Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Supplementary Information

Role of Al-based coagulants on hybrid ozonation-coagulation (HOC) process for WWTP effluent organic matter and ibuprofen removal

Xin Jin [1], *Yong Shi* [1], *Rui Hou*[1], *Weijie Zhang* [1], *Pengkang Jin* [1*], *Xiaochang Wang* [1]

[1] School of Environmental and Municipal Engineering, Xi'an University of Architecture and Technology, Xi'an, Shaanxi Province, 710055, China

Corresponding author: Pengkang Jin

Phone: +86 13379217572

E-mail: pkjin@hotmail.com

Number of pages:7
Number of text:1
Number of figures:10

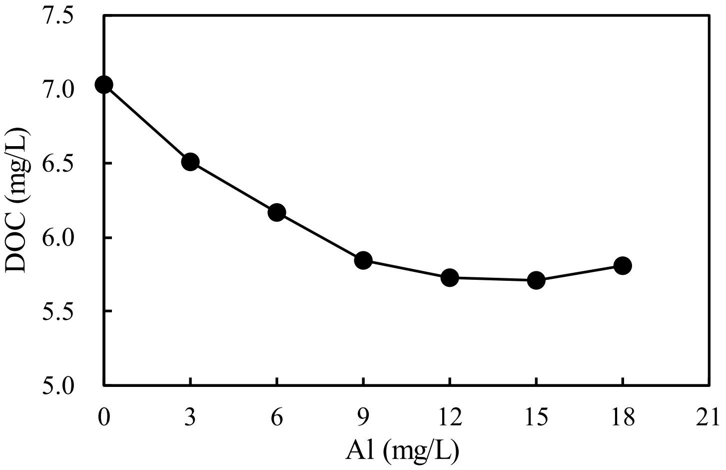


Fig. S1 DOC removal performance at different Al dosages at pH 8

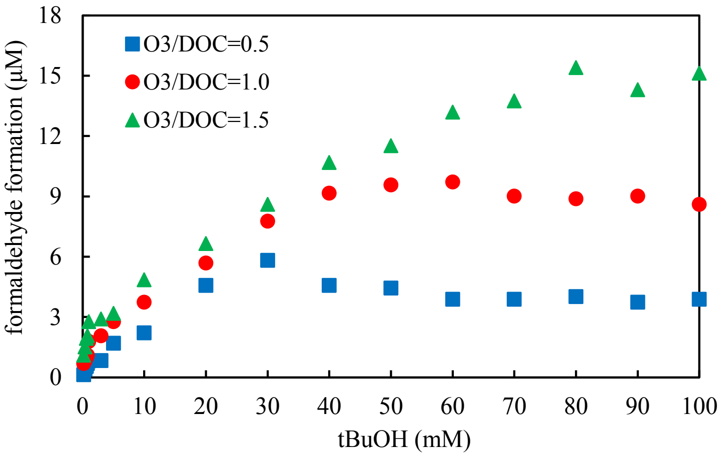


Fig. S2 Formaldehyde formation at different tBuOH dosages

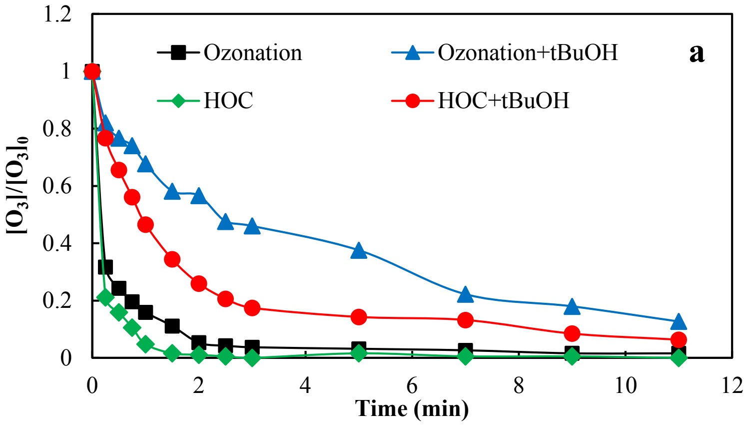
Text.S1. UV/H_2O_2 experiment procedures

UV/H_2O_2 experiment was used to obtain $\sum k_i[S_i]$. UV/H_2O_2 was used to generate •OH, and this experiment was conducted in ultrapure water. Experimental details were modified based on previous work[1]. A Low-pressure mercury lamp (254 nm, 40 W, Cnlight) positioned 5 cm above the water surface of the reactor (φ 5× 4 cm). The solution was adjusted to have concentrations of 12 mg/L [Al], 1 μM pCBA and 2 mM phosphate buffer (pH=8).

