, $[Fe(VI)]_0$ = 50~200 μM, $[sulfite]_0$ = 125~500 μM, and pH = 7.

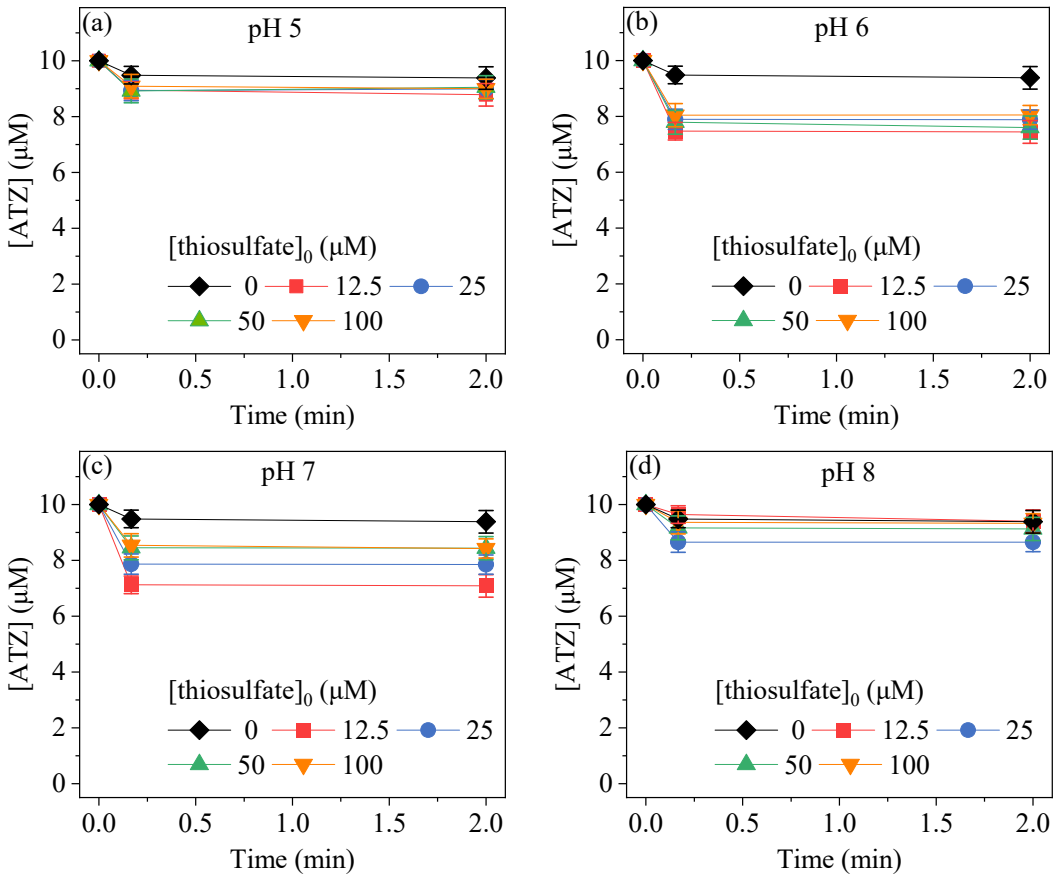


Fig. S4. The effects of pH and initial thiosulfate concentration on ATZ degradation in Fe(VI)/thiosulfate system. Experimental conditions: $[ATZ]_0$ = 10 μM, $[Fe(VI)]_0$ = 100 μM, $[thiosulfate]_0$ = 0~100 μM, and pH = 5~8.

