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# Degradation of trimethoprim by thermo-activated persulfate oxidation: Reaction kinetics and transformation mechanisms

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**Abstract**

Trimethoprim (TMP) is a dihydrofolate reductase inhibitor that is synergistically prescribed with sulfonamides to treat infectious disease in humans and animals. The widespread occurrence of TMP in natural environment may pose ecotoxicological risks to aquatic organisms and microalgae. In this work, we investigated the kinetics and mechanisms of TMP degradation by thermo-activated persulfate (PS) oxidation process in aqueous solution. Experimental results revealed that TMP could be effectively destructed at the temperature range of 50 – 65 $^{o}$C. Acidic pH facilitated the degradation of TMP. The pyrimidine moiety in TMP molecule was identified as the primary reactive site by comparison to substructural analogs. Solid phase extraction (SPE) coupled with liquid chromatography-electrospray ionization-triple quadrupole mass spectrometry (LC-ESI-MS/MS) was employed to identify the intermediate products. Thermo-activated PS oxidation of TMP produced several intermediates via hydroxylation and oxidation with $\alpha$-hydroxytrimethoprim (TMP-OH) and $\alpha$-ketotrimethoprim (TMP=O) being the major products. Water matrix affected TMP removal significantly, e.g., natural organic matter (NOM) and