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Comparison of UV/persulfate and UV/hydrogen peroxide processes for the degradation of organic micropollutants in tap water: kinetics, synergy, and selected transformation products

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This study systematically evaluated two ultraviolet (UV)-based advanced oxidation processes, UV/hydrogen peroxide (H_2O_2) and UV/persulfate, for the removal of nine organic micropollutants (OMPs): acesulfame, atenolol, carbamazepine, diclofenac, metoprolol, primidone, saccharin, sulfamethoxazole, and valsartan acid. The results show that increasing the concentration of hydrogen peroxide/persulfate, and extending the reaction time could improve the oxidation of the OMPs. Under optimized conditions, over 80% elimination was achieved for most OMPs. It was also observed that the transformation behavior varied among the investigated OMPs and appeared to be influenced by their physicochemical characteristics. For instance, diclofenac, as a photosensitive compound, exhibited rapid transformation. However, OMPs such as saccharin demonstrated limited degradation. The results indicate that persulfate showed superior degradation capability compared to H_2O_2 for atenolol, diclofenac and metoprolol. However, some OMPs including acesulfame and Valsartan acid showed better degradation using H_2O_2. Detectable levels of 2- and 3-hydroxylated carbamazepine derivatives occur only following UV/H_2O_2 treatment after 0.5–1.0 h and 1–2 mM H_2O_2. Another transformation product, acridone-9-carboxylic acid was predominantly detected under UV/persulfate. The study found that synergy between UV light and H_2O_2/persulfate often plays a major role in removing OMPs. In some cases, direct photolysis or direct oxidation by H_2O_2 or persulfate contributes more to OMP removal than the free radical-mediated oxidation generated during the advanced oxidation process.

KEYWORDS
contaminants of emerging concern (CECs), persistent and mobile substances (PM substances), persistent organic pollutants (POPs), persulfate activation, trace organic compounds (TOrCs), UV-based oxidation

1 Introduction

Many organic micropollutants (OMPs) cannot be fully removed by conventional drinking water treatment processes such as coagulation-flocculation, rapid sand filtration or chlorination (Yu et al., 2018; Ranjbar et al., 2024b; 2024a; Ahmadi et al., 2025). Coagulation-flocculation completely fails to remove most OMPs present in drinking

water due to their inability to aggregate with the coagulants and flocculants used in the process (Kooijman et al., 2020). Chlorination is commonly employed for water disinfection and many OMPs exhibit strong resistance to chlorine oxidation (Li et al., 2021; Ranjbar et al., 2026). Consequently, many OMPs occurring in raw water remain present after treatment with the aforementioned processes.

Advanced oxidation processes (AOPs) have emerged as promising technologies for OMP removal due to their ability to generate reactive oxygen species, particularly hydroxyl and sulfate radicals (·OH and $SO_4^{\cdot-}$), which exhibit high oxidative potential and rapid reaction kinetics (De Boer et al., 2022; Nadali Pishnamaz et al., 2023). Unlike biological treatments, which rely on microbial activity, and adsorption-based methods, which merely transfer pollutants to another medium, AOPs have the potential to mineralize OMPs to CO_2 and H_2O, minimizing the risk of secondary contamination (Gaur et al., 2022; Ranjbar et al., 2025a).

Among AOPs, UV-based processes have attracted significant research interest, as well as adoption by various industries and treatment plants, for the removal of OMPs (Šojić et al., 2012; Guerra-Rodríguez et al., 2021). Since UV lamps are commonly used for disinfection in many water treatment facilities, integrating UV-based oxidation processes becomes a cost-effective option for enhancing OMP removal (Rodríguez-Chueca et al., 2019). The UV/H_2O_2 process is capable of oxidizing many OMPs, including bisphenol A, carbamazepine, chloramphenicol, diclofenac, ibuprofen, naproxen, metoprolol, primidone, ronidazole, sulfamethoxazole and others (Wols et al., 2013; Ling et al., 2016). However, dissolved organic matter can substantially scavenge •OH, reducing the oxidation efficiency (Zhang et al., 2025). The formation of transformation products with significant structural similarity to the parent pollutants following AOP treatment was reported (Menacherry et al., 2022). This warrants greater attention, as emerging evidence indicates that many of them (e.g., certain transformation products derived from atenolol (Yan et al., 2023), carbamazepine (Donner et al., 2013), and diclofenac (Qiu et al., 2020)) can exhibit equal or even greater toxicity than their parent substances.

