

Atrazine Removal from Aqueous Solutions Using Hydrogen Peroxide-Modified Powdered Activated Carbon

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Abstract: Atrazine is a triazine herbicide that is commonly used in the Philippines to manage weeds in crops such as sugarcane, maize and rice. However, it has been polluting the surface and groundwater because of its persistence and solubility in water that causes health concerns such as endocrine disruption and cancer. Powdered activated carbon (PAC) is used as a treatment for the removing contaminants in drinking water treatment plants due to its high efficiency and low cost, but has problems with its regeneration and saturation limits. Therefore, this study involves the use of PAC and to modify it with H₂O₂ in order to improve atrazine removal by introducing oxidation by reactive radicals which allows the process to be more effective and sustainable. The spectrophotometric analysis at 450 nm indicated that the atrazine concentration was reduced consistently among the treatments. The results from the analysis suggest that with the increasing H₂O₂ concentration used for modification, the atrazine removal efficiency also increases which implies the importance of oxidative activation of adsorption capacity and the surface reactivity. Meanwhile, the optimal H₂O₂ concentration is the balance between enhanced surface functionality and structural stability, achieving maximum removal efficiency.

Keywords: Atrazine contamination, Hydrogen peroxide-modified activated carbon, Adsorption removal efficiency, Water treatment processes, Environmental health risks.

1. Introduction

A. Background of the Study

In the Philippines, atrazine is a triazine herbicide widely used in crops like maize, sugarcane, and rice. It works by inhibiting photosystem II that disrupts photosynthesis and causing weed death (He et al., 2019). Moreover, studies show that there has been an increased herbicide use in the Philippines due to intensified farming (Casimero, 2022). However, due to its widespread use, it has been detected on water treatment plants and drinking water sources in the Philippines because of its properties such as water solubility and environmental persistence which raised environmental and public health concerns. Due to agricultural runoff and irrigation practices, concentrations of atrazine were detected on water sources from

5.77 to 402 ng/L (0.00577 to 0.402 µg/L) (Lagunas-Basave et al., 2022).

Even at low concentrations, constant exposure of atrazine leads to many health issues in humans such as endocrine disruption which affects the development, behavior, and reproduction of humans (Vizioli et al., 2023). Meanwhile, in agriculture, atrazine is absorbed by plants and soil as herbicide. However, this could contaminate the environment as some of its residue spread into soils, sediments, crops, water bodies, and ground water (Deng et al., 2024). Pollution brought by atrazine also lowers soil microbial activity and disrupts nutrient cycles (Liu et al., 2024). Atrazine is also commonly detected in aquatic ecosystems which affects the development, reproduction, and behavior of aquatic animals and plants (Albuquerque et al., 2020).

However, despite the widespread atrazine use as herbicide in Philippine agriculture, current water treatment methods such as coagulation, sedimentation, and chlorination appear to be less efficient in removing atrazine (He et al., 2019). Because of the surface area and porosity of Powdered Activated Carbon (PAC), it is efficient in removing organic contaminants, such as atrazine. Although PAC is widely used for adsorption, there are still issues with regards to its lack of regeneration and its limits. Hence, there is a need for improved, cost-effective and environmentally friendly treatment such as modifying PAC with oxidation processes such as modifying PAC with H₂O₂. Nevertheless, research studying the utilization of these combined methods for atrazine removal in Philippine water system remains limited, implying a critical gap to address both environmental contamination and public health risk.

This study aimed to determine the efficacy of H₂O₂-modified PAC in lowering atrazine concentration in aqueous solutions through adsorption experiments and to determine the optimal concentration of H₂O₂ to PAC during modification in order to achieve high removal efficiency for atrazine residues. It seeks to optimize the adsorption and oxidation processes in order to develop a sustainable, low-cost, and efficient water treatment method which addresses atrazine contamination in the

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Philippines. The findings from this research will be helpful in designing a designated water treatment for removing atrazine.

