Supplementary Data

Enhancement of advanced Fenton process by weak magnetic field for the degradation of 4-nitrophenol

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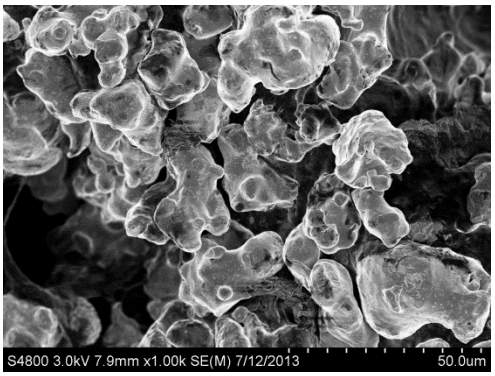
Number of Tables: 5

Text S1

To identify the existence of hydroxyl radicals, the electron paramagnetic resonance (EPR) signals of radicals trapped by 5,5-dimethyl-1-pyrroline-1-oxide (DMPO) were obtained using an EPR spectrometer (Bruker A200 ESP 300E) equipped with a Quanta-ray Nd/YAG laser system and an irradiation light source (k = 355 nm) at ambient temperature. The experimental condition was: the center field of 338.2 mT, sweep width of 5 mT, a sweep time of 110 s, microwave frequency of 9.80 GHz, and microwave power of 5.65 mW.

a



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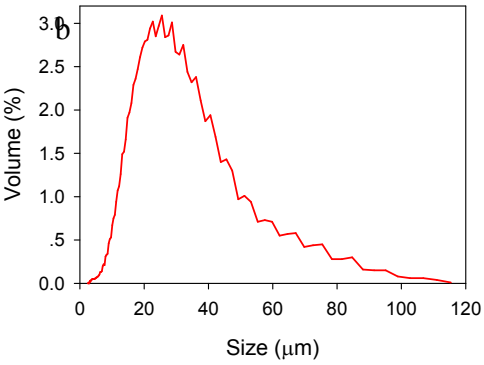


Fig. S1. (a) SEM image and (b) Particle size distribution of Fe^0 employed in this study.

