Supplementary Material for the artical:

Ferrate-acetylacetonate system to promote the degradation of sulfadimethoxine in mariculture tailwater

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Text:1

Figures: 3

Table: 3

Text S1.

The rate constant of the reaction of Fe(VI) with SDM can be expressed as:

$$-d[Fe(VI)]/dt = k[Fe(VI)]^{m}[SDM]^{n} \quad (1)$$

where [Fe(VI)] and [SDM] are the concentrations of Fe(VI) and sulfadimethoxine, m and n are the orders of the reaction, and k is the overall reaction rate constant.

The kinetic studies were carried out under pseudo-order conditions with sulfonamide in excess i.e. [SDM] >> [Fe(VI)] . under these circumstances Equation (1) can thus be re-written under pseudo-order conditions as:

$$-d[Fe(VI)]/dt = k_1[Fe(VI)]^{m} \quad (2)$$

$$\text{where } k_1 = k[SDM]^{n} \quad (3)$$

Reactions were monitored by measuring the absorbance of Fe(VI) at 510 nm wavelength as a function of time. The results indicate that the reaction is a first order reaction constant. Thus the reaction can be rewritten as

$$-d[Fe(VI)]/dt = k[Fe(VI)][SDM] \quad (4)$$

Figure

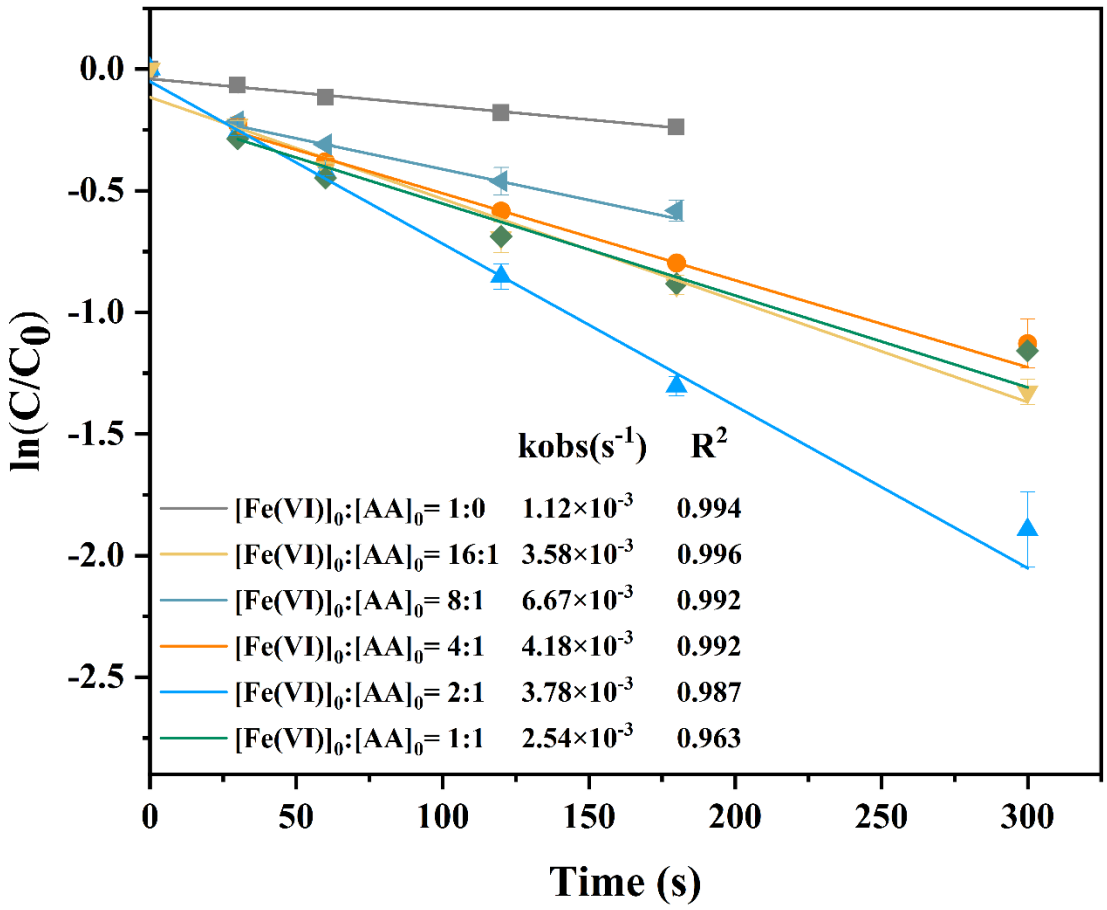

Fig. S1 Effect of $[Fe(VI)]_0$: $[AA]_0$ on the degradation kinetics of SDM ($[SDM]_0$ = 10 μM, $[Fe(VI)]_0$ = 200 μM, $[AA]_0$ = 0-200 μM, pH= 9, T = 25 °C)

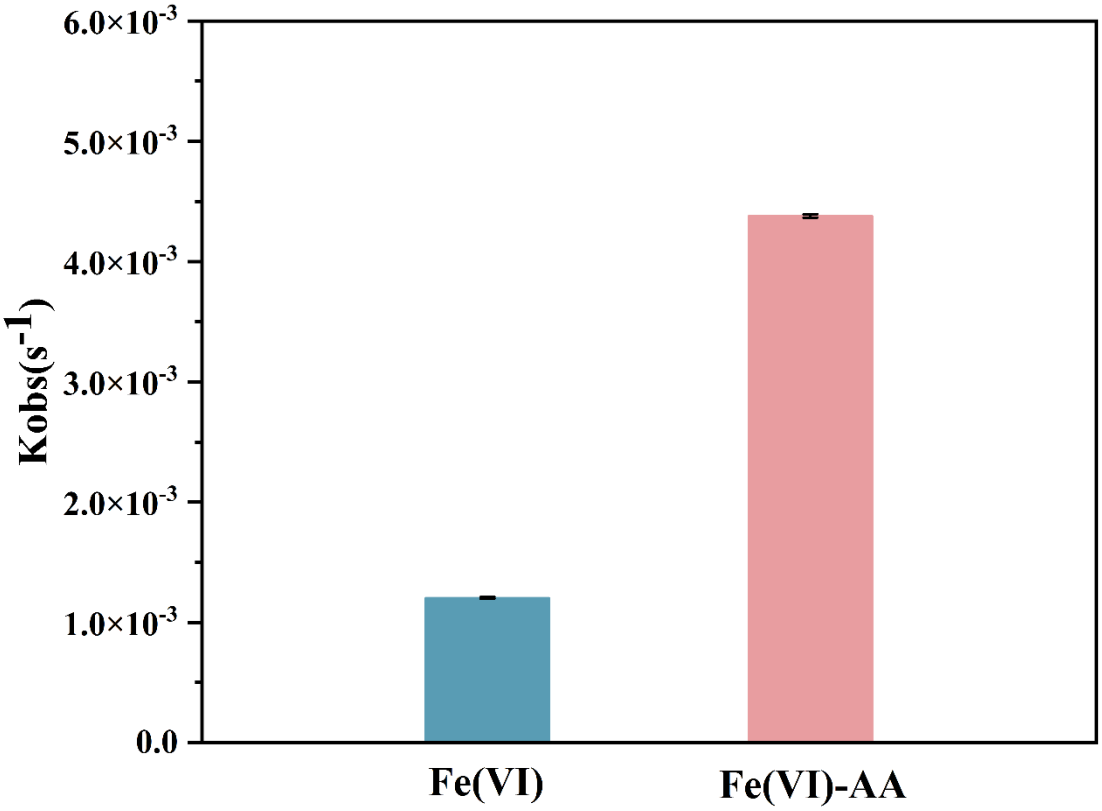

Fig. S2 Effect of actual mariculture tailwater on the Pseudo-first-order kinetic plot of SDM degradation