B. Research Questions

This research focused on how H₂O₂-modified PAC removes atrazine residues in aqueous solutions by answering the following questions:

1. How efficient is H₂O₂-modified PAC in reducing the atrazine concentrations in aqueous solutions through adsorption?
2. What is the optimal H₂O₂ concentration to achieve high efficiency in removing atrazine residues?

C. Review of Related Literature

1) Atrazine

Atrazine is known for its ability to control grassy weeds in agricultural sectors. Nevertheless, its persistence in both soil and water has led to excessive consumption of atrazine which leads to environmental pollution and contamination. Atrazine has chemical properties and stability allowing it to be in the environment for long periods of time which results to accumulation (Zhang *et al.*, 2019). This contamination poses risks as it disrupts photosynthesis and causes problems on impair growth and reproduction to organisms, such as aquatic plants and animals. In human health, the presence of atrazine's in drinking water sources cause potential impacts, including endocrine disruption and increased risk of certain diseases (Liu *et al.*, 2020).

2) Adsorption Mechanisms

Adsorption is a process where molecules of a specific substance attach to the surface of an adsorbent substance. This process has been used for wastewater treatments to remove contaminants. The efficiency of adsorption may be affected by factors such as pH level, temperature adsorbent surface, and concentration. Activated carbon is used as an adsorbent for water purification due to its porosity and high surface area. However, research indicates that activated carbon has limitations on its saturation and regeneration (Heidarinejad *et al.*, 2020).

3) Adsorption Properties of Hydrogen Peroxide

Hydrogen peroxide (H₂O₂) is an unstable compound that breaks down to produce oxygen and water accompanied by heat. At room temperature, H₂O₂ is relatively stable and presents itself as a colorless liquid. It is widely used as an oxidizing agent in an attempt to alter carbon-based adsorbents which increases the adsorption capacity of these substances (Liepins *et al.*, 2024). This improvement occurs as H₂O₂ breaks down into oxygen and water to form functional groups and high porosity are introduced on the adsorbent surface (Zhang *et al.*, 2021). Moreover, this process increases the physical surface area, improves chemical stability and ion exchange capacity which makes the adsorbent more efficient in the removal of heavy metals and other pollutants (Ibrahim *et al.*, 2024). Despite this, H₂O₂ is limited by its chemical instability, as it quickly decomposes when exposed to some factors such as impurities, which may affect its performance on adsorption.

4) Adsorption Properties of Powdered Activated Carbon

The common use of powdered activated carbon (PAC) as a

method to repel contaminants in drinking water treatment plants is likely due to its properties like low cost and high efficiency. PAC has properties which includes high surface area that is appropriate in the adsorption of contaminants like atrazine. Its adsorption efficiency is affected by the physical and chemical characteristics of PAC which include pore volume, functional groups and level of pH. On atrazine removal, PAC shows remarkable removal speed and efficiency and can achieve 80% atrazine reduction within one hour (Esquerdo *et al.*, 2020). However, PAC cannot be regenerated or used which can lead to waste management problems. Moreover, PAC requires a minimum contact time of 15 minutes to effectively remove contaminants which may affect treatment process design. A combination of PAC with oxidation processes can greatly improve its atrazine removal by achieving higher atrazine reduction rates within shorter times and can help with degrading oxidation by-products.

5) Hydrogen Peroxide-Modified Powdered Activated Carbon

Combining PAC with oxidation methods like hydrogen peroxide improves atrazine removal from water because oxidation produces reactive radicals that break down atrazine molecules more effectively than adsorption alone (Esquerdo *et al.*, 2020). Making the process more sustainable and low-cost is important for modifying activated carbon through treatments. Studies show that modified activated carbon combined with oxidation is a positive and eco-friendly way to reduce atrazine concentration on water sources.

6) Synthesis

Atrazine is widely used as an herbicide for controlling weeds, however, its persistence causes widespread environmental contamination. The properties of PAC allow it to be used in water treatments such as the removal of contaminants like atrazine. However, it poses a risk with regards to its regeneration. This issue may be addressed by introducing functional groups to PAC with the help of H₂O₂ in order to offer better adsorption capacities

D. Theoretical Framework

This research is based on the principles of adsorption, oxidation, and surface chemistry. Adsorption refers to the adhesion of contaminants in water to the surface of a solid adsorbent, such as PAC. The efficiency of the adsorption will depend on its pore size, surface area and chemical properties of the adsorbent and the contaminants. PAC's high surface area and microporous structure make it highly effective for removing organic contaminants from water.

