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Exploring the mechanism of Fe(III)-activated Fenton-like reaction based on the quantitative study

Hehe Qin [a], *Jinhong Fan* [a, b, c]*, *Shun Mao* [a, b]

[a] State Key Laboratory of Pollution Control and Resources Reuse, College of Environmental Science and Engineering, Tongji University, 200092 Shanghai, China

[b]Shanghai Institute of Pollution Control and Ecological Security, 200092 Shanghai, China

[c] Nangjing University & Yancheng Academy of Environmental Protection Technology and Engineering, Yancheng, Jiangsu Province, 224000, China

List of Authors:

Hehe Qin (AcademicQHH@163.com) (first author)

Jinhong Fan (jinhongfan@tongji.edu.cn) (corresponding author)

Shun Mao (Shunmao@tongji.edu.cn)

Text S1. Fenton mechanism equations

$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + \cdot OH + OH^-$ $k = 40 - 80\ M^{-1}s^{-1}$ (S1)

$\cdot OH + H_2O_2 \rightarrow H_2O + \cdot OH_2$ $k = 2.7\times10^7\ M^{-1}s^{-1}$ (S2)

$\cdot OH + Fe^{2+} \rightarrow Fe^{3+} + OH^-$ $k = 3\times10^8\ M^{-1}s^{-1}$ (S3)

$\cdot OH_2 + H_2O_2 \rightarrow H_2O + O_2 + \cdot OH$ $k = 3\ M^{-1}s^{-1}$ (S4)

$Fe^{3+} + H_2O_2 \rightarrow Fe^{2+} + \cdot HO_2 + H^+$ (S5)

$Fe^{3+} + H_2O_2 \rightarrow Fe(HO_2)^{2+} + H^+$ $k = 3.1\times10^{-3}\ M^{-1}s^{-1}$ (S5a)

$Fe(HO_2)^{2+} \rightarrow Fe^{2+} + \cdot HO_2$ $k = 2.7\times10^{-3}\ s^{-1}$ (S5b)

$Fe^{2+} + \cdot HO_2 + H^+ \rightarrow Fe^{3+} + H_2O_2$ $k = 1.2\times10^6\ M^{-1}s^{-1}$ (S6)

$Fe^{3+} + \cdot HO_2 \rightarrow Fe^{2+} + O_2 + H^+$ $k = 1.2\times10^6\ M^{-1}s^{-1}$ (S7)

$\cdot HO_2 + \cdot HO_2 \rightarrow O_2 + H_2O_2$ $k = 1\times10^6\ M^{-1}s^{-1}$ (S8)

Text S2. 4-CP degradation equations with different activators

$C_6H_5OCl + H_2O_2 \xrightarrow{light} C_6H_6O_2$ (HQ) or $C_6H_6O_2Cl$ (pCC) $+ H_2O$ (S9)

$C_6H_5OCl + 2H_2O_2 + Fe^{2+} \rightarrow C_6H_6O_2$ or $C_6H_6O_2Cl + OH^- + Fe^{3+}$ (S10)

$C_6H_5OCl + 4H_2O_2 + Fe^{3+} \rightarrow C_6H_6O_2$ or $C_6H_6O_2Cl + H_2O + Fe^{3+} + 2\cdot O_2H$ (S11)

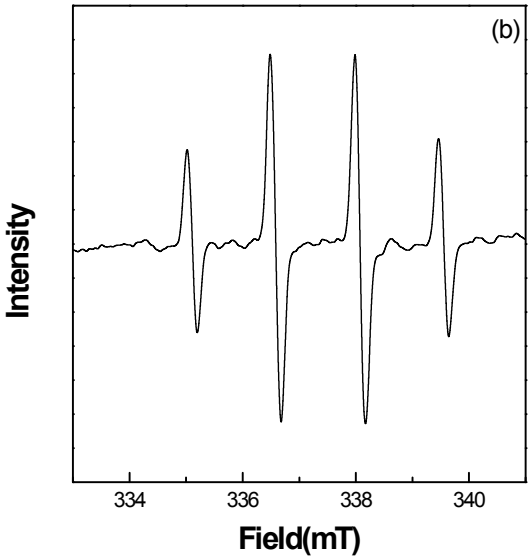
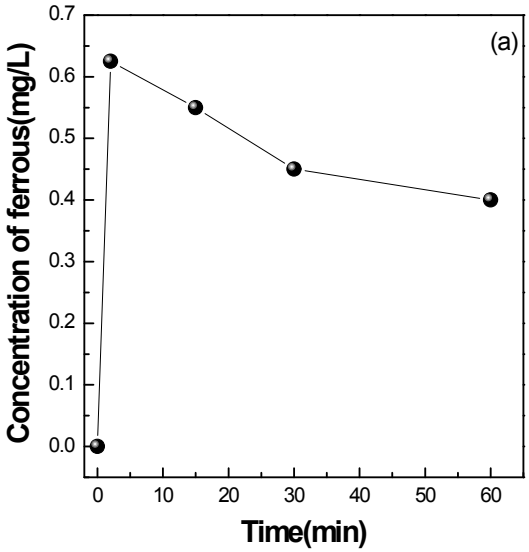