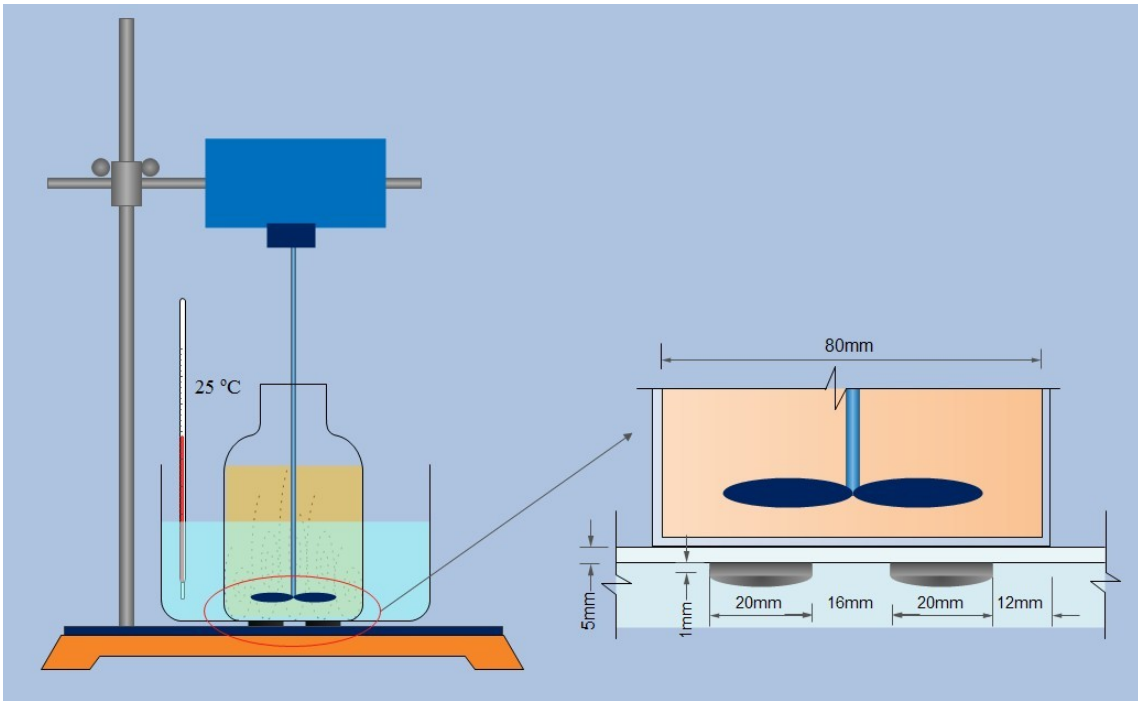


Fig. S2. The experimental setup of nonuniform MF.

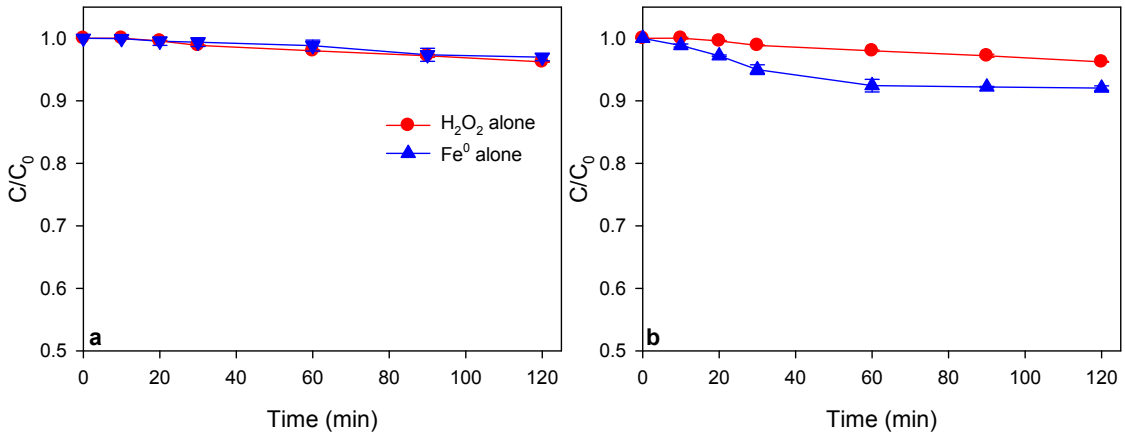


Fig. S3. Removal of 4-NP by H_2O_2 alone or Fe^0 alone (a, without WMF; b, with WMF). Reaction conditions: $[4\text{-NP}]_0 = 0.02$ mM, $[H_2O_2]_0 = 0.5$ mM, $[Fe^0]_0 = 0.5$ mM, $pH_{ini} = 4.0$, T = 25 °C.