Oxidation, through treatment with H₂O₂, modifies PAC by introducing oxygen-containing functional groups and enlarging the pores which will improve the physical and chemical adsorption properties. H₂O₂ effectively enhances GAC's surface chemistry which increases the adsorption capacity for contaminants (Zhou *et al.*, 2023).

Surface chemistry plays a crucial role by utilizing the presence of oxygen-containing functional groups on the carbon surface to increase its polarity and chemical reactivity in order to improve the attraction and binding of pollutants. These groups enhance the adsorbent's affinity for polar contaminants

by improving electrostatic interactions and hydrogen bonding (Zieliński *et al.*, 2022).

E. Hypotheses

This study is guided by the following hypotheses:

1. If PAC is modified with H₂O₂, then it will significantly reduce the concentration of atrazine residues in aqueous solutions.
2. If the concentration of H₂O₂ to PAC during modification is adjusted, then the atrazine removal will be highly efficient.

F. Objectives

This study aims to assess the efficiency of H₂O₂-modified PAC on removing atrazine residues. Specifically, this research aims to:

1. To evaluate the efficacy of H₂O₂-modified PAC in reducing atrazine concentration in aqueous solutions through adsorption experiments.
2. To determine the optimal concentration of H₂O₂ to PAC during modification in order to achieve high removal efficiency for atrazine residues.

2. Methods

This section contains the detailed procedures and materials involved in preparing, modifying, and testing the H₂O₂-modified PAC and atrazine solutions used in the research study.

A. Procurement of Materials

The 3% hydrogen peroxide (H₂O₂) solution and powdered activated carbon (PAC) were available at the researcher's residence. Meanwhile, a 6% H₂O₂ solution was purchased from a local drugstore. Atrazine standard powder was bought from a commercial store to ensure laboratory-grade quality which is suitable for experimental use. All chemicals were selected to maintain consistency and reliability in the research procedures.

B. Preparation of Hydrogen Peroxide (H₂O₂) Solutions



Fig. 1. Different H₂O₂ solutions

The 3% H₂O₂ concentration was diluted in order to prepare a 1% and 3% H₂O₂ solution. For 1% H₂O₂ solution, 33.33 mL of the 3% H₂O₂ was mixed with 66.67 mL of distilled water to make 100 mL. For 3% H₂O₂, the 3% H₂O₂ solution was used

directly without any dilution. Meanwhile, to prepare 5% H₂O₂, 83.33 mL of the 6% H₂O₂ was mixed thoroughly with 16.67 mL of distilled water in order to make 100 mL. The solutions were mixed thoroughly to ensure uniform concentration. This method follows standard dilution calculations where $C_1V_1=C_2V_2$ to ensure accurate preparation of desired concentrations needed for the modification experiment.

C. Preparation of Atrazine Solution

Atrazine standard powder was accurately weighed through a weighing apparatus to acquire 0.5 g, this was dissolved in a 1 L volumetric flask filled with distilled water in order to prepare stock solution with a concentration of 500 mg/L (0.5 g/L). From this stock solution, 10 mL was carefully measured and diluted with 100 mL distilled water to prepare a working solution of 50 mg/L atrazine solution.



Fig. 2. 50mg/L atrazine solution

D. Preparation of H₂O₂-Modified Powdered Activated Carbon (PAC)

1) Modification of PAC Using H₂O₂ Solution

Ten grams of PAC were accurately weighed and placed into 3 separate 250 mL beakers for each modification group (1%, 3% and 5% H₂O₂ solution). Each group was treated with 20 mL of H₂O₂ solution at a specific H₂O₂ concentration (either 1%, 3%, or 5% H₂O₂ concentration). Each mixture was mixed gently at room temperature (approximately 25°C) for 60 minutes, ensuring uniform and consistent mixing which promotes effective oxidation of the PAC surface.