SO_4•$^-$ has recently attracted interest due to the higher stability, longer life span, and higher standard redox potential (2.5–3.1 V) compared to •OH (Kilic et al., 2019; Zou et al., 2021; Ranjbar et al., 2023b; 2023a). The UV/persulfate process utilizes peroxymonosulfate (PMS) or peroxydisulfate (PDS) as precursors to generate SO_4•$^-$ (Lai et al., 2023). PDS is a stable and mild oxidizing agent with a high redox potential, which enables them to oxidize a wide variety of OMPs (Li et al., 2018). Compared to the conventional UV/H_2O_2 process, UV/persulfate may offer certain operational advantages under specific conditions. In particular, previous studies have reported that persulfate-based AOPs can be less sensitive to pH variations than hydroxyl radical-based systems; however, the extent of this effect depends on the activation method and water matrix composition. This relative stability has been attributed to the formation of sulfate radicals, which remain effective over a broader pH range compared to hydroxyl radicals (Xiao et al., 2016; Acero et al., 2018). The storage and transportation costs of persulfate are lower, as they are supplied as stable solid salts and do not require special storage conditions (Cai et al., 2021). These features make the UV/persulfate process more flexible in treating complex water matrices and demonstrate great potential for industrial applications (Priyadarshini et al., 2022). In comparison, hydrogen peroxide also offers important advantages, including its widespread availability and the possibility of *in-situ* production, which can reduce the need for transport and on-site chemical storage (e.g., via electrochemical or catalytic processes) (Liu et al., 2024). Overall, both oxidants present distinct operational benefits depending on the application context.

This study aims to evaluate the efficiency of UV-based AOPs for the degradation of OMPs in tap water, focusing on systems that generate hydroxyl and sulfate radicals. Unlike previous studies that have primarily examined UV/H_2O_2 or UV/persulfate individually, this work provides a systematic comparison of hydrogen peroxide and persulfate under identical experimental conditions at an environmentally relevant OMP concentration of 1 μg/L. In addition to comparing contaminant removal efficiencies, the study evaluates the formation of selected transformation products and investigates the influence of key operational parameters, including reaction time and oxidant dosage, on process performance. These findings provide insight into the relative effectiveness of hydroxyl- and sulfate radical-based UV-AOPs for drinking water treatment.

2 Materials and methods

2.1 Materials

Potassium persulfate ($K_2S_2O_8$, analytical grade, ≥99%, molecular weight: 270.33 g/mol, Merck, Germany) and H_2O_2 (35%, molecular weight: 34.02 g/mol, density: 1.13 g/mL, Carl Roth, Germany) were used as oxidizing agents. Sodium thiosulfate ($Na_2S_2O_3$, ≥99%, Merck, Germany) was employed as a quenching agent, prepared in ultrapure water (Milli-Q, 18.2 MΩ cm at 25 °C) and stored under dark, low-temperature (4 °C) conditions. Acesulfame, atenolol, carbamazepine, diclofenac, metoprolol, primidone, saccharin, sulfamethoxazole and valsartan acid were purchased from Merck, Germany.

2.2 Test solutions

Nine OMPs including acesulfame, atenolol, carbamazepine, diclofenac, metoprolol, primidone, saccharin, sulfamethoxazole, valsartan acid were spiked to the tap water to reach a concentration of 1 μg/L each. These compounds were selected based on their physicochemical properties, including polarity and hydrophobicity, as well as their frequent occurrence in European water samples reported in previous studies (Schulze et al., 2019; Neuwald et al., 2021). The list of selected OMPs and their characteristics is provided in Table 1. All tests were conducted using tap water from Berlin, Germany, with a pH of 7.3 ± 0.1, 4.5 ± 0.1 mg/L dissolved organic carbon (DOC) and an ultra-violet absorbance at 254 nm (UVA_{254}) of 0.08 ± 0.05 cm^{-1}.

Valsartan acid, a dominant and highly persistent transformation product derived from several widely used antihypertensive drugs (including valsartan, irbesartan, candesartan, and olmesartan) (Nödler et al., 2013), was intentionally selected for investigation over its parent compounds due to its widespread environmental

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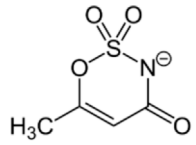
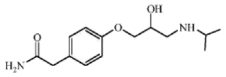
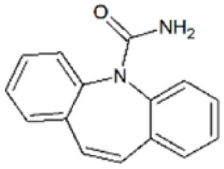
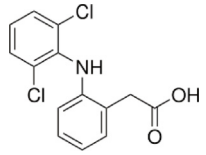
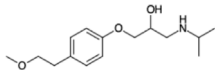
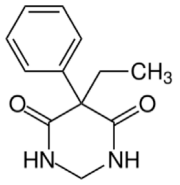
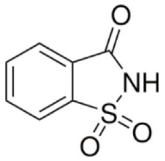
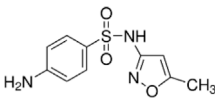
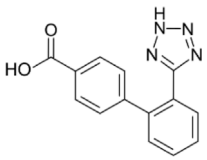
TABLE 1 Studied OMPs, their CAS numbers, molecular weights and structures.