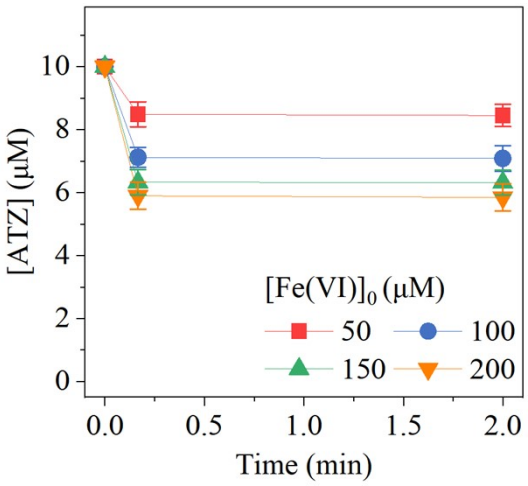


Fig. S5. The effects of initial Fe(VI) concentration on ATZ degradation in Fe(VI)/thiosulfate system. Experimental conditions: $[ATZ]_0$ = 10 μM, $[Fe(VI)]_0$ = 50~200 μM, $[thiosulfate]_0$ = 6.25~25 μM, and pH = 7.

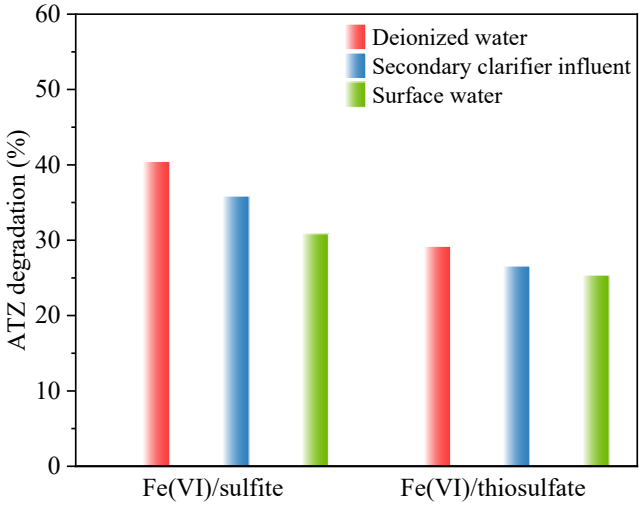
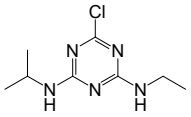
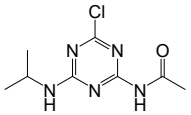
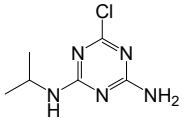
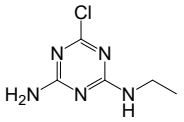
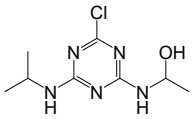
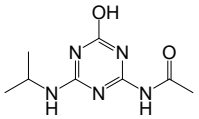


Fig. S6. Comparison of ATZ degradation by Fe(VI)/sulfur-containing reductants systems in deionized water, secondary clarifier influent and surface water. Experimental conditions: $[ATZ]_0$ = 10 μM, $[Fe(VI)]_0$ = 100 μM, $[sulfite]_0$ = 250 μM, $[thiosulfate]_0$ = 12.5 μM.

Table S1. Identified oxidation products of ATZ in Fe(VI)/sulfite and Fe(VI)/thiosulfate systems.

Products	[M + H^+]	Retention Time (min)	Chemical Structure
Atrazine (ATZ)	216.1	8.57	
I. atrazine amide (CDIT)	230.1	7.64	
II. desethyl-atrazine (DEA)	188.1	7.22	
III. desisopropyl-atrazine (DIA)	174.0	6.40	
IV. 2-hydroxy-4-(2-hydroxy-ethylamino)-6-isopropylamino-s-triazine (ONIT)	232.1	9.03	
V. N-(4-hydroxy-6-(isopropylamino)-1,3,5-triazin-2-yl) acetamide (ODIT)	212.2	2.98	