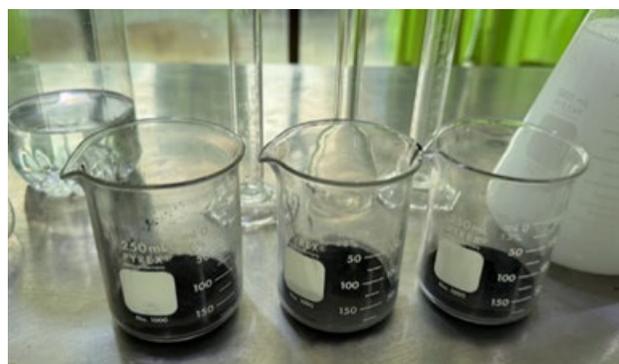


Fig. 3. PAC placed into 3 separate 250 mL beakers



Fig. 4. Mixing of H₂O₂ solution and PAC

2) Filtering and Drying of H₂O₂-modified PAC

After the modification process, the mixtures were filtered using a funnel and filter paper to separate the H₂O₂-modified PAC. The modified PAC was rinsed thoroughly with 50 mL of distilled water to remove any residual hydrogen peroxide. Lastly, to dry the samples, they samples were placed in an oven at 60°C for two hours in order to eliminate moisture in order to prepare for the adsorption experiments.

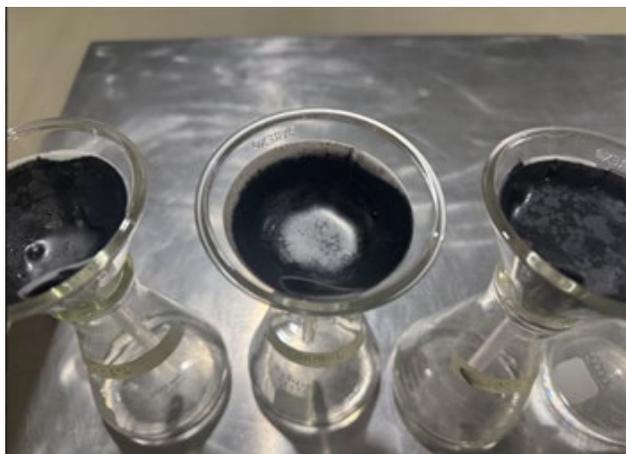


Fig. 5. Filtering of H₂O₂-modified PAC



Fig. 6. Drying of H₂O₂-modified PAC

E. Adsorption Process

In order to test its adsorption, three 250 mL beakers were labeled according to its specific H₂O₂ to PAC concentration and one 250 mL beaker was labeled as the control. One gram of each modified PAC sample was added to its respective beaker. Meanwhile, the control beaker received an untreated PAC sample without any modifications. This was followed by adding 100 mL of the 50 mg/L atrazine solution. The mixtures were gently stirred using a clean glass stirring rod at room temperature for 30 minutes to allow adsorption to occur.

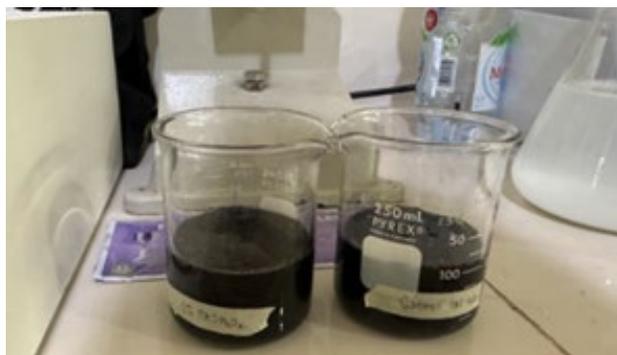


Fig. 7. Adsorption experiment of Control and 1% H₂O₂-modified PAC



Fig. 8. Adsorption experiment of 3% and 5% H₂O₂-modified PAC

1) Filtering of Modified PAC from Atrazine Solution

After stirring, the mixtures were filtered using a filter paper and funnel in order to separate the modified PAC from the atrazine solution. Each flask was also securely covered with parafilm layer to avoid contamination. The filtrates were then properly labeled and stored for UV-Vis spectrophotometer analysis.