OMP	Abbr	Molecular weight (g/mol)	CAS number	Structure
Acesulfame	ACE	163.15	55589-62-3	
Atenolol	ATN	266.34	29122-68-7	
Carbamazepine	CBZ	236.27	298-46-4	
Diclofenac	DFC	296.15	15307-86-5	
Metoprolol	MTP	267.37	51384-51-1	
Primidone	PRI	218.25	125-33-7	
Saccharin	SAC	183.18	81-07-2	
Sulfamethoxazole	SMX	253.28	723-46-6	
Valsartan acid	VSA	266.08	164265-78-5	

relevance and prior detection within local tap water matrices (unpublished monitoring data).

2.3 Experimental setup

The experiments were conducted in a UV reactor (Peschl Ultraviolet, Germany (Supplementary Figure S1)). To ensure safety, controllability, and efficiency, the system is composed of a UV protection cabinet, power control system, cooling system, sample containers and UV light source module. Inside of the UV reactor comprises sample containers, UV lamp, and quartz sleeve (Supplementary Figure S2). A low-pressure amalgam lamp emitting 254 nm at 20 W was used in this study. Four quartz sample containers (each with a capacity of 25 mL) are positioned symmetrically around the radiation source with reflectors installed, as shown in Supplementary Figure S2. Due to the high

UV transmittance of quartz, these containers maximize UV transmission, thereby enhancing the effectiveness of photochemical reactions. To avoid the impact of varying UV radiation intensities at different positions, only one position was used for all experiments. The sample container is equipped with an integrated magnetic stirrer, featuring independent stirring positions located beneath each sample container. This ensures uniform mixing of samples and continuous UV exposure throughout the experiment.

2.4 Removal experiments

To assess the impact of H_2O_2 and PDS dosages on OMP eliminations, a series of experiments was conducted with varying dosages (0.2, 0.5, 1.0 and 2.0 mM). Immediately after H_2O_2/PDS addition, all test solutions were wrapped with aluminum foil to prevent interference from external light sources. The prepared solution was transferred into a 25 mL quartz sample container. Once the sample was placed in the reactor, the magnetic stirrer was activated to ensure homogeneous mixing of the solution. The reactor door was then closed, and timing was initiated immediately after the UV lamp was turned on. Sampling time points were set at 30, 60, 120, and 240 min. Dark reaction control experiments were conducted under identical experimental conditions but without UV irradiation. The initial OMP concentrations, H_2O_2/PDS dose, and stirring speed were kept identical to those in the UV degradation experiment to ensure a valid comparison.

At the end of each experiment, 10 mL of the test solution was transferred from the reaction vessel to a clean beaker using a pipette. To terminate residual oxidants, an appropriate amount of $Na_2S_2O_3$ solution (tenfold higher than the H_2O_2/PDS dose on a stoichiometric basis (Kowalska et al., 2020; Maniakova et al., 2020; Ding and Hu, 2021)), was added as a quenching agent. $Na_2S_2O_3$ reacts efficiently with H_2O_2 and PDS, neutralizing excess H_2O_2/PDS and preventing continued degradation of OMPs after sampling. This is particularly important for ensuring the accuracy of experimental results, as residual oxidants could otherwise continue reacting during sample storage, causing misleading degradation rates. After quenching, samples were filtered (0.2 μm membrane), then transferred into 1.5 mL vials, sealed, and labeled. All vials were stored at 4 °C in a refrigerator until analysis.

2.5 Analyses

The concentrations of targeted substances and selected transformation products were determined using chromatography and tandem mass spectrometric (Agilent 1,290 infinity 2 Series UHPLC coupled with SCIEX QTRAP 6500+ triple quadrupole mass spectrometer) analysis. The chromatographic separation of these substances was carried out on a reverse phase C18 column (Agilent Zorbax Eclipse Plus C18, 150 mm × 2.1 mm, 3.5 μm particle size) against a gradient elution of 0.1% acetic acid and pure acetonitrile (0.4 mL/min flow rate and 20 μL injection volume). While most compounds were measured in the positive electrospray ionization (ESI) mode, negative ESI was used for the measurement of acesulfame and saccharin. The compound specific parameters used for mass spectrometric analysis were selected according to Hermes et al. (2018). Hydroxylated transformation products generated from carbamazepine, atenolol, metoprolol and diclofenac were quantified (more details provided in Table 2).