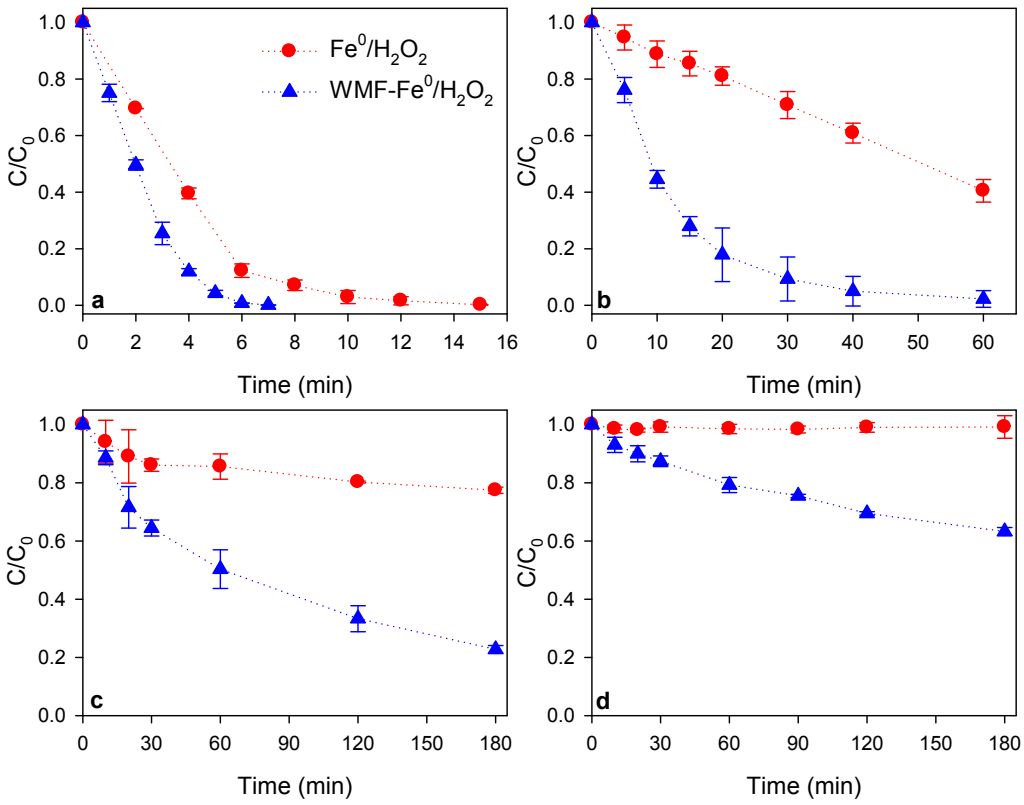


Fig. S4. Influence of WMF on 4-NP removal by Fe^0/H_2O_2 system at different pH_{ini} levels (a, pH_{ini} 3.0; b, pH_{ini} 4.0; c, pH_{ini} 5.0; d, pH_{ini} 6.0). Reaction conditions: $[4\text{-NP}]_0$ = 0.02 mM, $[H_2O_2]_0$ = 0.5 mM, $[Fe^0]_0$ = 0.5 mM, T = 25 °C.

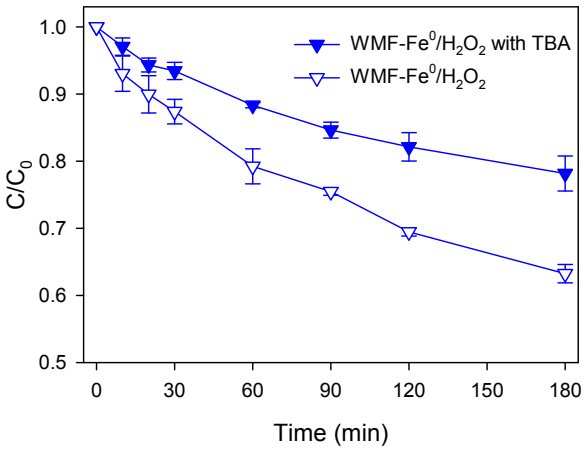


Fig. S5. Effect of radical quenching agent on 4-NP removal in WMF-Fe^0/H_2O_2 system at pH_{ini} 6.0. Reaction conditions: $[TBA]_0$ = 0.1 M, $[4\text{-NP}]_0$ = 0.02 mM, $[H_2O_2]_0$ = 0.5 mM, $[Fe^0]_0$ = 0.5 mM, T = 25 ^oC.

Fig. S6. (a) The MF strength distributions of the plane parallel to the applied uniform MF (with the applied flux densities of 5 mT, 10 mT and 20 mT, respectively) and through the center of a Fe^0 sphere; (b) The MF gradients around a Fe^0 sphere when the flux densities of applied MF are 5 mT, 10 mT and 20 mT, respectively. The arrow shows the direction of the applied uniform MF.