F. Waste Disposal

All waste materials including used H₂O₂ and atrazine liquids were carefully handled following the proper laboratory safety procedures. H₂O₂ of low concentration was diluted prior to disposal in order to make sure it had minimal environmental impact. High concentration wastes like 5% H₂O₂ or residues of atrazine were stored in a sealed container and were disposed as hazardous chemical waste. Solid residues like PAC were collected and disposed following environmental protocols.

Safety measures including gloves and face masks were observed during disposal steps.

G. Transportation of Filtered Samples for Spectrophotometer Analysis

The samples were placed inside a box after adsorption process to prevent any spillage during transport. Proper labels were put into each flask to avoid any confusion. Moreover, each flask was covered with parafilm in order to prevent any contamination and evaporation. The flasks were transported to WVN Research Laboratory located in Davao City for UV-Vis spectrophotometer analysis.

Absorbance values of the treated samples were recorded and compared with a calibration curve in order to determine atrazine concentration. To determine the efficiency of removal and the optimal concentration of PAC:H₂O₂, the results obtained after the analysis of the UV-Vis spectrophotometer were analyzed with the help of such statistical tools as the mean, one-sample t-test and standard deviation.

3. Results

The removal efficiencies show very high means, all near or above 99.4%, which indicates consistently strong atrazine removal across treatments. The 5% PAC:H₂O₂ treatment and the control had the highest mean removal efficiencies at 99.1% and 99.97% respectively. The smallest standard deviation (0.0141) is observed for both the 5% PAC:H₂O₂ and the control group which implies that these have the most consistent performance.

The statistical tool compared the average removal efficiency of the sample (99.785%) with a hypothesized mean value (50%) to determine if there is a significant difference. In the test, the t-statistic is extremely high 9477.04) and the p-value (two-tailed) is 2.03E-08, which is very far from the common significance (0.05). Hence, this result means that the probability of observing such a large difference by chance is negligible, so the null hypothesis is rejected.

Table 2
Table containing the one sample t-test

ONE SAMPLE T-TEST	
Statistic	Value
Mean	99.785
Variance	0.043567
n (Sample Size)	4
Hypothesized Mean	50
df	3
t Statistic	477.0362
p-value (one-tailed)	1.02E-08
t Critical (one-tailed)	2.353363
p-value (two-tailed)	2.03E-08
t Critical (two-tailed)	3.182446

*The alpha value or significance level for this analysis is set at 0.05

4. Discussion

A. Overview of Findings

The results obtained from the spectrophotometric analysis at 450 nm showed a consistent and pronounced reduction in atrazine concentration across all treatments using varying concentrations of hydrogen peroxide-modified powdered-activated carbon (H₂O₂-PAC). These results align with a study involving modifying PAC with H₂O₂ for enhanced adsorption of secondary effluent organic matter (Zhou et al., 2023), this research shows that modifying with H₂O₂ enhances the adsorption efficiency of PAC. The residual atrazine concentrations decreased from 0.29–0.25 µg/mL in the 1% PAC:H₂O₂ treatment, to 0.14–0.12 µg/mL in the 3% treatment, 0.05–0.04 µg/mL in the 5% treatment, and finally 0.01–0.02 µg/mL in the optimized PAC:H₂O₂ system. This progressive decline clearly indicates that increasing the concentration of H₂O₂ used in PAC modification enhances its capacity to remove atrazine from aqueous environments.

