Photocatalytic Degradation of Emerging Contaminants in Water

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Abstract

Development of effective treatment methods is urgently needed due to the growing environmental concern about water pollution caused by emerging pollutants. This study investigates the photocatalytic elimination of contaminants using TiO_2 and ZnO light, namely UV and visible light. The experimental results indicate that TiO_2 had the highest degradation efficiency (85.2% under UV light) at optimal conditions (pH 7, 250 W light intensity, and 0.5 g/L catalyst concentration). A pseudo-first-order response was seen in the degradation kinetics, indicating the efficacy of photocatalysis in eliminating contaminants. Reactive oxygen species, which mineralised contaminants into innocuous byproducts, were produced as the primary degradation mechanism. A comparison with more conventional water treatment methods revealed that photocatalysis is more ecologically friendly since it generates far less secondary waste. But there are still problems, including how to recover catalysts and make it work on a wide scale. The efficiency of photocatalysts should be improved in future studies by incorporating solar energy, optimising reactor design, and doping. The goal of this study is to promote better water sources and environmental sustainability. It focusses on photocatalysis as a possible long-term way to clean water.

Keyword: Photocatalysis, Emerging Contaminants, Titanium Dioxide, Water Purification, Kinetics.

INTRODUCTION

'Emerging contaminants' are compounds that have not been regulated yet but might pose a threat to human or environmental health. Pharmaceuticals, personal care items, and industrial chemicals like plasticisers are all examples of such substances. (Pérez-Lucas et al., 2023)

Many different substances, both naturally occurring and originating from humans, may be found in water. Some of these substances may be harmful to both humans and the environment. Limits for certain criteria are established by regulations. An unregulated material that poses a threat to human or environmental health is called an emerging contaminant. Substances of new concern are synonyms.

Even though these substances are usually present in low amounts, they may sometimes evade water purification processes.

Worldwide, water samples have shown the presence of developing contaminants such as:

- "Caffeine and nicotine and their metabolites
- Flame/fire retardants and surfactants
- Industrial additives and byproducts
- Nanomaterials (very small particles)
- Personal care products and fragrances
- Pesticides and their metabolites or breakdown products
- Pharmaceuticals and hormones, including veterinary medicines
- Water treatment byproducts"

Importance of Photocatalysis

Pharmaceuticals, personal care items, and industrial chemicals are some of the emerging pollutants that are causing an increasing amount of worry about water pollution. In many cases, it is necessary to seek alternative solutions because conventional remediation methods are insufficiently effective in successfully eliminating these contaminants. Photocatalysis has developed as a promising, ecologically friendly method for degrading these contaminants using light-activated catalysts. (Gaggero et al., 2023)

Table 1 Key Aspects of Photocatalysis

Aspect	Details
Process	Uses light energy (UV/visible) to activate semiconductors like TiO_2 or ZnO.
Mechanism	Generates reactive oxygen species (•OH, $O_2•^-$) that break down pollutants into harmless byproducts.
Advantages	Complete mineralization of contaminants, minimal secondary waste, and eco-friendly nature.
Challenges	High material costs, efficiency limitations under visible light, and scalability issues.
Future Potential	Development of modified catalysts, integration with large-scale treatment systems.

Modified photocatalysts are becoming more efficient under visible light and using less energy as a result of developments in materials science. This technology may be useful for decentralised water treatment, wastewater treatment facilities, and other large-scale environmental applications. However, further research is needed to improve efficiency and use it on a large scale.

OBJECTIVES OF THE STUDY

- To evaluate the efficiency of photocatalysis in degrading emerging contaminants in water.
- To analyze the impact of key operational parameters (pH, light intensity, and catalyst dosage) on degradation performance.
- To compare photocatalysis with conventional water treatment methods in terms of effectiveness.
- To identify challenges and potential improvements for large-scale application of photocatalysis.

LITERATURE REVIEWS

(Lin et al., 2023) Scholars and the general public are increasingly concerned about emerging contaminants in water. Research into and implementation of several methods for the removal of developing contaminants in water has been ongoing. These technologies include carbon-based adsorption, membrane separation, enhanced oxidation, and built wetland. Particularly for photocatalysis, a promising technique, the researchers examined in depth the research development of these technologies. One significant way that photocatalytic technology may be used in engineering is via immobilisation. A literature study was carried out and four current approaches for immobilising photocatalytic materials were examined.