The limits of detection and quantification (LOD and LOQ), provided in Supplementary Table S1, were determined from the signal-to-noise (S/N) ratios of the calibration standards following the method described by Taleuzzaman (2018). Calibration was performed prior to sample analysis by injecting a complete set of standards, with individual analyte concentrations ranging from 0 to 1,000 ng/L (except for acesulfame, which was prepared at twenty-fold higher concentrations). Due to limited availability, all analyses were conducted without the addition of internal standards. To ensure system consistency, blanks and quality control standards were analyzed after every 10 samples. Retention times and peak intensities were regularly monitored to check for standard degradation; however, no significant changes were observed throughout the study. Instrument control, data acquisition, peak review, and integration were performed using Analyst software (version 1.7.3; SCIEX).

2.6 Extent of AOP

The extent of synergy between UV light and the oxidants (H_2O_2 or PDS) in conducting AOPs for the removal of each OMP was calculated using Equation 1 (Guerra-Rodríguez et al., 2021).

$$S\,(\%) = \frac{k_{H_2O_2/PDS+UV} - k_{H_2O_2/PDS} - k_{UV}}{k_{H_2O_2/PDS+UV}} \times 100 \qquad (1)$$

$k_{H2O2/PDS}$, k_{UV} and $k_{H2O2/PDS+UV}$ represent the pseudo-first order rate constants for tests conducted using the H_2O_2/PDS in dark conditions, UV light without H_2O_2/PDS and the combined UV and H_2O_2/PDS conditions, respectively. It should be noted that UV irradiation of natural waters may lead to the formation of reactive species (e.g., hydroxyl radicals) from background constituents such as natural organic matter. However, under the conditions applied in this study using tap water, the contribution of these processes in the UV-only experiments is considered minor.

3 Results and discussion

3.1 Control tests

Compounds with strong UV absorbance, such as ACE, DFC, and SMX, exhibited notable photolytic degradation, indicating sensitivity to UV radiation (Figure 1). In contrast, other OMPs showed minimal degradation by UV. When H_2O_2 was used in the dark, complete degradation of DFC was achieved within 240 min, while the degradation of other OMPs remained relatively low. Using PDS alone in the dark, ATN, DFC, MTP, and SMX demonstrated transformation, suggesting direct reactivity between PDS and these OMPs. Similar direct oxidation of OMPs by H_2O_2, PDS and PMS has also been reported in previous studies (Maniakova et al., 2020; Guerra-Rodríguez et al., 2021; Ranjbar et al., 2025a; 2025b).

TABLE 2 Selected transformation products, their parents and molecular weights.

Metabolite name	Molecular weight (g/mol)	Parent	References
Hydroxy atenolol	282.34	Atenolol	Tay et al. (2011)
2-hydroxy carbamazepine	252.27	Carbamazepine	Trognon et al. (2024)
3-hydroxy carbamazepine	252.27		
10,11-dihydro-10-hydroxy carbamazepine	254.28		
4-hydroxy diclofenac	312.15	Diclofenac	Lonappan et al. (2016)
α-hydroxy metoprolol	283.36	Metoprolol	Voigt et al. (2021)

