The acute toxicity evolution during ozonation of mono-chlorophenols and initial identification of high toxic intermediates

Supporting information

Dehua Ma[1], Jianjian Wei[1], Hongbo Zhang[1], Yukun Zhou[1], Jinyou Shen[1], Lianjun Wang[1,*], Peng Zhang[2,*]

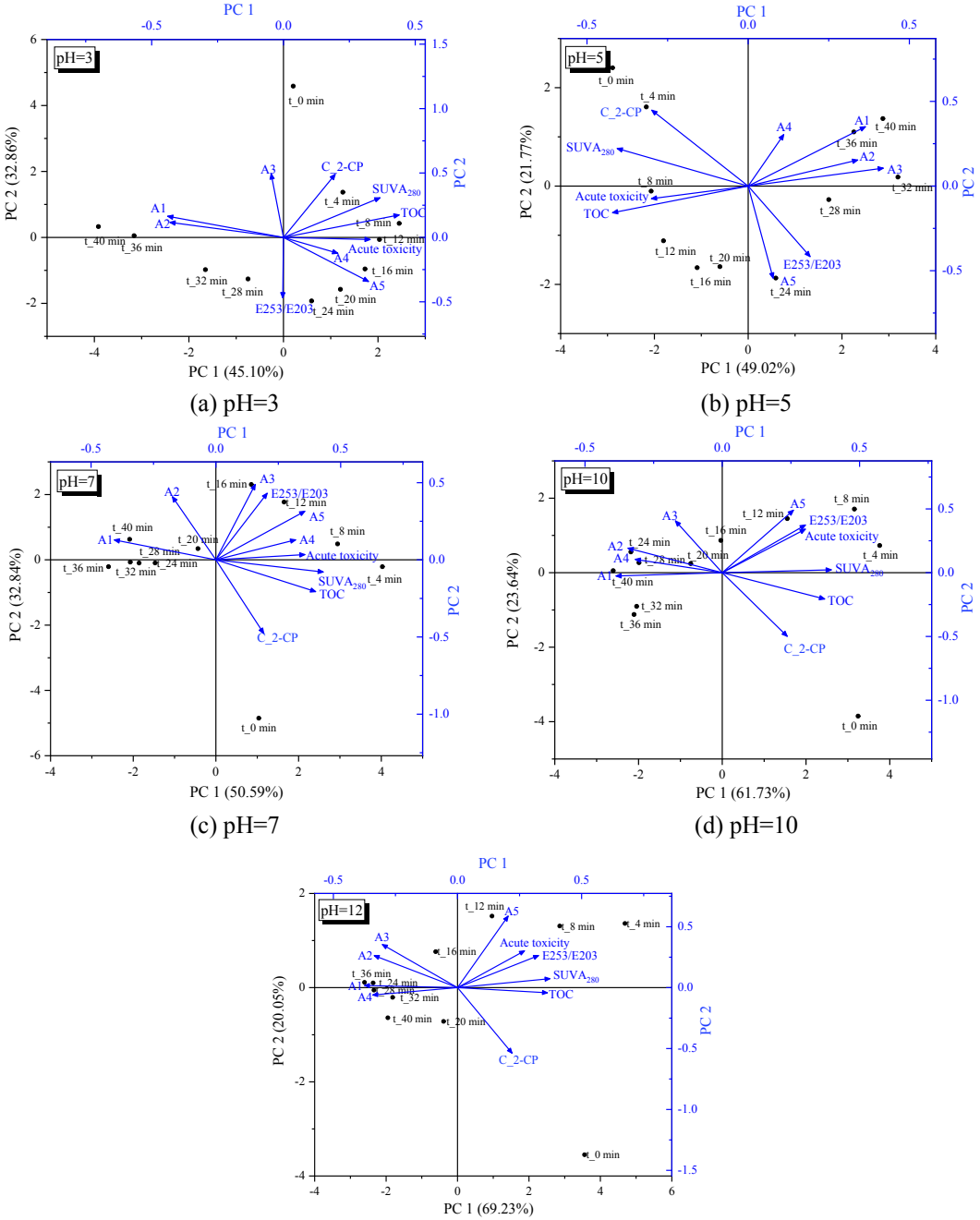
1. Key Laboratory of New Membrane Materials, Ministry of Industry and Information Technology; School of Environmental and Biological Engineering, Nanjing University of Science & Technology, Nanjing 210094, China