([SDM]$_0$ = 10 μM, [Fe(VI)]$_0$ = 200 μM, [AA]$_0$ = 25 μM, pH= 9, T = 25 °C)

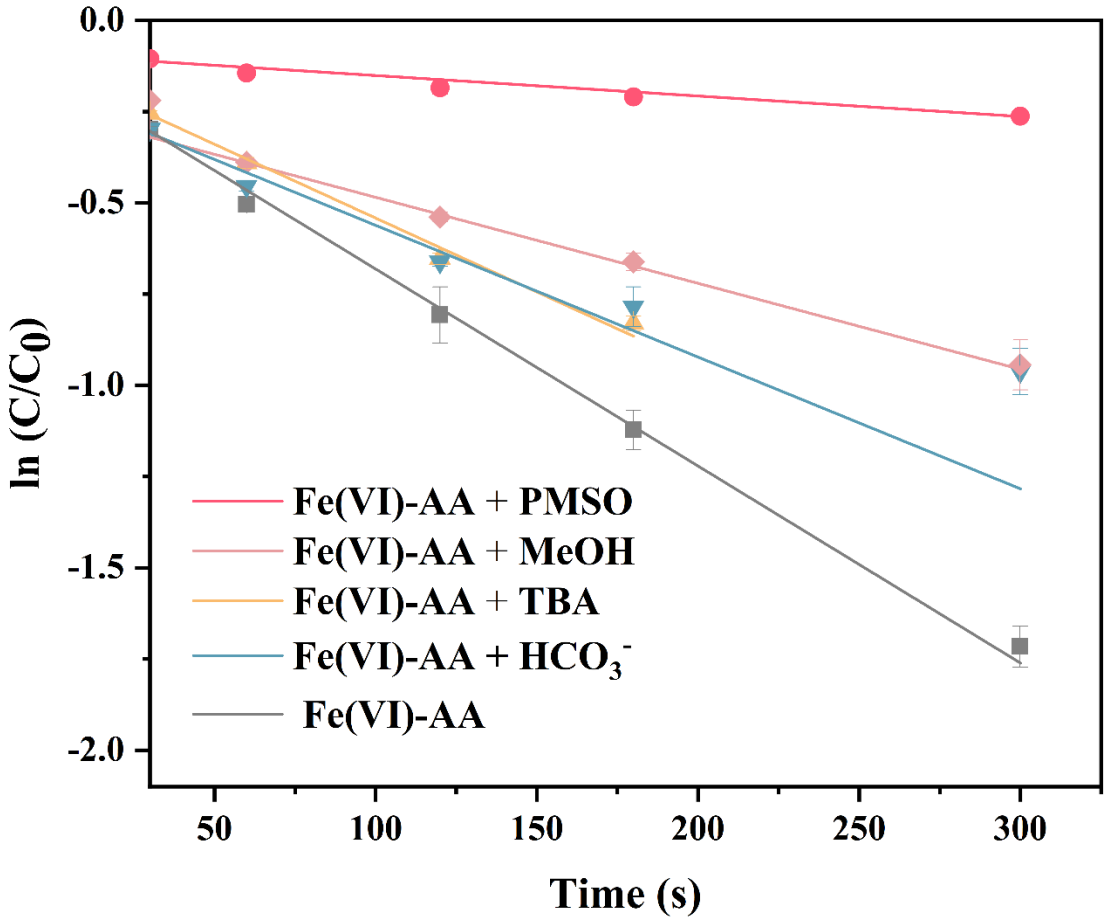

Fig. S3 Effects of PMSO, TBA, HCO_3^- and MeOH on the degradation kinetics of SDM in the Fe(VI)-AA system at a salinity background of 20 ppt ($[SDM]_0$ = 10 μM, $[Fe(VI)]_0$ = 200 μM, $[AA]_0$ = 25 μM, pH= 9, T = 25 °C)