Figure S1 ESR pattern in the Fe(III)/H_2O_2 system

Condition: $[Fe(III)]_0 = 2$ mM, $pH_0 = 2.45$, $[H_2O_2]_0 = 1.6$ mM



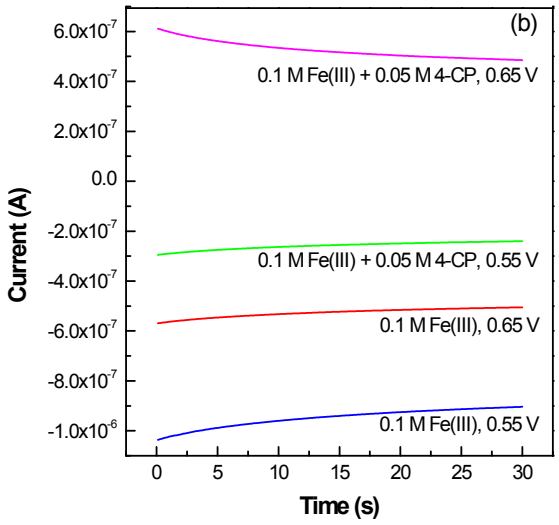
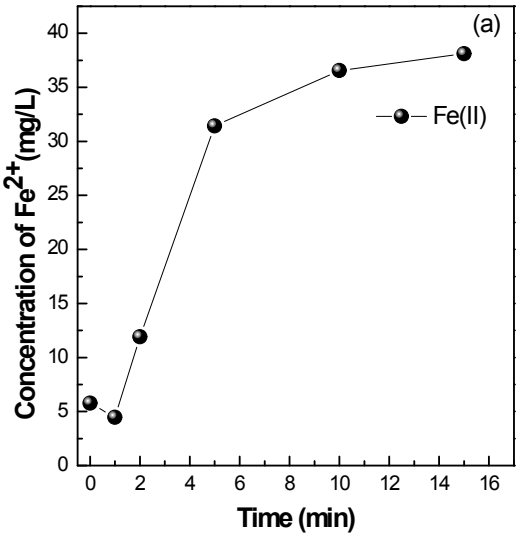


Figure S2. Yield profiles of ferrous ion in reaction of 4-CP with ferric (a) and Amperometric i-t curve ferric and mixture of ferric and 4-CP solution

Condition: $[4\text{-CP}]_0 = 0.4$ mM for (a) and 50 mM for (b), $[Fe(III)]_0 = 2$ mM for (a) and 100 mM for (b), $pH_0 = 2.45$



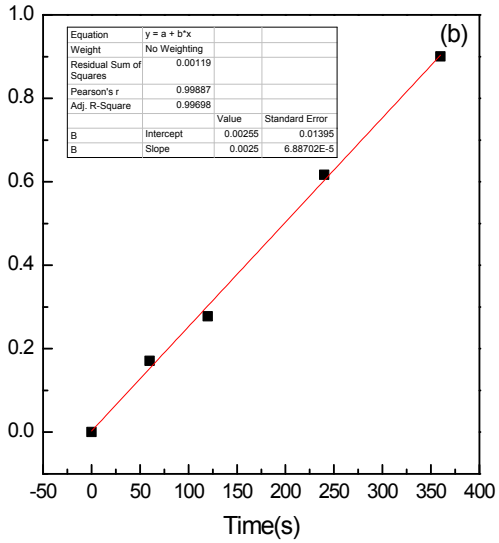


Figure S3. (a) Yield profiles of ferrous ion in reaction of BQ with ferric; (b) pseudo first-order kinetic fitting of BQ degradation

Condition: $[Fe(III)]_0 = 1$ mM, $[HQ]_0 = [BQ]_0 = 0.4$ mM, $[H_2O_2]_0 = 0.8$ mM, $pH_0 = 2.45$