Supplementary Data

For

Remediation of PAHs contaminated industrial soils by hypochlorous acid: Performance and mechanisms

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Table S1 The physical and chemical properties of the contaminated industrial soil

Parameter	Value	Unit
Moisture content	27.50	%
Cation exchange capacity	20.20	cmol/kg
pH (in water)	7.30	
Soil organic matter	6.90	%
Gravel	0.07	%
Silt	22.96	%
Clay	76.97	%
Cu	62.40	mg/kg
Ni	57.20	mg/kg
Hg	3.13	mg/kg
As	21.90	mg/kg
Pb	87.80	mg/kg
Cd	0.50	mg/kg

Table S2 The composition of PAHs in the contaminated industrial soil.

PAH Congener	Concentration (mg kg^{-1})	Proportion (%)
Naphthalene	13.8	0.6
Acenaphthylene	66.7	2.7
Acenaphthene	22.1	0.9
Fluorene	33.3	1.3
Phenanthrene	144.3	5.8
Anthracene	56.5	2.3
Fluoranthene	368.0	14.9
Pyrene	356.3	14.4
Benzo[a]anthracene	219.3	8.9
Chrysene	169.7	6.9
Benzo[b]fluoranthene	205.9	8.3
Benzo[k]fluoranthen	109.5	4.4
Benzo[a]pyrene	285.1	11.5
Indeno[1,2,3-cd]pyrene	189.3	7.7
Dibenz[a,h]anthracene	54.1	2.2
Benzo[ghi]perylene	176.1	7.1
Sum	2469.9	100

Table S3 Degradation of PAHs with different oxidizing agents [1-10]

Number	Oxidant	PAHs	Initial concentration of PAHs	Degradation rate
Ref. 1	PS	light PAHs	1.559 mg/kg	31%
		Heavy PAHs	2.667 mg/kg	45%
		16-PAHs	4.226 mg/kg	39%
Ref. 2	PS	16-PAHs	1189±40 mg/kg	16.16%
Ref. 3	PS	PAHs	16.98 mg/kg	69.14%
Ref. 4	PS	16-PAHs	214±21 mg/kg	47.66%
Ref. 5	CP/PS/OA-Fe^{2+}	total-PAHs (2-6ring)	137.8 mg/kg	70.8%
Ref. 6	Fenton	16-PAHs	263.6±73.3 mg/kg	54.1%
	$KMnO_4$			90.0%
	Activated persulfate			81.5%
Ref. 7	Soluble Fe(II) +citric acid or oxalic acid	Naphthalene	0.2730 mg/kg	89.5%
		Acenaphthene	0.3380 mg/kg	
		Fluoranthene	0.1440 mg/kg	
		Anthracene	2.0580 mg/kg	
Ref. 8	$KMnO_4$	Phenanthrene	340 mg/kg	40.8%
		Benz[a]anthracene	218 mg/kg	41.0%
		Benzo[a]pyrene	202 mg/kg	46.0%
Ref. 9	$KMnO_4$-Fenton	27-PAHs	3090 mg/kg	71%
Ref. 10	O_3/H_2O_2	Fluoranthene	31.32 ng/mL	89%
		Phenanthrene	107.15 ng/mL	66%
		Anthracene	32.35 ng/mL	71%
This work*	HClO	16-PAHs	2469.9 mg/kg	93.33%

Table S4 Integration details of pseudo-first-order dynamics

Equation	y=a+b×x				
Cl_2 (mg/L)	1000	2000	3000	4000	5000
Weight			Instrument		
Intercept	0.41358±0.00753	0.65518±0.03212	0.74979±0.01938	1.39288±0.02403	1.53888±0.03343
Slope	0.00194±0.00117	0.01043±0.00201	0.02339±0.00186	0.02308±0.00273	0.02454±0.00152
Sum of squares of residuals	168.41485	38.93052	20.16404	7.34146	7.2901
Pearson's	0.59433	0.93301	0.98448	0.97316	0.99427
R^2(COD)	0.35323	0.87051	0.96921	0.94704	0.98858
Adjusted R^2	0.22388	0.83813	0.96305	0.9338	0.98477

Detailed equations were listed as follows. And statistical data were shown in Table S4.