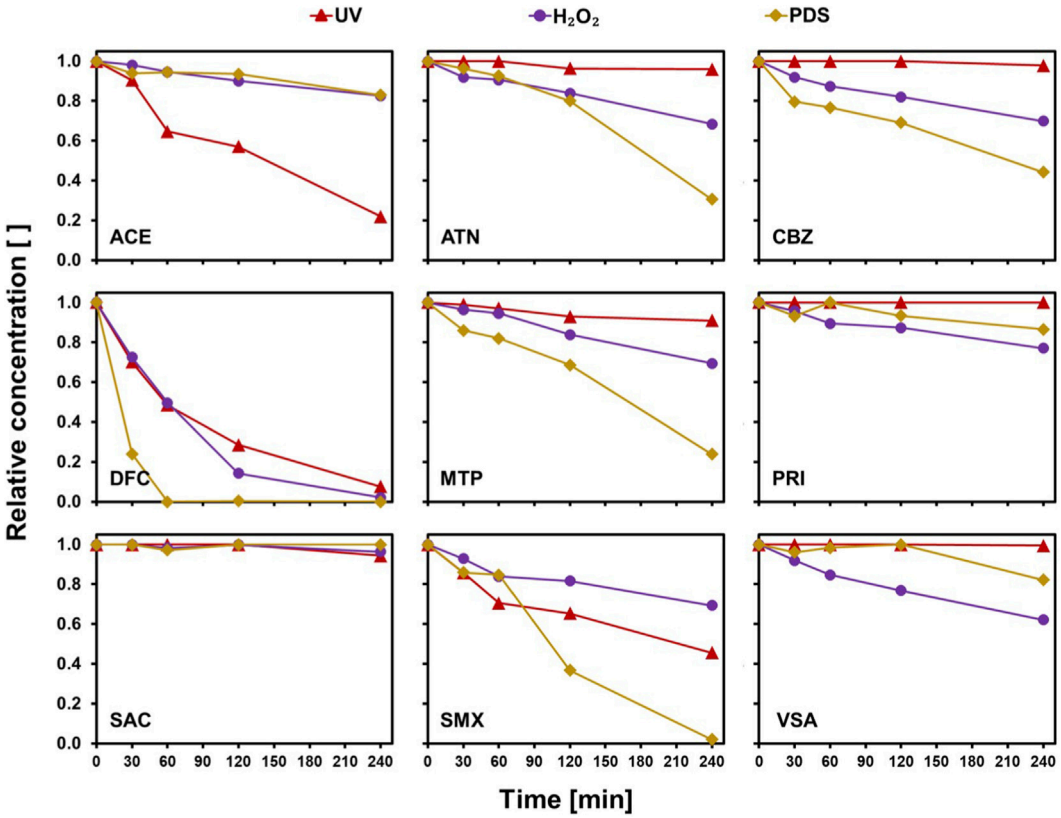


FIGURE 1
Relative concentration (C/C_0) of OMPs (ca. 1 μg/L initial concentration each) in control experiments conducted at room temperature (ca. 20 °C) in drinking water using UV irradiation, 2 mM H_2O_2, or 2 mM PDS separately.

3.2 OMP removals with UV/H_2O_2

Increasing the H_2O_2 dosage and extending the irradiation time led to a significant enhancement in the removal of OMPs (Figure 2). At 2.0 mM H_2O_2 dosage and 240 min of irradiation, all compounds except SAC achieved transformation exceeding 80%. Specifically, ACE and DFC showed the most rapid degradation, achieving more than 70% elimination within 120 min even at lower H_2O_2 doses. On the other hand, PRI exhibited higher stability, requiring a longer reaction time to achieve significant removal even at higher H_2O_2 dosages. Varying H_2O_2 doses indicated that most OMPs showed low initial degradation at a dose of 0.2 mM. However, when the H_2O_2 dose was elevated to 1.0 and 2.0 mM, a substantial enhancement in the degradation of most OMPs was observed.

3.3 OMP removal by UV/PDS

Within 240 min of reaction, increasing the PDS dosage resulted in elimination percentages exceeding 80% for all compounds except SAC and VSA (Figure 3). Notably, ATN, MTP, and SMX, exhibited relatively high degradation in the first 60 min, whereas ACE and PRI showed slower degradation. Furthermore, higher PDS concentrations led to improved degradation. For instance, after