B. Efficiency of H₂O₂-Modified PAC in Reducing Atrazine Concentrations

The data above indicates that H₂O₂-modified PAC shows high efficiency in reducing atrazine concentration by adsorbing and catalytically oxidizing the compound. The modification of PAC with H₂O₂ also present functional groups, like carbonyl, hydroxyl groups and carboxylic acid groups on the carbon surface. These functional groups work to enhance the hydrophilicity and surface polarity of PAC that enhances a stronger interaction with polar or moderately polar contaminants like atrazine

The trend from 1% and 5% PAC:H₂O₂ show that their adsorption efficiency was dependent on the dose. The 1% treatment that had atrazine residual levels of 0.29 and 0.25 µg/mL has a limited oxidative activation which is why only a small portion of atrazine molecules was captured by the adsorption sites. The 3% treatment improved removal efficiency by nearly half which signifies that there are additional active sites and an enhanced electrostatic interaction between the atrazine molecules and oxygenated surface of PAC. Lastly, the 5% treatment has the most significant decline among the concentrations with residual atrazine concentrations dropping to as low as 0.04 µg/mL.

This pattern proves that the adsorptive and oxidative elimination of atrazine by H₂O₂ modification of PAC increases which is consistent with literature reviews that oxidized activated carbon shows higher affinity for nitrogen-containing herbicides and aromatic compounds. Adsorption is also enhanced by the oxidation process which is likely because of the involved partial degradation of atrazine into less persistent intermediates by attack with hydroxyl radicals.

Table 1
Table containing the removal efficiency on trial 1 and trial 2, mean, and standard deviation

Treatments	TRIAL 1			TRIAL 2			Mean (%)	SD
	C ₀ (µg/ml)	C _f (µg/ml)	Removal Efficiency	C ₀ (µg/ml)	C _f (µg/ml)	Removal Efficiency		
1% PAC:H ₂ O ₂	50	0.29	99.42%	50	0.25	99.5%	99.46	0.0566
3% PAC:H ₂ O ₂	50	0.14	99.72%	50	0.12	99.76%	99.47	0.0283
5% PAC:H ₂ O ₂	50	0.05	99.9%	50	0.04	99.92%	99.91	0.0141
PAC (Control)	50	0.01	99.98%	50	0.02	99.96%	99.97	0.0141

C. Optimal H₂O₂ Concentration for Maximum Atrazine Removal

The PAC:H₂O₂ (Control) system had the lowest residual atrazine level of 0.01–0.02 µg/mL in the aqueous solution. Here, the PAC surface had the best combination of surface oxygen functionalities, pore volume and active sites required in adsorption and formation of radicals.

When excessive H₂O₂ is used in modification, which may cause partial pore collapse or over-formation of acidic groups which can force back neutral or weakly basic organic molecules such as atrazine. On the other hand, low H₂O₂ levels may result to incomplete oxidation and fewer reactive sites. Therefore, an optimized concentration provides the right balance of sufficient oxidation for high reactivity without damaging the structural framework of the carbon.

5. Conclusion

The experimental results show that H₂O₂-modified PAC is highly effective for lowering atrazine from solutions. The efficiency of atrazine reduction increases with increasing H₂O₂ concentration used for modification hinting the importance of oxidative activation in enhancing adsorption capacity and surface reactivity. Meanwhile, the optimal condition was achieved with the PAC:H₂O₂ system, which had the lowest residual atrazine concentration (0.01–0.02 µg/mL) having almost complete removal.

1. H₂O₂-modified PAC efficiently reduces atrazine concentrations through combined adsorption and oxidative degradation.
2. The optimal H₂O₂ concentration yields a balance between enhanced surface functionality and structural stability, achieving maximum removal efficiency.

These findings confirm that H₂O₂ modification significantly improves the adsorptive and catalytic performance of PAC, offering a promising and sustainable approach for pesticide remediation in contaminated water systems.

6. Recommendation

Future research should explore a broader range of hydrogen peroxide concentrations in order to identify the optimal level for maximizing atrazine removal efficiency. It is also recommended to test the comparison of different sources of activated carbon in terms of adsorption capabilities and cost-efficiency. Additionally, exploring the possibility of H₂O₂-modified PAC in removing other organic contaminants is also recommended. The pH level of the modification process should be carefully monitored and regulated because it affects the adsorption capacity and chemical stability of the modified carbon.

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