Degradation of bisphenol A by ozonation and determination of degradation intermediates by gas chromatography–mass spectrometry and liquid chromatography–mass spectrometry

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**Highlights**

- The stoichiometric ratio between ozone and BPA was calculated to be 10.30 at pH 3.0.
- Mineralization of the BPA solution is not as successful as the oxidative degradation.
- Ten oxidation products are identified during BPA ozonation.
- Henry’s constant, $k_{H}$, increased 5.5% depending on growth of ionic strength of BPA solution.

**Abstract**

In this study, bisphenol A (BPA), an endocrine disruptor, was removed by ozonation process. During ozonolysis, degradation kinetics and degradation intermediates of BPA were determined and degradation stoichiometry was also calculated. The degradation of BPA was found to be optimal at pH 3.0 and BPA solution with 0.509 mM concentration was completely degraded after 25 min ozonation time. The stoichiometric ratio between ozone and BPA were calculated to be 10.30. The pseudo-first order degradation rate constant, $k_{obs}$, decreased in the range of 19.3–13.3 s$^{-1}$ when the initial concentration of BPA was raised from 0.051 to 0.509 mM. In addition, the second order rate constant, $k_{app}$ (BPA), was also calculated in the range of $2.18 \times 10^{-2} - 3.56 \times 10^{4}$ M$^{-1}$ s$^{-1}$. Henry’s constant, $k_{H}$, increased as 5.5% depending on growth of ionic strength of BPA solution during ozonation. As a result of the increase of $k_{H}$, dissolved ozone reduced throughout the ozonation. Ten different intermediates occurred during the ozonation of BPA and were identified via GC–MS and LC–MS/MS. Malonic and oxalic acids were observed among the intermediates in the first 5 min of ozonation and taken as markers of mineralization. $k_{0,TOC}$ value was calculated as 2.11 M$^{-1}$ min$^{-1}$ for BPA mineralization and the mineralization of ozonation was achieved about 30% at the end of 25 min ozonation.

1. Introduction

2,2-Bis(4-hydroxyphenyl)propane (bisphenol A, BPA) is a dimer of two para-hydroxyphenyls bonded through a methylene bridge and indispensable monomer for the production of various polymeric materials such as polycarbonate, epoxy resins, polyacrylates since the polymerization of the para-hydroxyphenyl rings of BPA can be easily controlled. Hence, the production of BPA has been found increasing market demand. For example, $7.6 \times 10^{8}$ and $5.6 \times 10^{7}$ kg of BPA are produced in the United States and China, respectively per year [1]. Notwithstanding its high commercial value, it has been shown that BPA is an endocrine disruptor even at a low concentration (1.0–10.0 mg L$^{-1}$) and can cause to detrimental health problems on people such as carcinogenesis [2–5]. Therefore, governments limited legally total BPA intake around 50 μg per