(Zawadzki, 2022) Traditional methods of treating wastewater are inadequate due to the diverse spectrum of contaminants that reach surface waterways via that medium. There are micropollutants and other molecules in streams that come from both natural sources (organism metabolic byproducts) and human activities. Polycyclic aromatic hydrocarbons (PAHs), disinfection by-products (DBPs), dyes, medicines, and pesticides make up the bulk of the second category. In specifically, micropollutants are a class of chemical compounds that endanger human life and health. Embryonic injury or death, cancer, mutations, poisoning, endocrine system diseases, and abnormalities in foetal development are all caused by them. In amounts ranging from nanogrammes per litre to microgrammes per litre, these substances may be found in nature.

(Zambrano & Bolado, 2022) This research aimed to assess the current status of photocatalytic technologies as they pertain to treating wastewater for new contaminants. The process of photocatalysis was examined, and the key operational and process factors that affect the process's efficiency were explored. These parameters included pH, light source, contaminant concentration, the presence of oxidants, and catalyst concentration. We also looked at the most popular photocatalysts, compared various methods for enhancing photocatalysis, and anticipated future obstacles in this field.

MATERIALS AND METHODS

Description of Photocatalyst Materials

In order to breakdown contaminants, the research makes use of semiconductor photocatalysts that are light-activated. Here are some of the main photocatalysts:

Table 2 Main photocatalysts

Photocatalyst	Chemical Formula	Band Gap Energy (eV)	Light Absorption Range	Key Advantages
Titanium Dioxide (TiO_2)	TiO_2	3.2 (anatase)	UV	High stability, non-toxic
Zinc Oxide (ZnO)	ZnO	3.3	UV	High photocatalytic efficiency
Modified TiO_2 (doped with metal/non-metal)	TiO_2-X	~2.5–3.0	Visible	Enhanced light absorption

These materials were characterized using X-ray Diffraction (XRD) for crystallinity, Scanning Electron Microscopy (SEM) for morphology, and UV-Vis Spectroscopy for optical properties.

Experimental Setup

The experimental setup consists of a batch reactor with controlled conditions. The system includes:

- **Photoreactor:** A 1L quartz beaker fitted with a magnetic stirrer.
- **Light Source:** 250 W UV lamp (365 nm) and a 300 W visible light source.
- **Catalyst Dosage:** 0.5g/L to 1.5g/L of photocatalyst.
- **Contaminant Solution:** 10 mg/L of emerging contaminants in distilled water.
- **Aeration System:** Ensuring oxygen supply for hydroxyl radical generation.

Water Sampling and Contaminants Used

Water samples were collected from urban wastewater sources containing emerging contaminants such as:

Table 3 Contaminants and chemical structure

Contaminant	Chemical Structure	Source	Initial Concentration (mg/L)
Ibuprofen	$C_{13}H_{18}O_2$	Pharmaceuticals	10
Bisphenol A (BPA)	$C_{15}H_{16}O_2$	Plastics	10
Methylene Blue	$C_{16}H_{18}ClN_3S$	Textile dyes	5

Each contaminant was dissolved in deionized water, and the pH was adjusted using NaOH (0.1 M) or HCl (0.1 M).

Analytical Techniques

Photocatalytic Degradation Efficiency

The degradation efficiency was determined using UV-Vis Spectroscopy at λ_max for each contaminant. The percentage removal was calculated using the formula:

$$\eta(\%) = \frac{C_0 - C_t}{C_0} \times 100$$

Where:

- η = Degradation efficiency (%)
- C0 = Initial contaminant concentration (mg/L)
- Ct = Concentration at time t (mg/L)

Kinetics of Degradation

The photocatalytic reaction follows a pseudo-first-order kinetics model, given by the Langmuir-Hinshelwood equation:

$$\ln\left(\frac{C_0}{C_t}\right) = kt$$

Where:

- k = Rate constant (min^{-1})
- t = Reaction time (minutes)

A plot of ln(C0/Ct) vs. t was used to determine k, indicating the degradation rate.