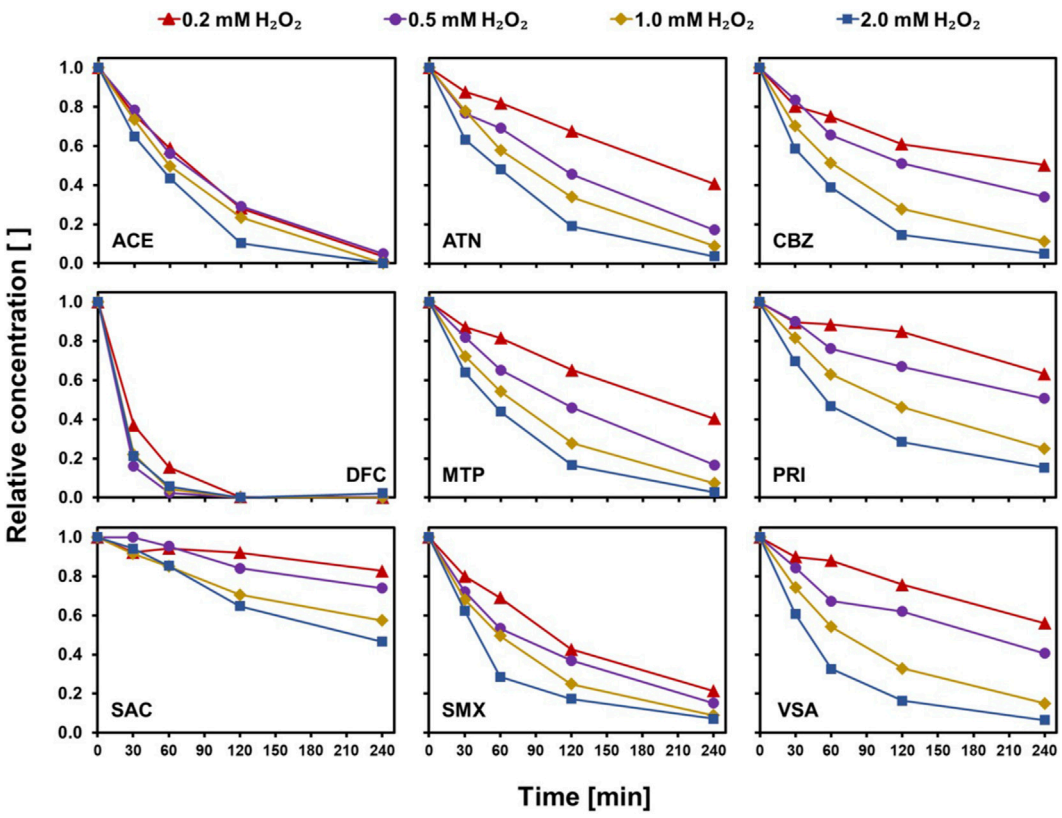


FIGURE 2
Relative concentration (C/C_0) of OMPs (ca. 1 µg/L initial concentration each) in drinking water during UV/H_2O_2 treatment at room temperature (ca. 20 °C) at different H_2O_2 doses (0.2–2.0 mM).

120 min of reaction, the degradation of CBZ at 1.0 mM PDS was much higher than that at 0.2 mM PDS.

3.4 Comparison of H_2O_2 and PDS

Although both oxidants (H_2O_2 and PDS) accelerated the degradation, variations in oxidation were observed among different compounds, and their removal efficiency depended on the intrinsic properties of each OMP. For example, DFC and SMX are highly sensitive to photolysis and attained high eliminations within a relatively short reaction time (30 min), whereas more stable compounds like CBZ and PRI required higher H_2O_2/PDS dosages to achieve significant degradation, as reported in a recent study (Thor et al., 2025). A comparison between H_2O_2 and PDS reveals that while some OMPs are effectively removed by H_2O_2, others respond better to PDS. However, cost-benefit evaluations indicate that PDS-based AOPs remain more expensive, as PDS currently costs nearly three times as much as H_2O_2 (Rodríguez-Chueca et al., 2018). Nevertheless, with increasing demand and continued optimization and commercialization of production processes, the cost of PDS is expected to decrease in the future (Fang et al., 2019).

The differences in degradation behavior can also be interpreted considering the reaction characteristics of the reactive oxygen species generated during the AOPs. In the UV/H_2O_2 process, hydroxyl radicals are the predominant oxidizing species and generally react with organic compounds through hydrogen abstraction, hydroxyl addition, and electron transfer in a largely non-selective manner. In contrast, UV/PDS systems may generate both sulfate radicals and hydroxyl radicals, with sulfate radicals typically exhibiting greater selectivity and reacting preferentially via electron transfer with electron-rich moieties, such as aromatic rings and electron-donating functional groups (Kilic et al., 2019; Zou et al., 2021; Doroudian et al., 2025). Consequently, the degradation rates of individual OMPs may be influenced by their molecular structure and physicochemical properties, including aromaticity, electron density, and acid-base characteristics. In addition, dissolved organic carbon (DOC = 4.5 mg/L) present in the tap water can compete with OMPs for reactive radicals, thereby reducing the effective oxidant availability (Rizzo et al., 2019). However, because the DOC concentration remained constant throughout all experiments, its scavenging effect was the same for both UV/H_2O_2 and UV/PDS systems and did not affect the relative comparison between the two processes.

3.5 Identification of transformation products

In the UV/H_2O_2 system, only two hydroxylated derivatives of carbamazepine (2-hydroxylated carbamazepine) were identified

