

Article



Heterogeneous Catalytic Ozonation of Aniline-Contaminated Waters: A Three-Phase Modelling Approach Using TiO₂/GAC

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Supplementary Materials



Figure S1. Utilization efficiencies of ozone in a TiO₂/GAC catalytic system at different pHs (**a**) ¹ and inlet ozone concentrations (**b**) ² in the experimental ozonation system. Experimental conditions: $Q_G = 4 \text{ L} \text{ min}^{-1}$; $M_{CAT} = 3.3 \text{ g} \text{ L}^{-1}$; $T = 18.0 \text{ }^{\circ}\text{C}$; P = 1 atm; $V_{reac} = 1.5 \text{ L}$; (*Agitation*) = 60 rpm. ¹ Co₂in = 11.3 mg L⁻¹. ² pH = 7.0.



Figure S2. Effect of the ozone dose on the control stage during catalytic ozonation of aniline with the TiO₂/GAC catalyst. Experimental conditions: $Q_G = 4 \text{ L} \text{ min}^{-1}$; pH = 7.0; $M_{CAT} = 3.3 \text{ g} \text{ L}^{-1}$; T = 18.0 °C; P = 1 atm; $V_{reac} = 1.5 \text{ L}$; (*Agitation*) = 60 rpm.



Figure S3. Analysis of some by-products formed during the TiO₂/GAC ozonation of aniline in terms of TOC. Effect of catalyst dosage on the evolution of: (**a**) oxalic and (**b**) oxamic acid during ozonation. Experimental conditions: $Q_G = 4 \text{ L} \text{ min}^{-1}$; $C_{O_3^{\text{in}}} = 5.4 \text{ mg } \text{L}^{-1}$; pH = 7.0; *T* = 18.0 °C; *P* = 1 atm; *V*_{reac} = 1.5 L; (*Agitation*) = 60 rpm.



Figure S4. Analysis of the main intermediates in the aniline catalytic ozonation with TiO₂/GAC in terms of TOC, excluding oxalic and oxamic acid in different cases: (**a**) molecular attack of ozone at pH = 3.0; (**b**) ozone in excess and dominance of radicalary attack (pH = 7.0 and ozone dose of 20.1 mg L⁻¹); and (**c**) most favourable conditions (pH = 7.0, 5.4 mg L⁻¹ ozone concentration) or combined molecular radicalary attack. Experimental conditions: $Q_G = 4 \text{ L min}^{-1}$; $M_{CAT} = 3.3 \text{ g L}^{-1}$; T = 18.0 °C; P = 1 atm; $V_{reac} = 1.5 \text{ L}$; (*Agitation*) = 60 rpm.