During the UV/H_2O_2 experiment, the rate of •OH generation can be calculated from Eq. (S1)[2].

$$r_{OH\bullet} = \Phi_{OH\bullet}.I_0 f_{H_2O_2}(1-e^{-A}) \tag{S1}$$

Where $\Phi_{\bullet OH}$ is the quantum yield of •OH at 254 nm, and $\Phi_{\bullet OH}$ is 1.00 in the bulk solution[3]. I_0 is the incident light intensity at 254 nm, and it was measured by an illuminometer (ST-51X, SENTRY, Taiwan); A is the fraction of light absorbed by the bulk solution, and is given by $A = 2.303b(\varepsilon_{H2O2}C_{H2O2}+\varepsilon_{HO2-}C_{HO2-}+\varepsilon_S C_S)$, where ε_{H2O2}=17.9-19.6 M^{-1} cm^{-1}, ε_{HO2-}=220 M^{-1} cm^{-1}, $\varepsilon_S C_S$ is the absorbance of other compounds in the water matrix at 254 nm, and b is the water path length. In this case, $AlCl_3 \cdot 6H_2O$ had no UV adsorption at 254 nm. Parameter f_{H2O2} is the fraction of absorbed light that is absorbed by H_2O_2 and HO_2^-, and is given by $f_{H2O2}=2.303b(\varepsilon_{H2O2}C_{H2O2}+\varepsilon_{HO2-}C_{HO2-})/A$. Based on Eq.(S1), •OH formation during UV/H_2O_2 experiment can be obtained in both ultrapure water and WWTP effluent (Fig. S5).



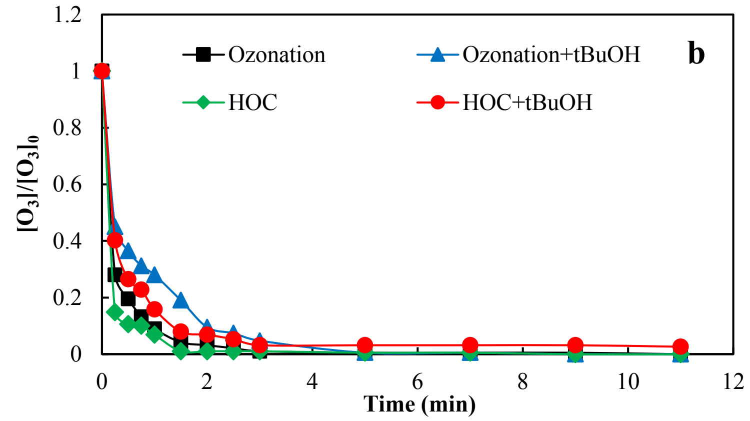


Fig. S3 Ozone depletion at pH 8 in the ozonation and HOC processes.

a: ultrapure water; b: WWTP effluent. tBuOH dosage: 10mM.

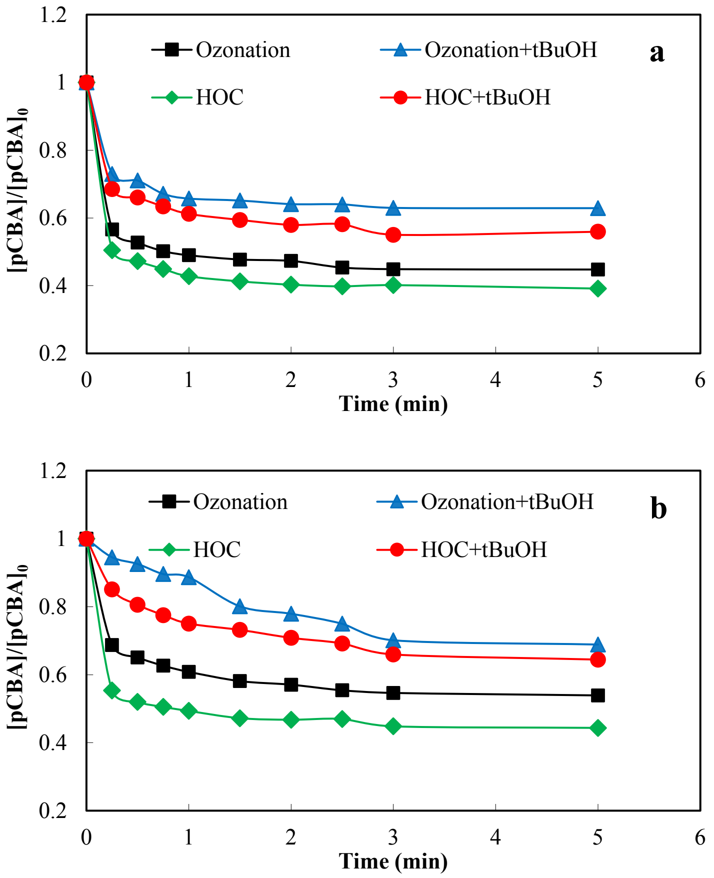


Fig. S4 pCBA decomposition at pH=8 in the ozonation and HOC processes.