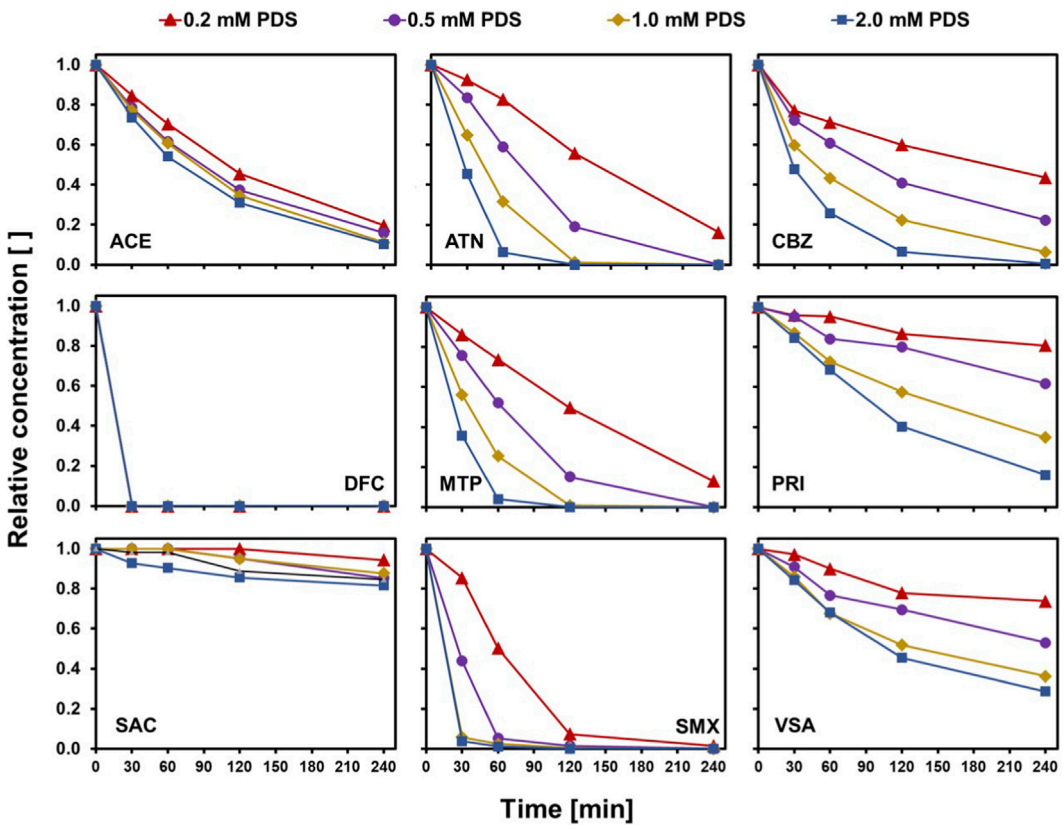


FIGURE 3
Relative concentration (C/C_0) of OMPs (ca. 1 μg/L initial concentration each) in drinking water during UV/H_2O_2 treatment at room temperature (ca. 20 °C) at different PDS doses (0.2–2.0 mM).

among the studied transformation products. The peak concentration of 2-hydroxycarbamazepine was observed at 30 min UV irradiation, reaching up to 30 ng/L. While 3-hydroxycarbamazepine peaked at 58 ng/L after 60 min irradiation at the highest tested H_2O_2/PDS dosage of 2 mM. Another transformation product of carbamazepine, 9-acridinecarboxylic acid, was also detected, with concentrations reaching up to 18 ng/L. However, its formation was more pronounced at lower oxidant dosages (0.2 mM H_2O_2). Continued exposure to the oxidizing species ultimately led to the complete degradation of these transformation products, as evidenced by their absence at longer irradiation times.

In the UV/PDS system, acridone-9-carboxylic acid was produced at concentrations of approximately 27, 42, 38, and 40 ng/L for PDS dosages of 0.2, 0.5, 1.0, and 2.0 mM, respectively. A notable difference between the UV/PDS system and the UV/H_2O_2 process is the absence of 2- and 3-hydroxylated carbamazepine derivatives under the experimental conditions applied in the present study. While the partial conversion of sulfate radicals into hydroxyl radicals is expected to occur in the UV/PDS system, sulfate radicals remain the dominant oxidant. Because sulfate radicals react highly selectively via single-electron transfer rather than hydroxyl radical addition (Menachery et al., 2018; Nair et al., 2022), the system preferentially generates ring-contraction products like 9-acridinecarboxylic acid instead of hydroxylated adducts. This mechanistic difference is strongly supported by the higher concentrations of 9-acridinecarboxylic acid observed in the UV/PDS system (up to 40 ng/L) compared to the UV/H_2O_2 process (<20 ng/L).

3.6 Comparison of UV photolysis, direct chemical oxidation and AOP

Pseudo-first-order kinetic constants were calculated to measure the possible synergistic effect of the AOP components, i.e., UV light and oxidants (H_2O_2 or PDS) (Supplementary Table S2). Then, for each OMP at various oxidant dosages, the degree of synergy was calculated and shown (Figure 4). This calculation was not performed for DFC in the UV/PDS system due to insufficient data, as DFC was oxidized too rapidly. The results show that the extent of synergy between UV light and oxidants (H_2O_2 and PDS) varies for different OMPs, likely due to the generation of reactive species such as •OH and SO_4•$^-$.