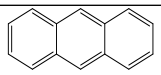
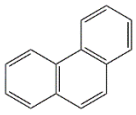
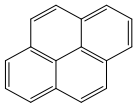
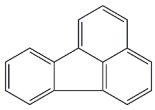
Reaction kinetics could be described by a pseudo-first order model which was explicated in equation (1) and (2):

$$-\frac{dC}{dt} = k_{obs}t \quad (1)$$

$$ln\frac{C_0}{C_t} = k_{obs}t \quad (2)$$

Where k_{obs} was the rate constant of pseudo-first-order reaction, t was the corresponding reaction time, C_0 and C_t were the initial and instantaneous concentrations of PAHs, respectively.

Table S5 The chemical structures and physicochemical characteristics of anthracene, phenanthrene, pyrene and fluoranthene.

PAH congener	Chemical structure	molecular weight g mol^{-1}	solubility mg L^{-1}	vapor pressure mm Hg	log K_{ow}
Anthracene [a]		178.2	1.3	$6.56x10^{-6}$	4.45
Phenanthrene [a]		178.2	1.2	$1.21x10^{-4}$	4.46
Pyrene [a]		202.3	0.14	$4.50x10^{-6}$	4.88
Fluoranthene [a]		202.3	0.12	$9.22x10^{-6}$	5.16

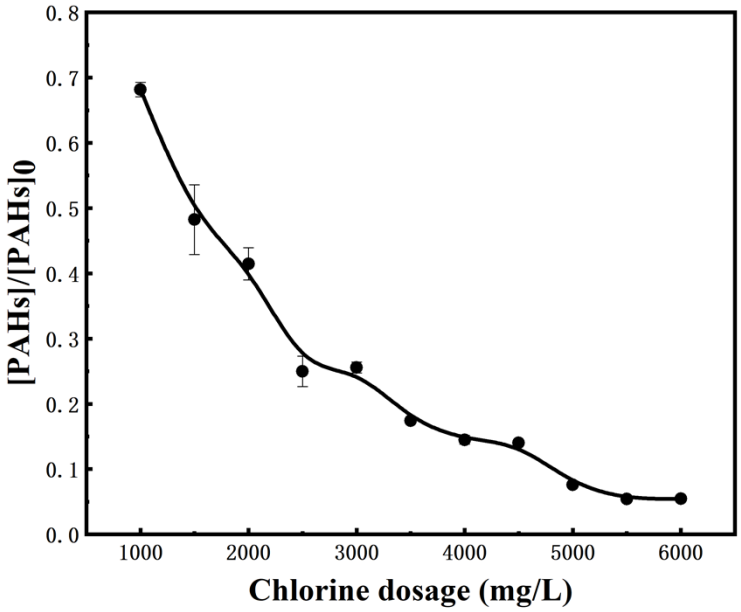


Fig. S1. The degradation of PAHs with different effective chlorine dosages.

To select the dose of effective chorine, preliminary experiments were conducted. With an initial concentration of 2469.9 mg/kg, PAHs were degraded gradually by HClO oxidation with effective chlorine dosages ranging from 1000 to 6000 mg/L (Figure S1). It could be found that the degradation efficiency of PAHs increased with the increase of chlorine dosages. Moreover, when the chlorine dosage was higher than 5000 mg/L, the degradation efficiency of PAHs only increased slightly. Therefore, we set chlorine dosage as 1000, 2000, 3000, 4000, and 5000 mg/L for the time-dependent degradation of PAHs.