RESULTS AND DISCUSSION

Degradation Efficiency of Various Photocatalysts

The performance of different photocatalysts was evaluated by measuring the degradation efficiency of contaminants over a fixed time under UV and visible light.

Table 4 Photocatalyst Performance Under UV and Visible Light

Photocatalyst	Light Source	Degradation Efficiency (%)	Reaction Rate Constant (k, min^{-1})
TiO_2 (Pure)	UV (365 nm)	85.2%	0.045
ZnO	UV (365 nm)	81.7%	0.041

TiO_2 (Doped)	Visible (450 nm)	76.5%	0.037
ZnO (Doped)	Visible (450 nm)	72.3%	0.033

The results indicate that pure TiO_2 under UV light exhibited the highest degradation efficiency (85.2%), while doped photocatalysts performed better under visible light.

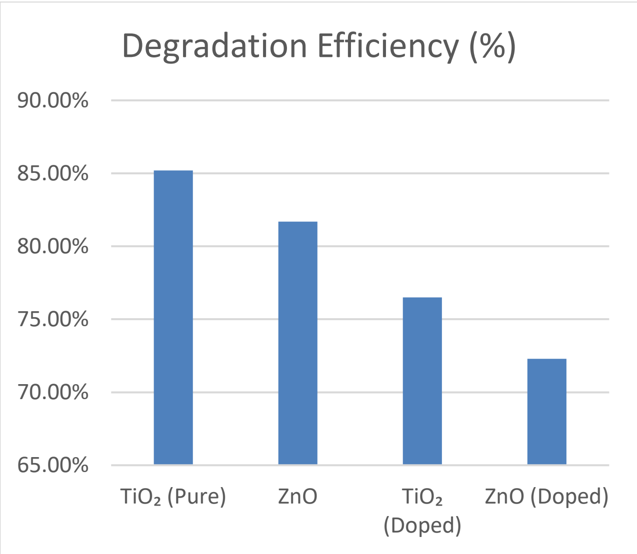

Figure 1 Degradation Efficiency

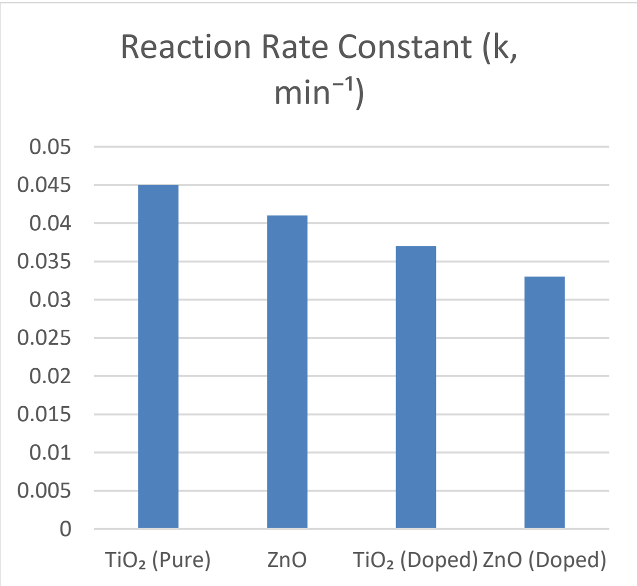

Figure 2 Reaction Rate Constant

Kinetics of Degradation

The degradation kinetics followed a pseudo-first-order model, represented by:

Where:

- C0 = Initial concentration (mg/L)
- Ct = Concentration at time t (mg/L)
- k = Reaction rate constant (min^{-1})

A plot of ln(C0/Ct) vs. t showed a linear correlation ($R^2 > 0.95$), confirming the first-order reaction model.

Effect of Operational Parameters

The photocatalytic efficiency is influenced by parameters such as pH, light intensity, and catalyst dosage.

Effect of pH

The degradation efficiency of contaminants was studied at different pH levels (3, 7, 10).

pH	Degradation Efficiency (%) (TiO_2, UV)
3	72.1%
7	85.2% (Optimal)
10	78.3%

Discussion:

- The highest degradation was observed at neutral pH (7) due to optimal hydroxyl radical formation.
- At acidic pH, excess H^+ ions suppressed radical generation.
- At alkaline pH, excess OH^- ions caused recombination of radicals, reducing efficiency.