Fig. S7 Aggregation of Fe^0 particles under a uniform MF of 50 mT.

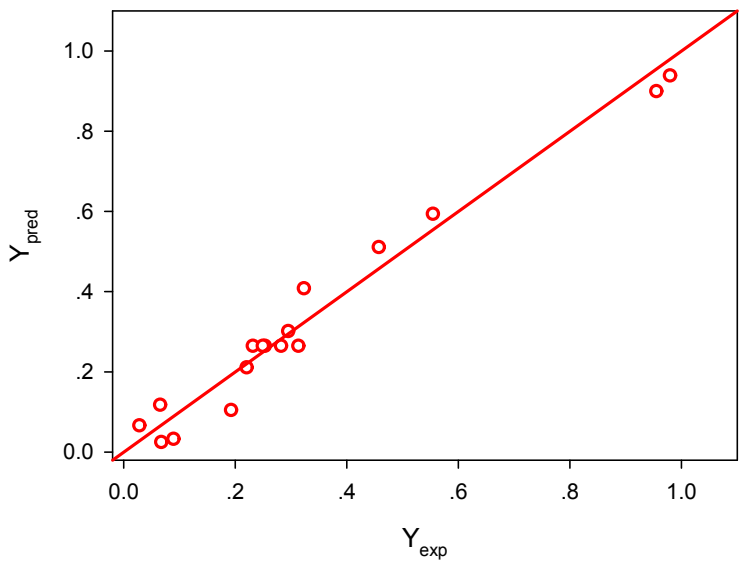


Fig. S8. Comparison between the calculated and experimental values of the output.