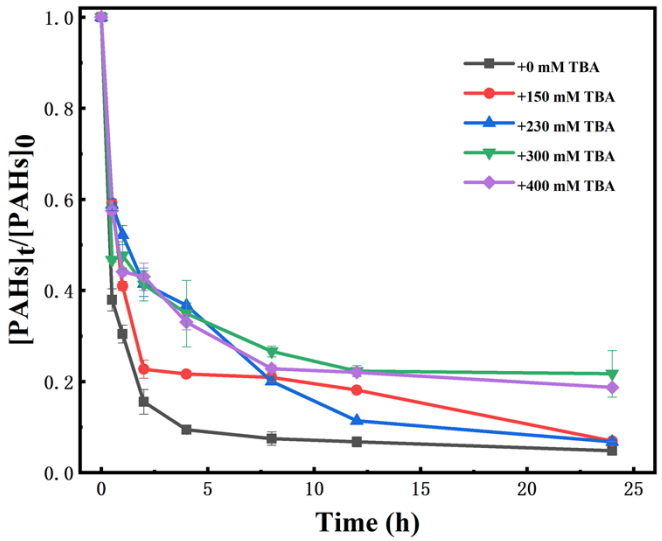


Fig.S2. The effect of TBA dosages on the PAHs degradation in the contaminated industrial soil by HOCl oxidation. Experimental