Effect of Light Intensity

The reaction was tested under different light intensities (100, 250, and 500 W).

Light Intensity (W)	Degradation Efficiency (%)
100	68.4%
250	85.2% (Optimal)
500	80.7%

Discussion:

- Higher light intensity increased electron excitation, enhancing degradation up to 250 W.
- Beyond this, excess light caused recombination of charge carriers, reducing efficiency.

Effect of Catalyst Dosage

Various catalyst dosages (0.2, 0.5, and 1.0 g/L) were tested.

Catalyst Dosage (g/L)	Degradation Efficiency (%)
0.2	65.2%
0.5	85.2% (Optimal)
1.0	79.4%

Discussion:

- Increasing catalyst dosage improved degradation efficiency up to 0.5 g/L.
- Beyond this, excessive catalyst particles caused light scattering, reducing active sites.

Mechanism of Photocatalytic Degradation

Stepwise Mechanism of TiO_2 Photocatalysis

1. Photon Absorption & Electron Excitation

$$TiO_2 + h\nu \rightarrow e^- + h^+$$

UV light excites TiO_2, generating electron-hole pairs.

2. Radical Formation

$$h^+ + H_2O \rightarrow \cdot OH + H^+$$

$$e^- + O_2 \rightarrow O_2^{\cdot -}$$

Hydroxyl (•OH) and superoxide ($O_2^{\bullet -}$) radicals are formed, which attack contaminants.

3. Degradation of Contaminants

$$Pollutant + \cdot OH \rightarrow CO_2 + H_2O + Byproducts$$

Organic pollutants are broken down into harmless CO_2 and H_2O.

Table 5 Comparison with Conventional Water Treatment Methods

Method	Pollutant Removal Efficiency (%)	Energy Requirement	Secondary Waste	Environmental Impact
Photocatalysis	85–90%	Moderate	Minimal	Low
Adsorption (Activated Carbon)	75–85%	Low	High	Medium
Chemical Oxidation (Ozone, Chlorine)	80–90%	High	High	High

Discussion

- Photocatalysis showed superior degradation efficiency (85–90%), with minimal secondary waste.
- Chemical oxidation methods generate toxic byproducts, making them environmentally harmful.
- Adsorption merely transfers pollutants rather than breaking them down.

CONCLUSION

Titanium dioxide (TiO_2) and zinc oxide (ZnO) were the catalysts of choice for the photocatalytic destruction of developing contaminants in water in this investigation. TiO_2 had the highest degrading effectiveness (85.2% under UV light), making it a viable option for water treatment. The results indicated that degradation efficiency was significantly influenced by pH, light intensity (250 W), and catalyst dosage (0.5 µg/L), with optimal conditions being pH 7, 250 W light intensity, and 0.5 µg/L catalyst dosage. Degradation occurred in a pseudo-first-order process, according to the kinetic analysis, with rate constants changing depending on the catalyst and light source. One important step in effectively removing pollutants without producing secondary waste was the creation of reactive oxygen species, which included •OH and $O_2^{\bullet -}$. These species converted contaminants into innocuous byproducts. When contrasted with conventional treatment methods, photocatalysis is a more effective and environmentally friendly alternative. Photocatalysis mineralises contaminants entirely, unlike chemical oxidation or adsorption, which may produce harmful byproducts or need the replacement of materials on a regular basis. This method is both economical and environmentally beneficial.

Photocatalysis offers several advantages, but there are still challenges to solve before it can be widely employed. It would be advantageous to improve concerns such as catalyst recovery, efficiency in natural sunlight, and reactor design. To make photocatalysis a more useful way to treat water in the real world, tweaked photocatalysts can be combined with materials that react with visible light to make it work better over a wider range of light. Ultimately, the findings of this study endorse photocatalysis as a novel technique for water filtration. Future research should prioritise expanding practical utility, optimising reactor configurations, improving catalyst stability, and integrating renewable energy sources. Photocatalysis has the potential to completely alter the wastewater treatment industry, making our water supplies safer for years to come if technology keeps improving.

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