Paraquat degradation by Fenton's reagent: parametric and kinetic analysis

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Paraquat is a quaternarium ammonium salt with a large agriculture application due to its low price and high efficacy. It is mainly used as a non-selective contact herbicide for weed control but, due to its high availability, paraquat is very reported as suicide intention way. Some reports about paraquat toxicity for human health have been published and a great concern, for example, about water deliberate contamination with paraquat has been generated. According to the EU Council of 1998, the maximum individual pesticide concentration in drinking water is 0.1 μg/L [1]. Therefore, there is the need of effective technologies able to degrade paraquat in water matrices.

Advanced oxidation processes (AOPs) have been chosen as decontamination treatment for a large type of pollutants in water matrices. Fenton's reagent is an example of an AOP and it was chosen for the present study. Since this work intends to evaluate the Fenton's reagent response in case of water contamination with paraquat, a parametric study was performed to verify the influence of some operation conditions on paraquat degradation and mineralization performances. The parameters tested were: initial pH (pH = 2, 3, 4 and 5), H_2O_2 concentration (from 2×10^{-3} to 5×10^{-2} M), Fe^{2+} concentration (from 9×10^{-5} to 4.6×10^{-4} M), initial paraquat concentration (2×10^{-4}, 4×10^{-4} and 8×10^{-4} M), temperature (in the range 10-70 ºC), and finally iron catalyst source ($FeSO_4.7H_2O$ or $Fe_2(SO_4)_3.xH_2O$). Experiments were carried out in a cylindrical jacket reactor being the pH and the temperature monitored (and the last controlled) along the reaction. Periodically, samples were taken from the reactor and were analyzed in a HPLC and in a Shimadzu 5000A TOC analyzer for paraquat degradation and mineralization evaluation, respectively.

Under the best conditions tested, >99% of paraquat degradation and 40% of total organic carbon (TOC) removal were reached after 4 h of reaction. Degradation of Gramoxone (commercial product with 25.6% (w/w) of paraquat dichloride) was also tested under the previous conditions. Finally, a simple semi-empirical mathematic model proposed by Behnajady *et al*. [2] was used to simulate the reaction kinetics and predict process performance under the different conditions tested. A remarkable adherence of the model to the experimental paraquat concentration histories was obtained, with such a simple model [2]:

$$\frac{C}{C_0} = 1 - \frac{t}{m + bt} \tag{1}$$

where C is the paraquat concentration at time t (min), C_0 is the initial paraquat concentration and b and m are two model characteristic constants [2]. The effect of the operating conditions in these constants is discussed.

REFERENCES
[1] – EU council, directive on the quality of water intended for human consumption, 98/83/EC, 1998.
[2] – M. A. Behnajady, N. Modirshahla, F. Ghanbary, J. Hazard. Mat. 148, 98-102 (2007).