a: ultrapure water; b: WWTP effluent

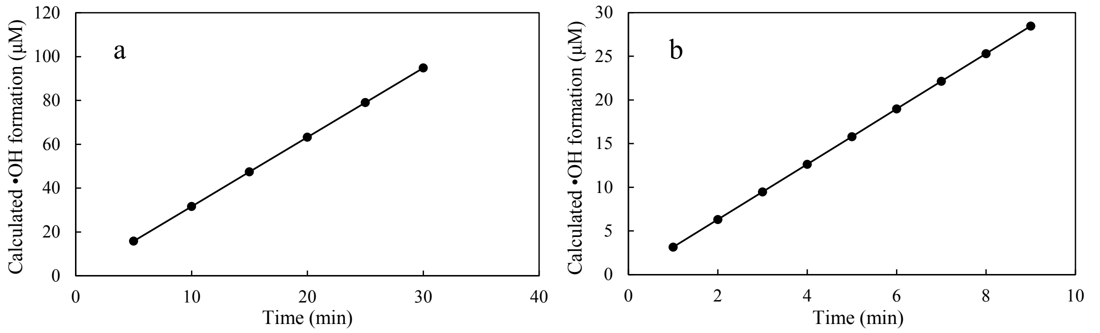


Fig. S5 •OH formation during UV/H_2O_2 experiment in ultrapure water (a) and WWTP effluent (b)

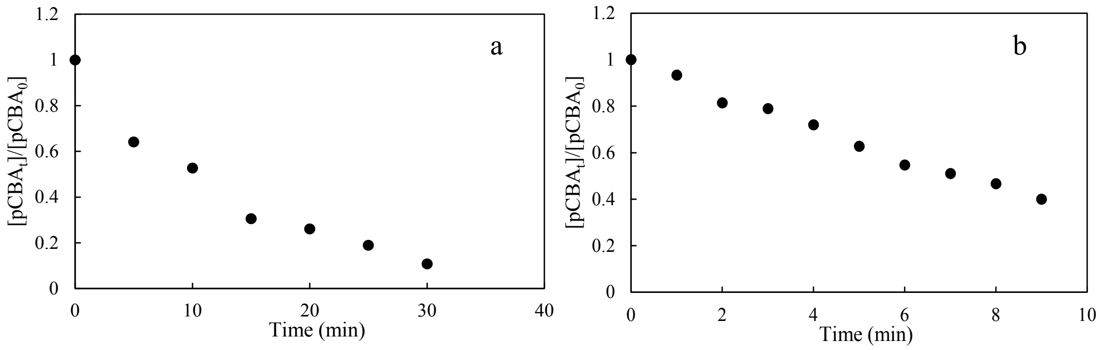


Fig. S6 pCBA removal during UV/H_2O_2 experiment in ultrapure water (a) and WWTP effluent (b)

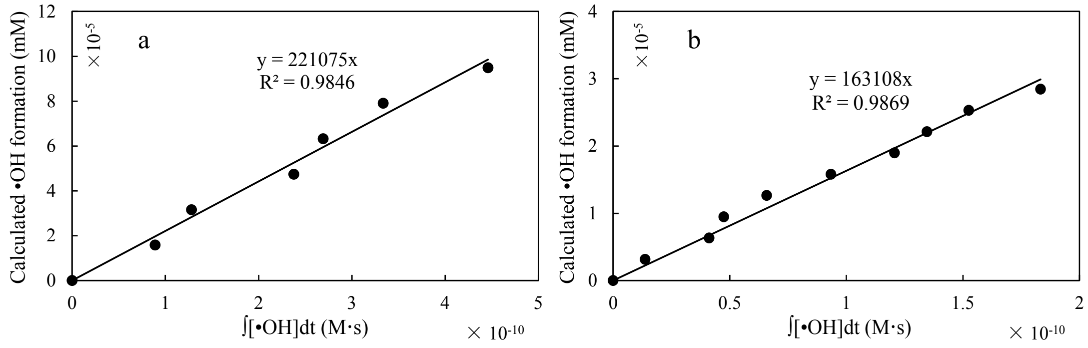


Fig. S7 $\sum k_i[S_i]$ calculation in (a) ultrapure water (P = 1E-5) and (b) WWTP effluent (P = 1E-7) (Calculated •OH formation vs. ∫[•OH]dt), the slope indicates $\sum k_i[S_i]$