While most OMPs exhibited an AOP level exceeding 80%, compounds such as ACE, DFC, and SMX showed a lower degree of AOP. This can be attributed to their direct elimination by UV irradiation and direct reactions with H_2O_2/PDS, which contribute to their degradation alongside radical-mediated pathways. This effect is most noticeable for ACE, whose elimination reached around 100% and 90% in

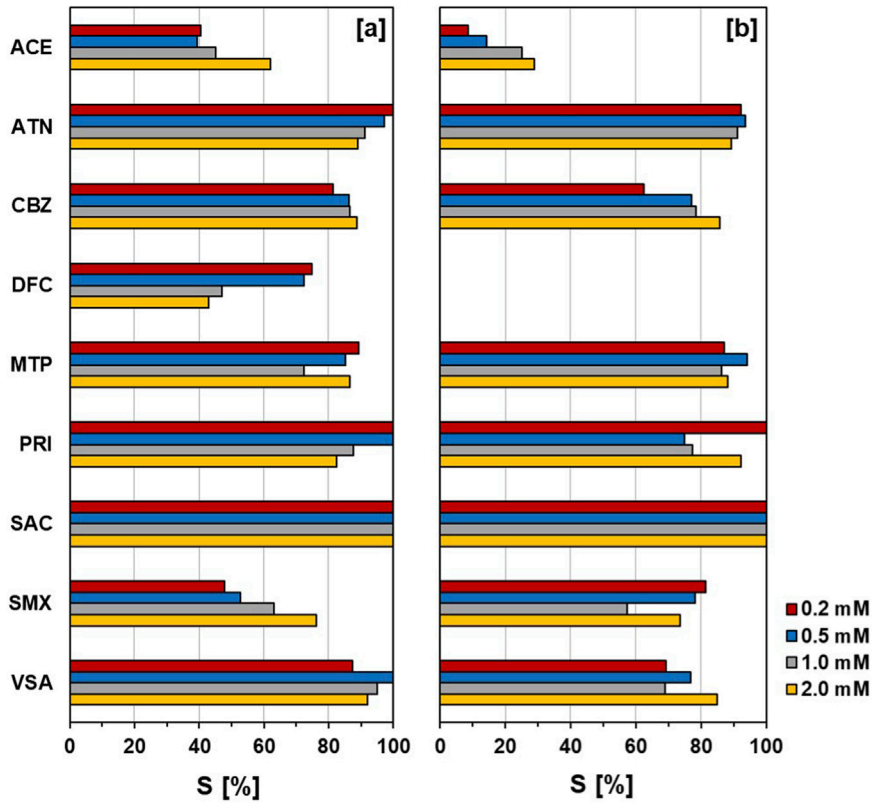


FIGURE 4
Extent of synergy between AOP components in **(a)** UV/H_2O_2 and **(b)** UV/PDS treatments at the different oxidant doses for removal of OMPs (ca. 1 μg/L initial concentration each) at room temperature (ca. 20 °C).

the UV/H_2O_2 and UV/PDS systems, respectively, using 2 mM H_2O_2/PDS after 2 h, while the estimated AOP levels were roughly 60% and 30%.

4 Conclusion

The results showed that oxidant (H_2O_2 or PDS) selection in a UV-based AOP system significantly influences degradation of OMPs. Some OMPs such as ATN, DFC, MTP can be rapidly removed in UV/PDS process. However, some OMPs such as ACE and VSA were better oxidized by UV/H_2O_2 process. Photosensitive substances like DFC were rapidly degraded under UV irradiation alone, whereas some other compounds such as PRI and SAC required higher H_2O_2/PDS doses and prolonged exposure for effective removal. The study of the extent of synergy between UV light and H_2O_2/PDS revealed that, while AOP accounts for a significant portion of OMP removal in most cases, the degree of AOP varies depending on the specific OMP and H_2O_2/PDS used. For some compounds, photolysis or direct oxidation by the oxidant contributes more to removal than the formation of free radicals generated by the AOP. Despite the elimination of the parent compounds, the formation of structurally similar transformation products remains a concern. Future studies can focus on in-depth investigation of OMP degradation mechanisms, identification of key intermediate products, and comprehensive assessment of their ecotoxicological impacts. Future studies may also explore optimization of process parameters to minimize the formation of toxic by-products, thereby ensuring the safety of treated drinking water quality. In addition, toxicity prediction tools, such as the Ecological Structure–Activity Relationship (ECOSAR) model, could be employed to evaluate the toxicity of intermediate compounds formed during OMP degradation and to assess the potential environmental impacts of UV-based AOPs.

Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

Author contributions

ER: Conceptualization, Investigation, Methodology, Supervision, Validation, Writing – original draft. JP: Data curation, Investigation, Methodology, Software, Visualization, Writing – original draft. SM: Data curation, Formal Analysis, Methodology, Validation, Writing – review and editing. AR: Conceptualization, Investigation, Methodology, Project administration, Resources, Supervision, Validation, Writing – review and editing.

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Conflict of interest

The author(s) declared that this work was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Supplementary material

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fenvs.2026.1905650/full#supplementary-material

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