conditions: $[PAHs]_0$=2469.9 mg/kg, $[Cl_2]_0$=5000 mg/L, pH=5.

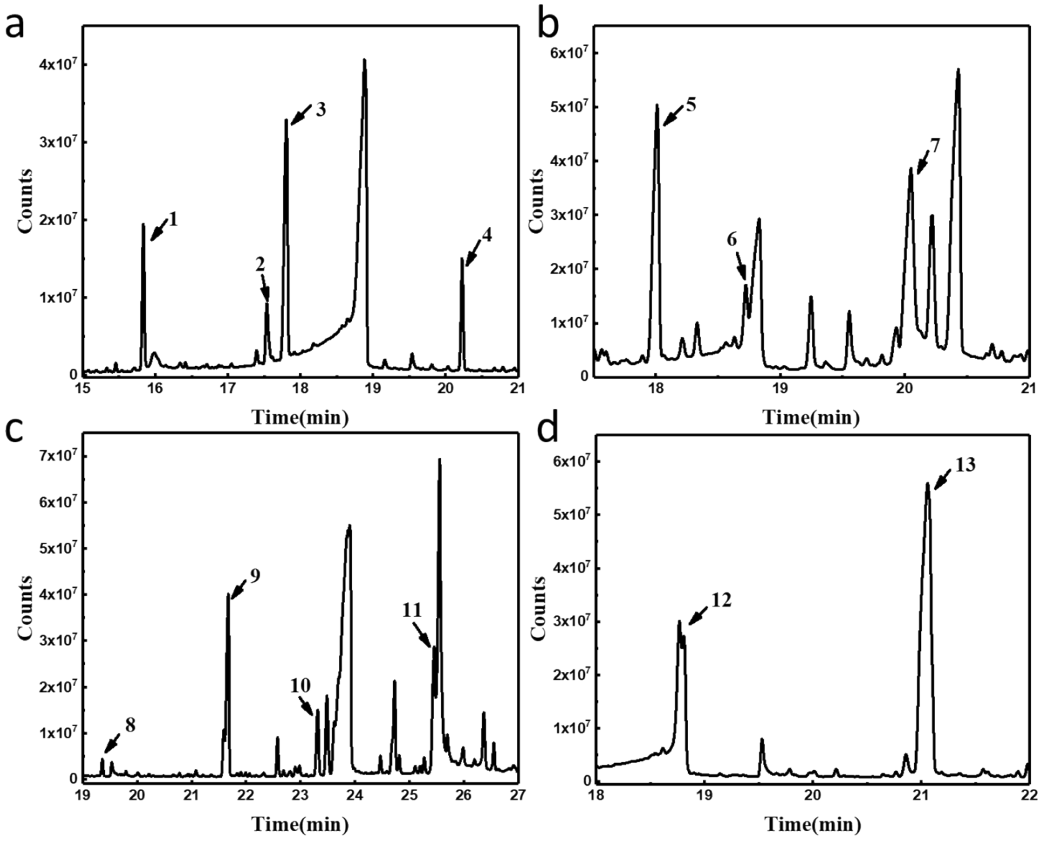
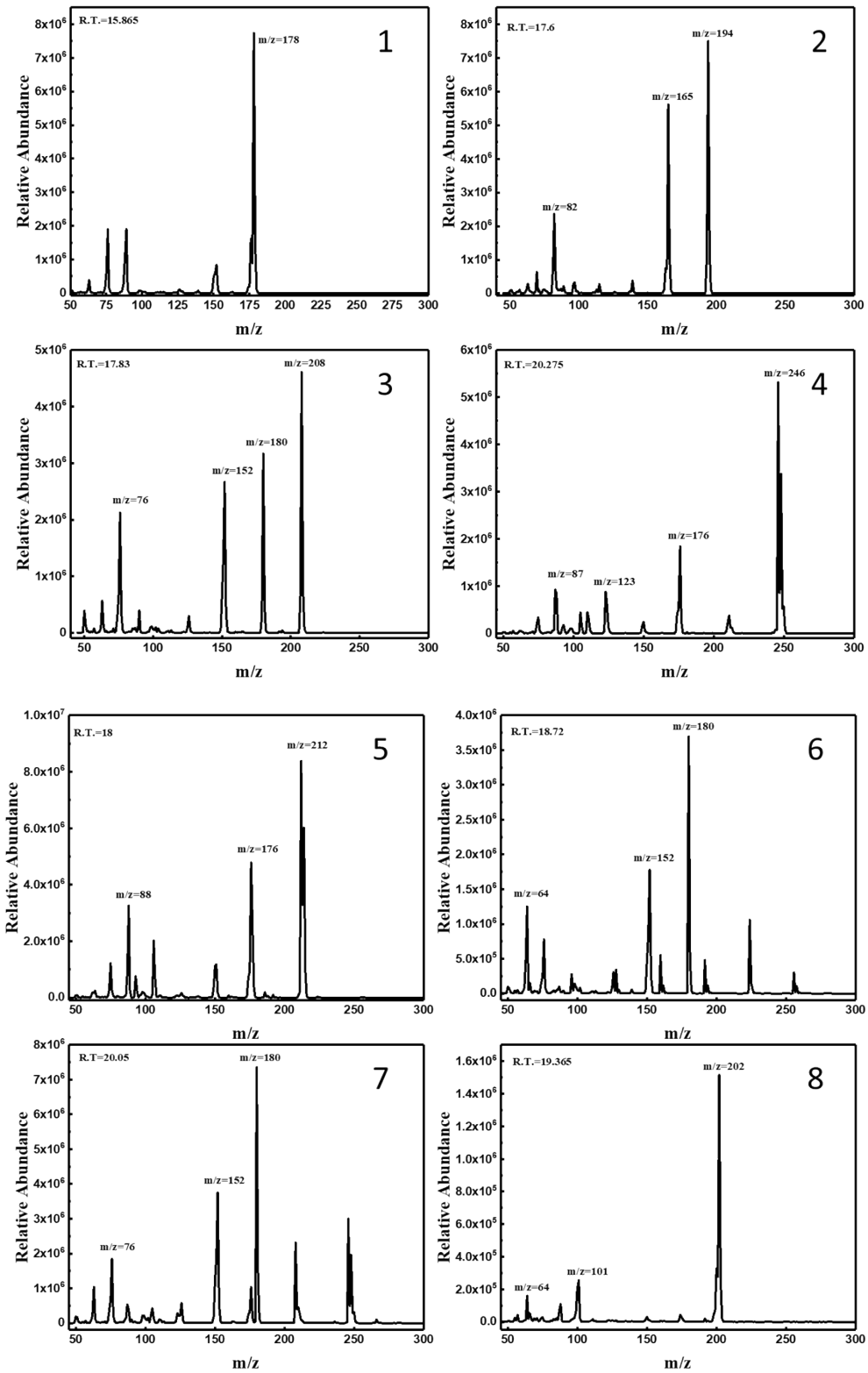