2. Transportation Institute of JSTI Group, Nanjing 211112, China

Corresponding author:

wanglj@njust.edu.cn (Lianjun Wang),

zp298@jsti.com (Peng Zhang)

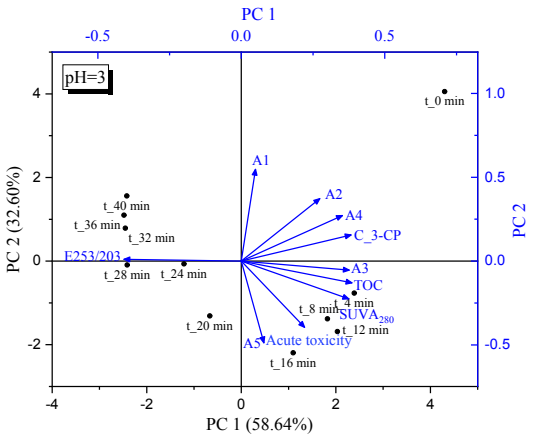


(a) pH=3 (b) pH=5

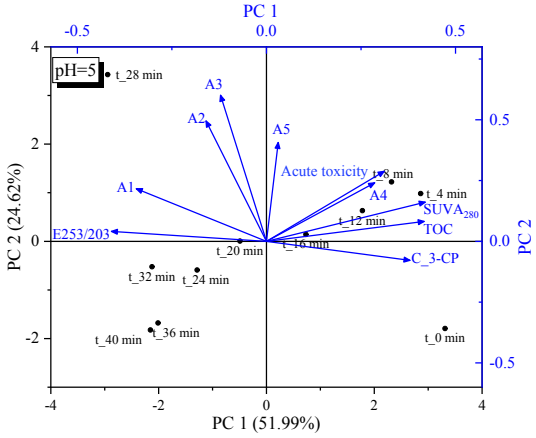
(c) pH=7 (d) pH=10

(e) pH=12

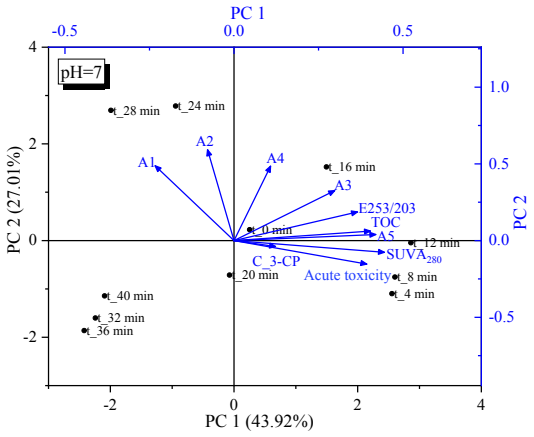
Fig. 1S Biplot for first two principal components of acute toxicity and other physiochemical parameters during the ozonation of 2-CP at different pH. The arrowhead lines intersecting at (0,0) represent the selected variables. Dots with black squares represent the ozonated samples.



