Advanced Oxidation: Theoretical VS. Actual Values

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Introduction

UNC Charlotte is collaborating with a water utility company conducting a series of water quality tests addressing groundwater contamination. The contamination is a result of an industrial solvent called 1,4 dioxane.1,4 dioxane is known to be carcinogenic to humans and also not biodegradable.[2]

To treat the contamination, water samples from various wet wells are undergoing water quality testing, and treatment through Advanced Oxidation Process (AOP). AOP is known as "an effective treatment technology for the removal of a variety of organic pollutants ".[1]

Through AOP hydroxyl radicals are released and help break down the presence of contaminants in water. In the design of AOP, it is important to evaluate how much the contaminants (1,4 dioxane) and the natural matter in the water samples are competing for the hydroxyl radicals. This competition or parameter is known as the scavenging term (ST).

Objectives

Purpose

- To perform water quality tests including pH, nitrate, nitrite, alkalinity, and Total Organic Carbon (TOC) on samples collected from groundwater wells
- To analyze water samples undergoing AOP which includes the use of UV light and hydrogen peroxide.
- To measure (actual) ST from AOP experiment
- To perform theoretical ST calculations
- To compare the actual values experimentally derived ST values to theoretical ST values

Method

Water Quality Testing

Water samples were analyzed for nitrates, nitrites, pH, TOC, and alkalinity. TOC used the Standard Method 5310B. Alkalinity was measured by titration method using a Hach digital titrator, Nitrates and nitrite used Hach test kits.

Hydrogen Peroxide Analysis (AOP)

The method used was the triiodide method.[3] Levels of hydrogen peroxide were measured by mixing 200mL of sample water with 0.376 mL of hydrogen peroxide. 0.125 mL of the mix sample was combined with 0.563 mL of reagent A and B. The sample was placed in the spectrophotometer for analysis. The is was done 3 times per sample.

UV Light Exposure (AOP)

50 mL of the water sample mixed with hydrogen peroxide and methylene blue were exposed under UV light for a specific time. The specific time was calculated using the UV dose excel calculator. After each exposure is completed 10 mL of the sample is placed in the spectrophotometer for analysis. There were a total of 6 exposures per set and 3 sets per water sample.

Calculating Theoretical Values

Using equation one this gives the theoretical ST. Actual ST values were gathered from the experiment. To determine the accuracy of the theoretical values percent differences between actual values and theoretical ST were calculated.

Figure 1: AOP Set Up (Spectrophotometer on the right and UV lamp with water sample on the left)

$$\left(\text{TOC} \times \frac{3.6 \times 10^8}{12{,}000}\right) + \left(\text{Alkalinity} \times \frac{8.5 \times 10^6}{50{,}000}\right)$$

Equation 1: Theoretical Scavenging Term

Results

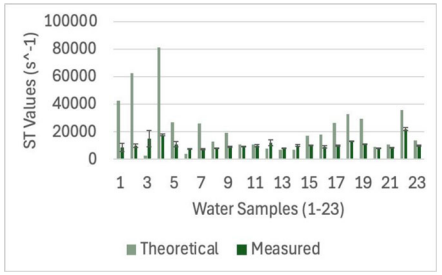

Figure 2: Measured vs. Theoretical Scavenging Term

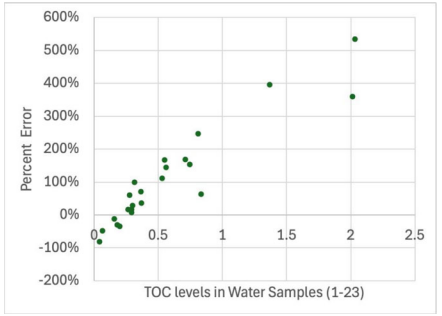

Figure 3: TOC Percent Difference between Theoretical and Actual Values

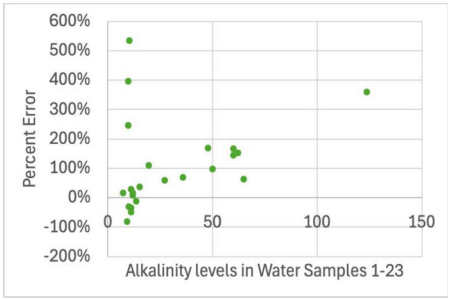

Figure 4: Alkalinity Percent Difference between Theoretical and Actual Values

Conclusions

- Theoretical values help in understanding how water quality testing helps determines ST.
- Each water quality parameter plays a role in determining the actual ST, but the one to have the strongest correlation is TOC
- Measured (actual) values are needed in order to see if the AOP hydroxyl radical are combatting contaminants.
- By relying on the theoretical value this allows for either a overdesign or underdesign of the AOP. Therefore, the ST has to be measured experimentally.

References

[1] Keen, O. S., McKay, G., Mezyk, S. P., Linden, K. G., & Rosario-Ortiz, F. L. (2014). Identifying the factors that influence the reactivity of effluent organic matter with hydroxyl radicals. Water Research, 50, 408–419. https://doi.org/10.1016/j.watres.2013.10.049

[2] Technical Fact Sheet - 1,4-Dioxane. (2017). United States Environmental Protection Agency.https://19january2021snapshot.epa.gov/sites/static/files/2014-03/documents/ffrro_factsheet_contaminant_14-dioxane_january2014_final.pdf

[3] Klassen, Normal V., et al. "H2O2 Determination by the I3- Method and by KMnO4 Titration." *Analytical Chemistry (Washington)*, vol. 66, no. 18, 1994, pp. 2921–25, https://doi.org/10.1021/ac00090a020.