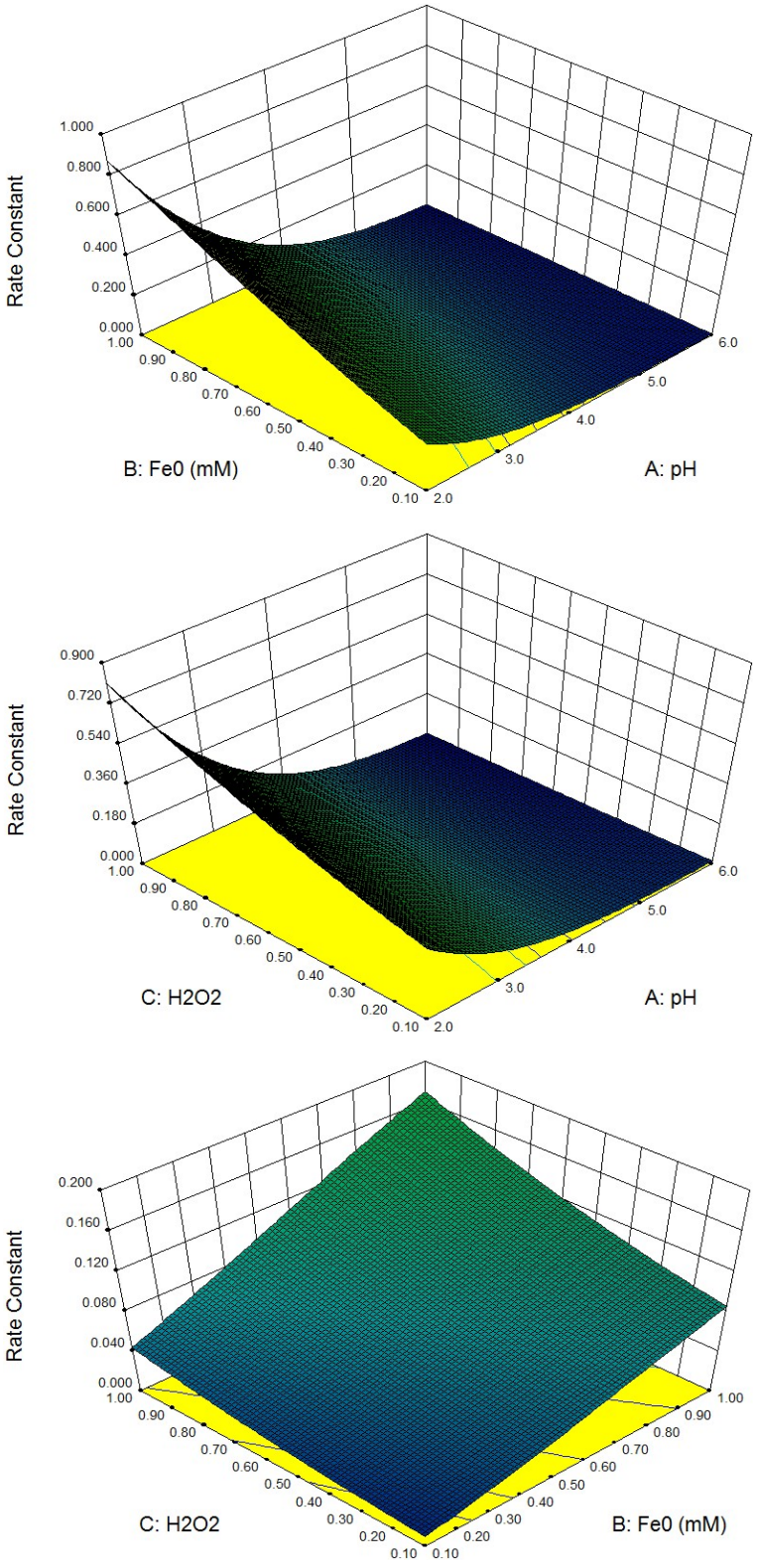


Fig. S9. Response surface plots of the rate constant of 4-NP for the three most important pair of factors.

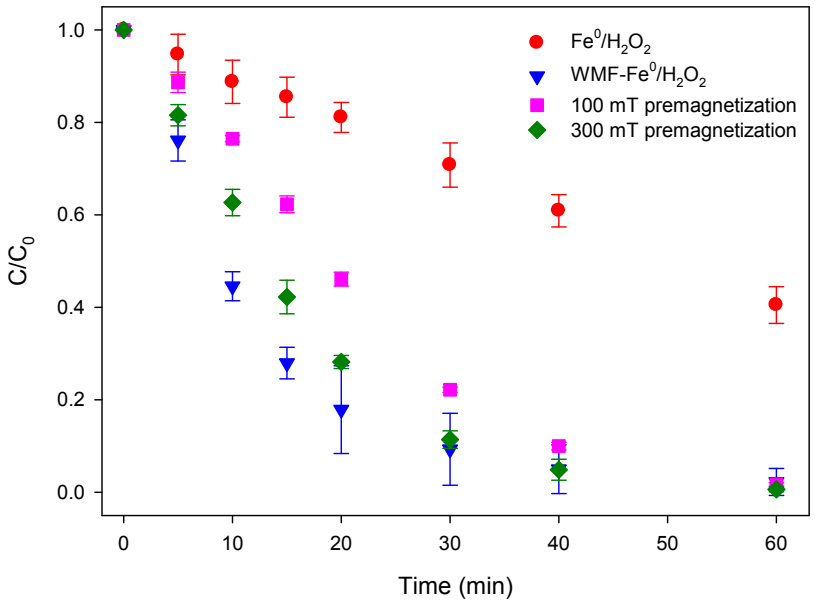


Fig. S10. Influence of premagnetization on 4-NP removal by Fe^0/H_2O_2. Reaction conditions: $[4\text{-NP}]_0$ = 0.02 mM, $[H_2O_2]_0$ = 0.5 mM, $[Fe^0]_0$ = 0.5 mM, pH_{ini} = 4.0, T = 25 °C.