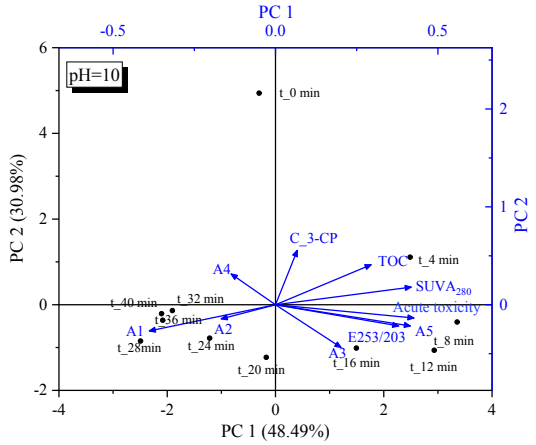
(a) pH=3



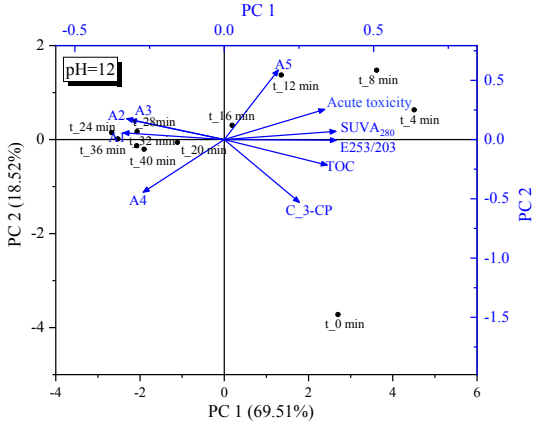
(b) pH=5



(c) pH=7

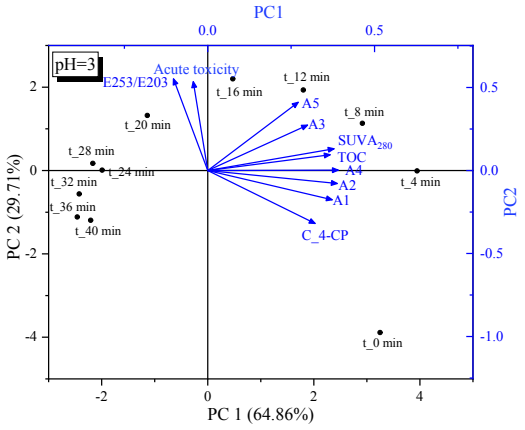


(d) pH=10

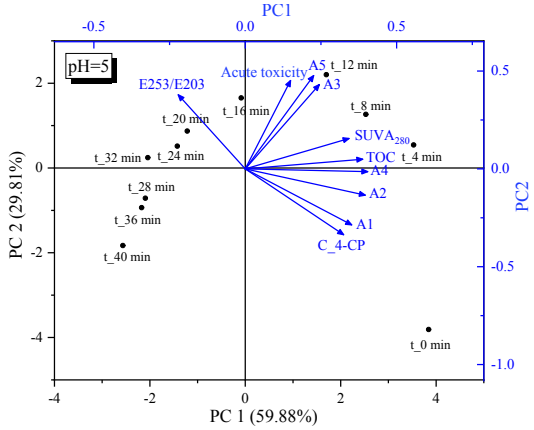


(e) pH=12

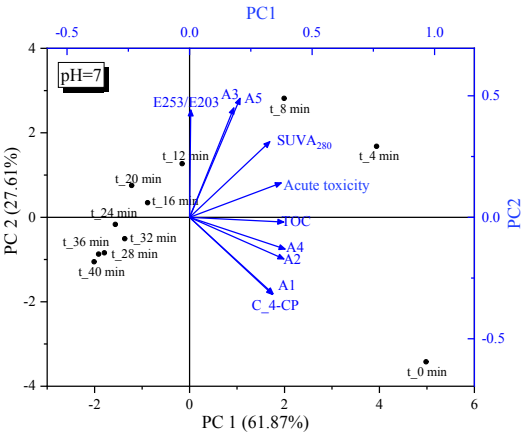
Fig. 2S Principal component analysis of acute toxicity with other physiochemical parameters during the ozonation of 3-CP at different pH.



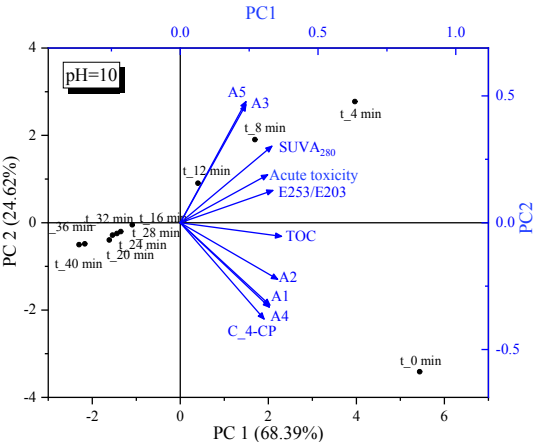
(a) pH=3



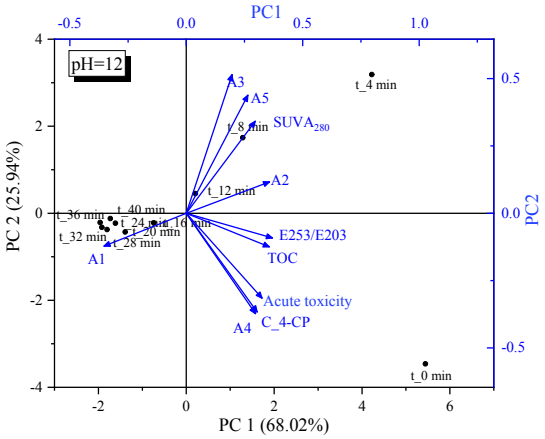
(b) pH=5



(c) pH=7



(d) pH=10



(e) pH=12

Fig. 3S Principal component analysis of acute toxicity with other physiochemical parameters during the ozonation of 4-CP at different pH.