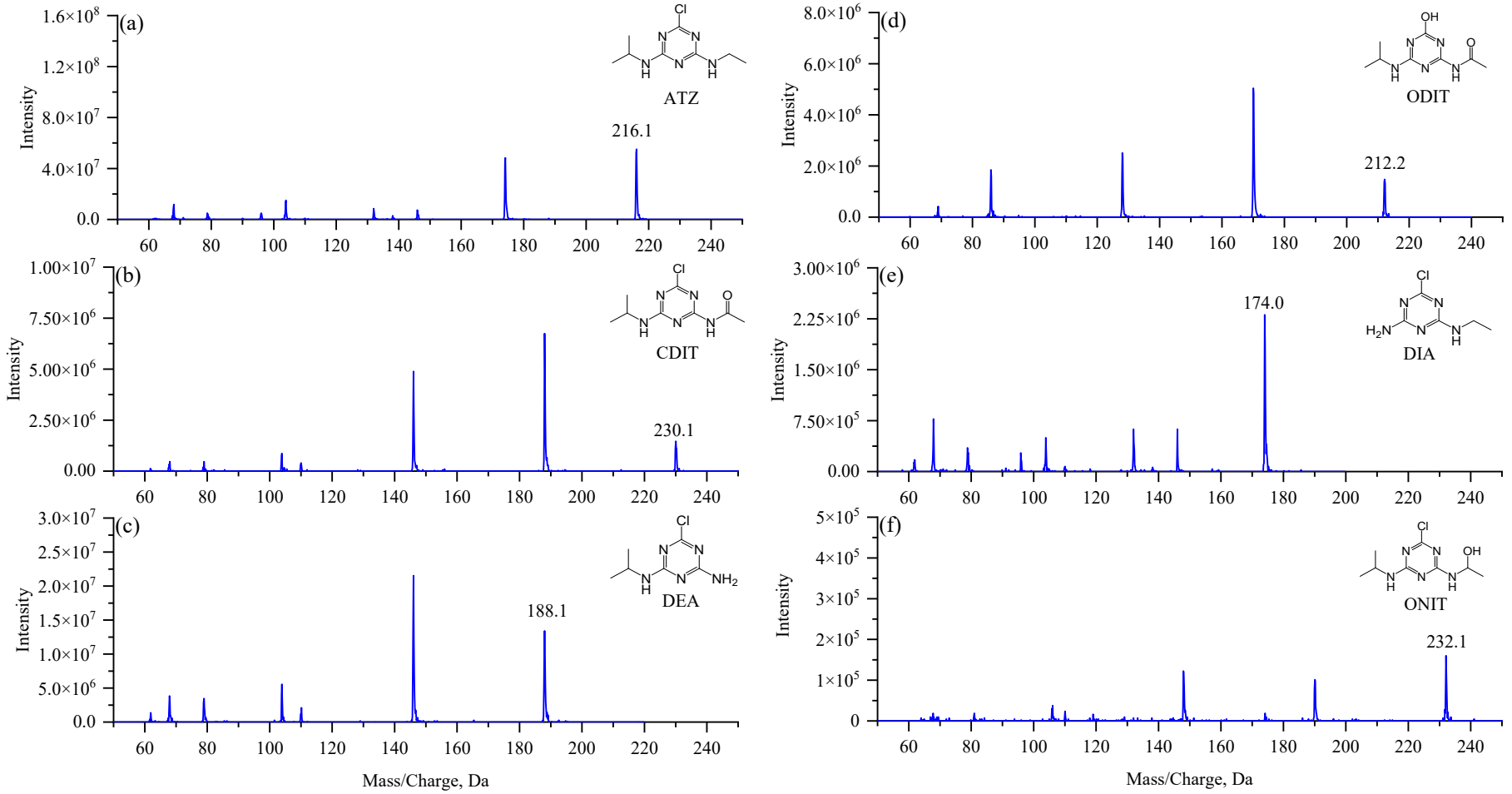


Fig. S7. The MSMS spectra of ATZ and its oxidation products generated by Fe(VI)/sulfite and Fe(VI)/thiosulfate systems.

Table S2. The detailed value of LC_{50} and ChV of ATZ and its oxidation products.