Table

Table.S1. Fukui index(d) of SDM

Atom index	f^-	f^+	f^0
1(C)	0.0375	0.0353	0.0364
2(C)	0.031	0.0763	0.0536
3(C)	0.041	0.0457	0.0434
4(C)	0.0185	0.0422	0.0303
5(C)	0.0352	0.0512	0.0432
6(C)	0.019	0.0686	0.0438
7(N)	0.0766	0.0502	0.0634
8(S)	0.0166	0.0447	0.0307
9(N)	0.0283	0.0151	0.0217
10(O)	0.0354	0.0417	0.0385
11(O)	0.0444	0.0448	0.0446
12(C)	0.0207	0.0346	0.0276
13(N)	0.0297	0.0217	0.0257
14(C)	0.0276	0.0184	0.023
15(N)	0.032	0.0381	0.0351
16(C)	0.0304	0.0384	0.0344
17(C)	0.0932	0.0171	0.0551
18(O)	0.0395	0.0212	0.0303
19(C)	0.0155	0.0106	0.013
20(O)	0.049	0.0135	0.0313
21(C)	0.0152	0.0088	0.012
22(H)	0.0217	0.0284	0.025
23(H)	0.0222	0.031	0.0266
24(H)	0.0143	0.0255	0.0199
25(H)	0.0146	0.0324	0.0235
26(H)	0.0281	0.0312	0.0297
27(H)	0.0283	0.03	0.0291
28(H)	0.0117	0.0096	0.0107
29(H)	0.0303	0.0136	0.0219
30(H)	0.0177	0.0138	0.0158
31(H)	0.0141	0.0094	0.0117
32(H)	0.0139	0.009	0.0115
33(H)	0.0176	0.0124	0.015
34(H)	0.0145	0.0077	0.0111
35(H)	0.0148	0.008	0.0114

Table.S2. The LC/MS data of SDM and main intermediates produced in the Fe(VI)-AA process.

Produce	Chemical Formula	Rt(min)	Theoretical Mass m/z	Detected Mass m/z	Mass error (ppm)
SDM	$C_{12}H_{14}N_4O_4S$	11.75	311.08085	311.08032	-1.7
P1	$C_5H_7N_3O_2$	2.24	142.06110	142.06078	-2.2
P2	$C_{11}H_{12}N_4O_2$	12.76	233.10330	233.10448	5.0
P3	$C_6H_9N_3O_2$	2.14	156.07675	156.07638	-2.3
P4	$C_{12}H_{14}N_4O_2$	7.35	247.11895	247.11806	-3.6
P5	$C_{12}H_{14}N_4O_5S$	11.56	327.07576	327.07516	-1.8
P6	$C_{12}H_{12}N_4O_7S$	13.75	357.04994	357.04898	-2.6
P7	$C_6H_9N_3O_5S$	2.09	236.03356	236.03316	-1.6
P8	$C_{12}H_{12}N_4O_5S$	9.55	325.06011	325.05963	-1.4
P9	C_6H_7NO	11.71	110.06004	110.06014	0.9
P10	$C_6H_7NO_3S$	2.04	174.02194	174.02145	-2.8

147
148 **Table.S3. ECOSAR toxicity analysis of SDM and intermediate**

ECOSAR

Compound	Acute toxicitty(mg/l)			Chronic toxicitty(mg/l)		
	Fish(96-hr-LC_{50})	DapHnid(48-hr-LC_{50})	Green algae(96-hr-EC50)	Fish	DapHnid	Green algae
SDM	1410	739	402	126	58.3	88.8
P1	3630	10400	6970	296	112	130
P2	856	455	257	77.3	36.8	57.9
P3	2630	1310	557	220	87.5	108
P4	631	340	206	58.1	28.8	48.1
P5	3990	2010	909	338	140	182
P6	1650	866	469	147	68.1	103
P7	7020000	2490000	267000	395000	65900	24600
P8	583	320	208	54.8	28.5	50.7
P9	1640	816	355	137	55.5	69.7
P10	6590000	2570000	403000	413000	87700	45600

	Not harmful		Harmful
	Toxic		Very toxic

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