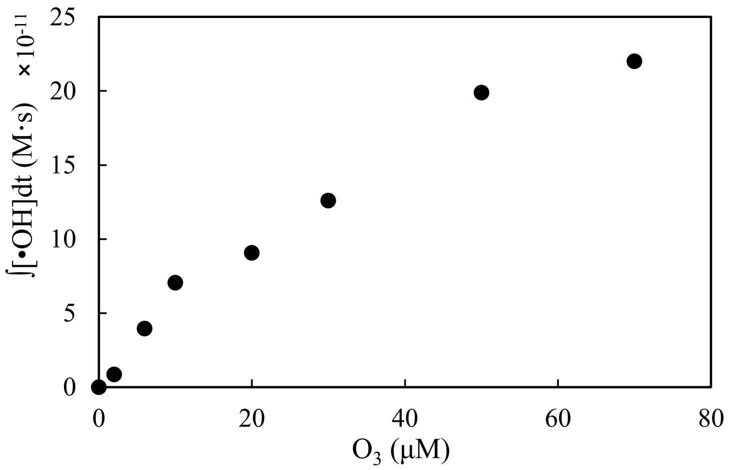


Fig. S8 ∫[•OH]dt at different ozone dosages in the HOC process in the ultrapure water

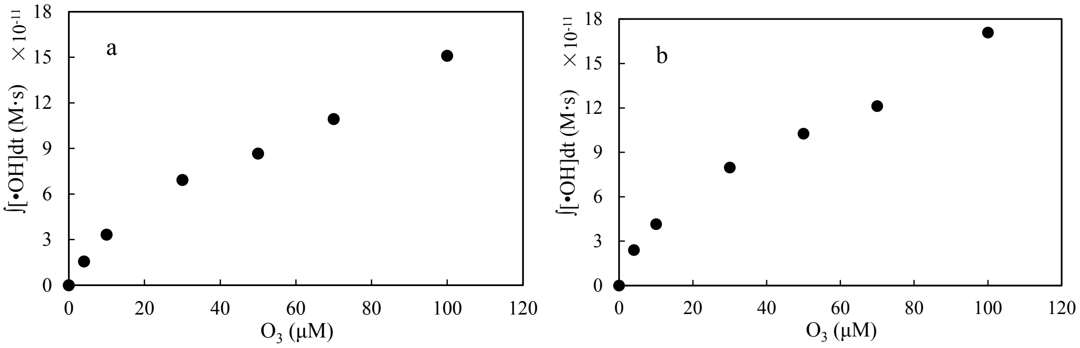


Fig. S9 ∫[•OH]dt at different ozone dosages in the HOC process in WWTP effluent. a: without $AlCl_3•6H_2O$; b: with $AlCl_3•6H_2O$

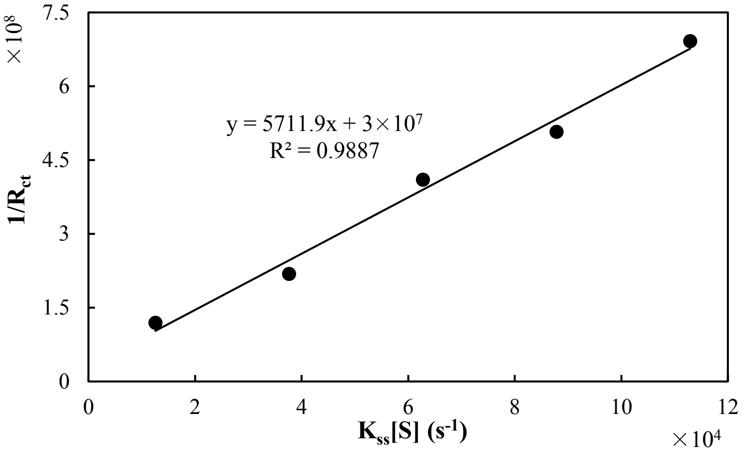


Fig. S10 The plots of $1/R_{ct}$ vs. (k_{SS}[S]) in ultrapure water without $AlCl_3$•$6H_2O$ (P = 5E-4)

References

1. Y. Liu, J. Jiang, J. Ma, Y. Yang, C. Luo, X. Huangfu, Z. Guo, Role of the propagation reactions on the hydroxyl radical formation in ozonation and peroxone (ozone/hydrogen peroxide) processes. *Water Res.*, 2015, **68**, 750-758.
2. J. C. Crittenden, S. Hu, D. W. Hand, S. A. Green, A kinetic model for H_2O_2/UV process in a completely mixed batch reactor. *Water Res.*, 1999, **33**, 2315-2328.
3. J. Baxendale, J. Wilson, The photolysis of hydrogen peroxide at high light intensities. *Transactions of the Faraday Society*, 1957, **53**, 344-356.