	LC_{50} (mg/L)			ChV (mg/L)		
	Fish	Daphnid	Green Algae	Fish	Daphnid	Green Algae
ATZ	32.7	20.0	20.4	3.49	2.41	6.31
DEA	243.0	135.0	92.7	23.2	12.5	23.2
CDIT	645.0	346.0	203.0	58.9	28.7	46.7
DIA	534	286	167	48.7	23.7	38.3
ODIT	1340	696	355	118	52.6	75.9
ONIT	3493	1730	743	291	117	145

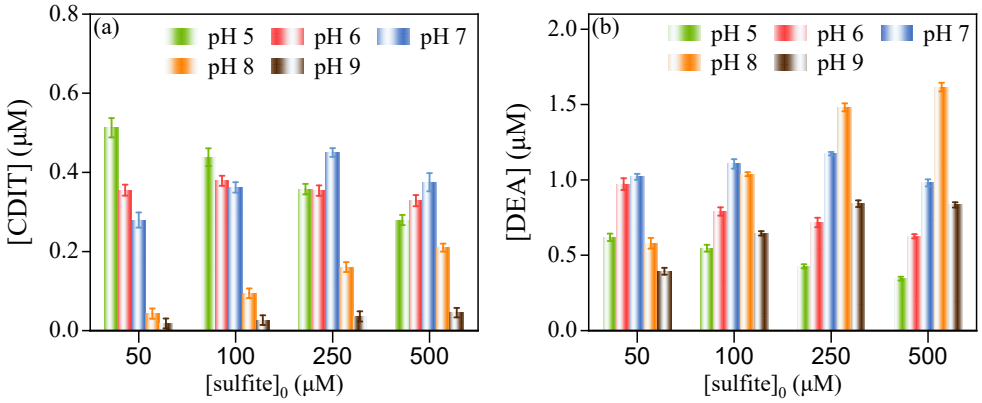


Fig. S8. The production of CDIT (a) and DEA (b) in ATZ degradation by Fe(VI)/sulfite system. Experimental conditions: $[ATZ]_0$ = 10 μM, $[Fe(VI)]_0$ = 100 μM, $[sulfite]_0$ = 50~500 μM, and pH = 5~9, and reaction time of 2 min.

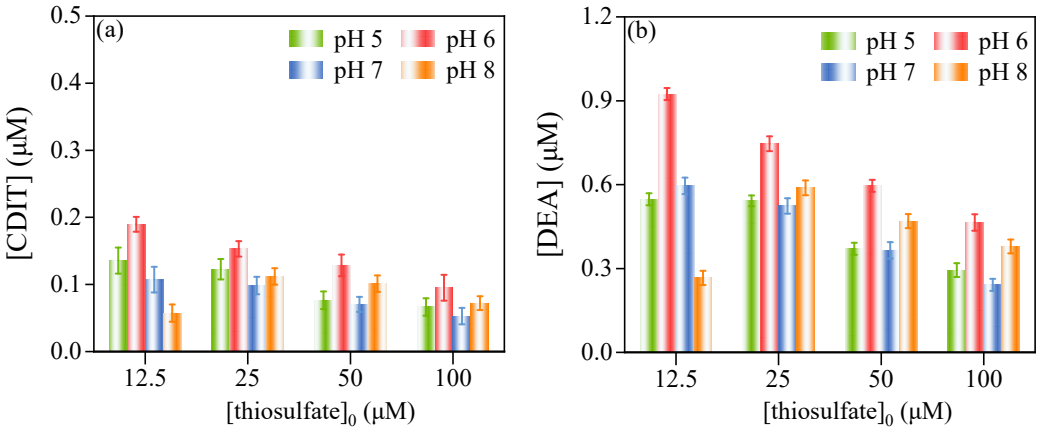


Fig. S9. The production of CDIT (a) and DEA (b) in ATZ degradation by Fe(VI)/thiosulfate system. Experimental conditions: $[ATZ]_0$ = 10 μM, $[Fe(VI)]_0$ = 100 μM, $[thiosulfate]_0$ = 12.5~100 μM, and pH = 5~8, and reaction time of 2 min.