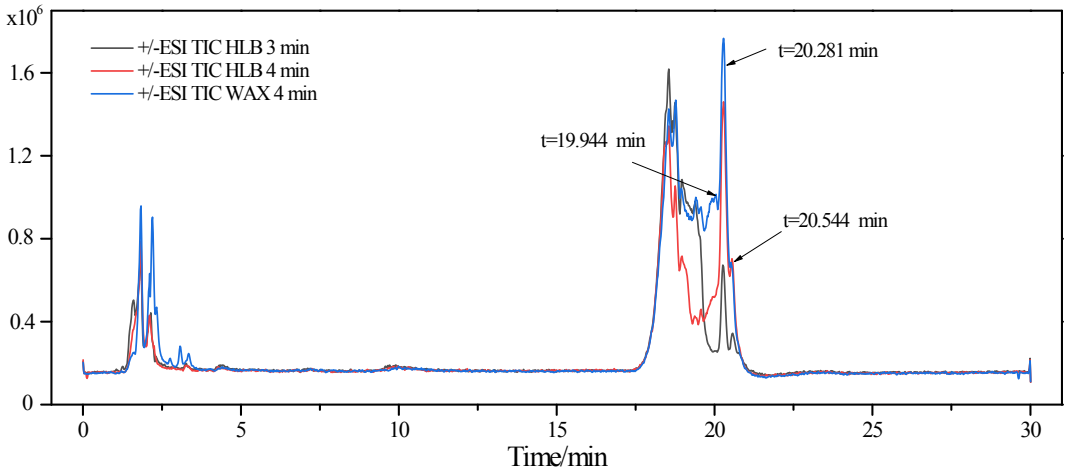


Fig. 4S Chromatogram of fractions HLB_3 min, HLB_4 min, WAX_4 min of 3-CP by LC-MS

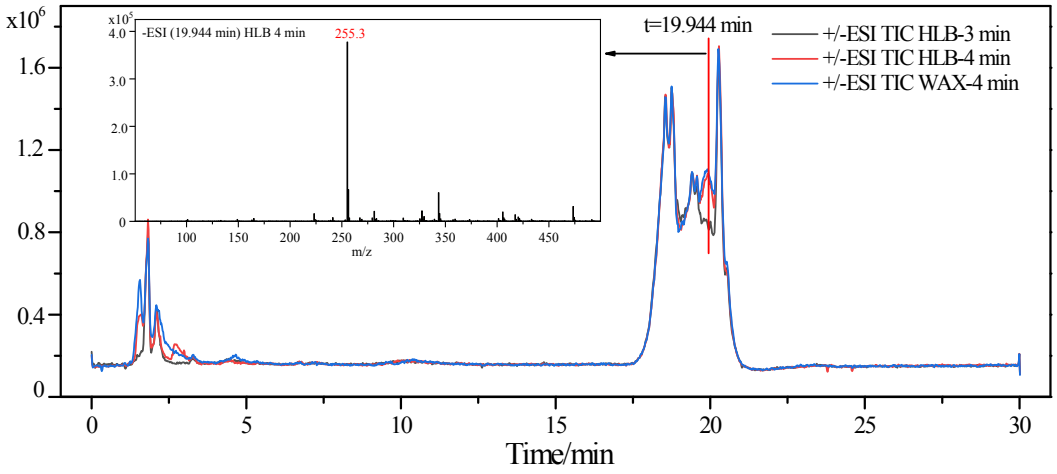


Fig. 5S Chromatogram of fractions HLB_3 min, HLB_4 min, WAX_4 min of 4-CP and mass spectrum of HLB_4 min at 19.944 min by LC-MS