Table S1 Details of the LC-MS/MS gradient program.

Time (min)	0.1% FA-Water (%)	0.1% FA-Acetonitrile (%)	Flow rate (mL min^{-1})
0	95	5	0.4
1	80	20	0.4
3	55	45	0.4
6	0	100	0.4
9	0	100	0.4
9.5	95	5	0.4
11.5	95	5	0.4

Table S2 Experimental range and levels of the independent variables.

Independent factors	Units	Symbol	Coded levels		
			-1	0	+1
pH	-	A	2.0	4.0	6.0
Fe^0 dosage	mM	B	0.10	0.55	1.00
H_2O_2 dosage	mM	C	0.10	0.55	1.00

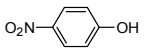
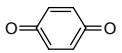
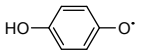
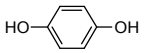
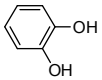
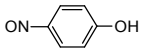
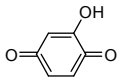
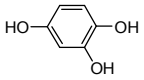
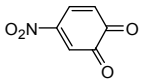
Table S3 ANOVA test for response function Y.

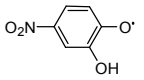
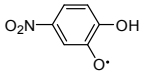
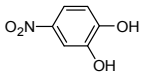
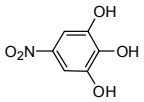
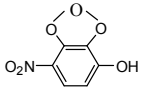
Source	Sum of squares	d.f.	Mean square	F-ratio	P-value
Model	1.1863	9	0.1318	24.6245	0.0002
A-pH	0.9086	1	0.9086	169.7338	< 0.0001
B-Fe^0	0.0777	1	0.0777	14.5089	0.0066
C-H_2O_2	0.0263	1	0.0263	4.9114	0.0622
AB	0.0532	1	0.0532	9.9293	0.0161
AC	0.0397	1	0.0397	7.4121	0.0297
BC	0.0000	1	0.0000	0.0000	0.9992
A^2	0.0799	1	0.0799	14.9273	0.0062
B^2	0.0010	1	0.0010	0.1774	0.6862
C^2	0.0002	1	0.0002	0.0380	0.8511
Residual	0.0375	7	0.0054		
Lack of Fit	0.0334	3	0.0111	10.7975	0.0218
Pure Error	0.0041	4	0.0010		
Cor Total	1.2238	16			

Table S4 Comparison of the experimental and predicted values of the response for diffierent experimental points.

pH	Fe^0 (mM)	H_2O_2 (mM)	Sqrt(k_{obs})	
			Observed	Predicted
3.75	1.00	0.10	0.3028	0.3455
3.75	0.55	0.55	0.2559	0.3064
5.50	0.55	1.00	0.0678	0.0717

Table S5 Summary of intermediates detected in various processes for 4-NP oxidation ("√" stands for detected and "-" stands for non-detected).

MW (m/z)	Chemical structure	Ultrasonic Irradiatio[33]	Electro-Fenton[31]	Plasma-TiO_2[34]	UV/H_2O_2[32]	Photo-Fenton[35]	Wet electrocatalytic oxidation[36]	Ozonatio[37]	WMF-Fe^0/H_2O_2 (This study)
139					√ Detected	- Undetected			
94		-	-	√	-	-	-	√	-
108		√	√	√	√		√	√	-
108		-	-	-	-	-	-	√	-
109		√	-	√	-	-	-		-
110		√	√	√	√		√	√	-
110		-	-	√	-	-	-	√	-
123		-	-	-	-	-	-	-	√
124		-	-	-	-	-	√	-	-
126		-	√	-	√	-	√	-	-
153		-	-	-	-	√	-	-	-

154		-	-	-	-	-	-	-	√
154		-	-	-	-	-	-	-	√
155		√	√	-	√	√	√	-	√
171		-	√	-	√	-	-	-	√
189		-	-	√	-	-	-	-	-