Fig.S3 Total ion chromatogram of degradation products by HOCl oxidation of (a) anthracene, (b) phenanthrene, (c) pyrene, and (d) fluoranthene. Experimental conditions: $[PAHs]_0$= 1 mg/L, $[Cl_2]_0$=100 mg/L, pH=5, reaction time=12 h.


1
R.T.=15.865
m/z=178
2
R.T.=17.6
m/z=194
m/z=165
m/z=82
3
R.T.=17.83
m/z=208
m/z=180
m/z=152
m/z=76
4
R.T.=20.275
m/z=246
m/z=176
m/z=87
m/z=123
5
R.T.=18
m/z=212
m/z=176
m/z=88
6
R.T.=18.72
m/z=180
m/z=152
m/z=64
7
R.T=20.05
m/z=180
m/z=152
m/z=76
8
R.T.=19.365
m/z=202
m/z=101
m/z=64
Relative Abundance
m/z

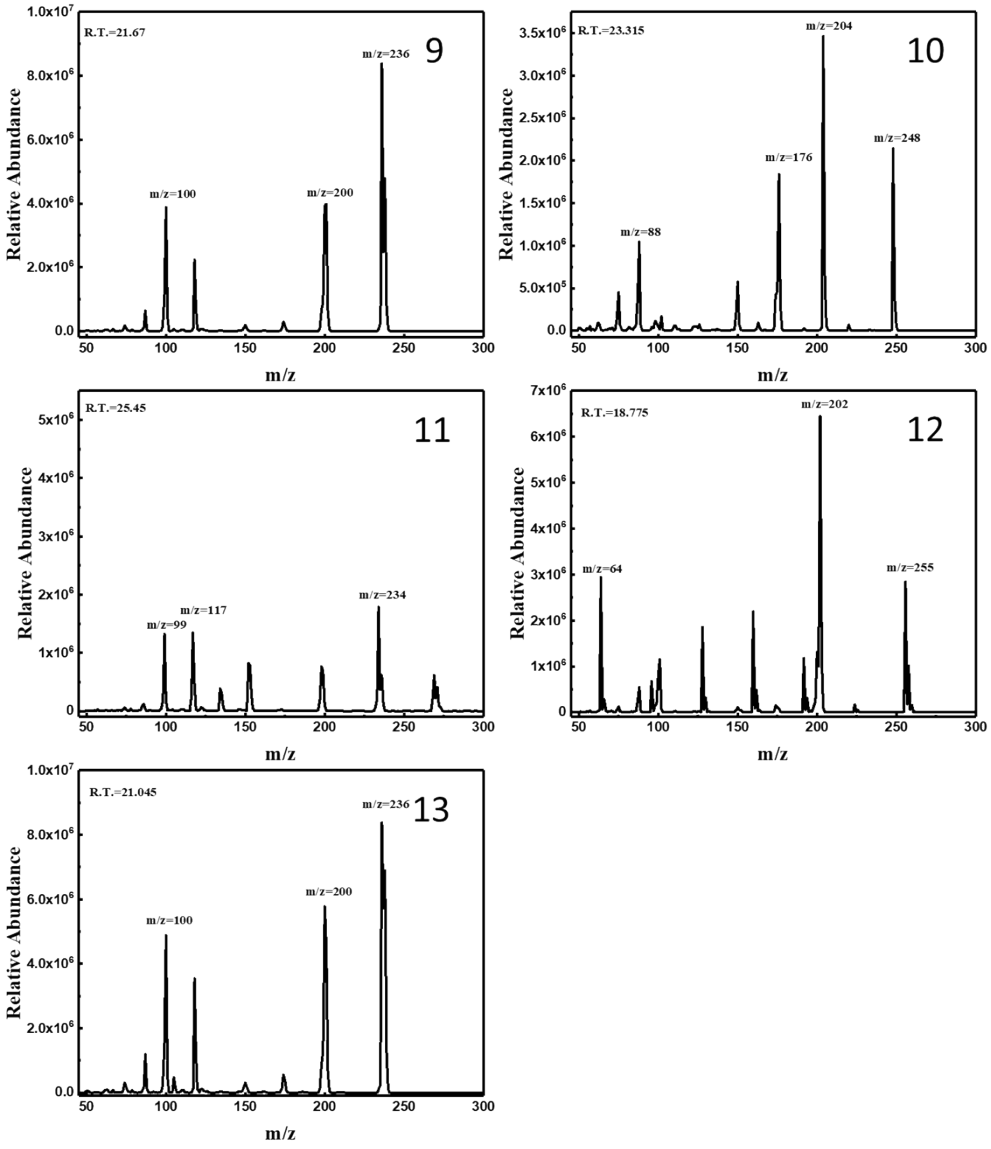


Fig. S4 Mass spectra of anthracene, phenanthrene, pyrene, fluoranthene and their degradation intermediates by HOCl oxidation. R.T.=retention time. Experimental conditions: $[PAHs]_0$= 1 mg/L, $[Cl_2]_0$=100 mg/L, pH=5, reaction time=12 h.

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