

Photodecomposition of sodium dodecyl sulfate under high-intensity pulsed UV radiation of continuous spectrum and hydrogen peroxide

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ABSTRACT

Surfactants are widely used in industry and households, although they are typically non-toxic, their self-degradation products could have potential health and environmental effects. Therefore, the improvement of water purification technology from these substances is an essential problem. Within this paper, the features of the photochemical decomposition of an anionic surfactant (sodium dodecyl sulfate) under the combined effect of high-intensity pulsed UV radiation of continuous spectrum and hydrogen peroxide are investigated. All experiments were conducted with an initial pollutant concentration of 10 mg L⁻¹. Direct photolysis has proven to be an extremely inefficient method due to the low process rate and high energy consumption. However, the addition of hydrogen peroxide to a solution irradiated by polychromatic light drastically enhances the photodecomposition rate. The decomposition efficiency rises from 90% to more than 99% and the energy consumption significantly decreases with an increase in the molar ratio of hydrogen peroxide and sodium dodecyl sulfate concentrations. The obtained values of electrical energy per order in conjunction with other process aspects demonstrate that the use of UV/H₂O₂ technology with a xenon flashlamp as a radiation source is advantageous for the purification of solutions from the investigated contaminant.

Keywords: Xenon flashlamp; UV; Water purification; Advanced oxidation processes; Sodium dodecyl sulfate

1. Introduction

Surfactants form a group of compounds belonging to one of the most frequently used substances in industry and households. Nowadays, there is a growing trend towards the use of biodegradable surfactants which exhibit improved decomposition characteristics. However, their relatively low but harmful concentrations can still be detected in treated sewage and surface water [1].

Sodium dodecyl sulfate C₁₂H₂₅OSO₃Na (SDS) is one of the widely used anionic surfactants. It is mainly employed as a detergent in industry, pharmacology, and cosmetics. Water purification from SDS is crucial since its presence in natural environments negatively affects the survival rate of fish, yeast, and bacteria [2]. For instance, according to the current legislation of the Russian Federation, the threshold limit value (TLV) of sodium alkyl sulfates in fishery water is 0.5 mg L⁻¹.

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Both traditional and recently developed methods have been proposed for water purification from SDS: ultrafiltration [3], glow discharge [4], and adsorption [5,6]. Among others, advanced oxidation processes (AOPs) are considered to be the best alternative due to their high efficiency and versatility [7]. The AOPs are based on the generation of hydroxyl radicals which are capable of initiating a cascade of reactions that could result in the total degradation or mineralization of the most recalcitrant organic and inorganic contaminants. Different AOPs mainly based on UV radiation were successfully used for the decomposition of SDS: heterogeneous photo-Fenton process [8], homogeneous photo-Fenton process using solar radiation [9] or low-pressure mercury lamps [10], and ozonation combined with ultraviolet irradiation in the presence of hydrogen peroxide ($O_3/H_2O_2/UV$) [11].

Currently, low-pressure mercury lamps (MLs) with monochromatic spectrum emitting at 253.7 nm wavelength are primarily used as a source of UV radiation in photochemical AOPs. However, such radiation selectivity is not efficient to both direct photolysis of organic compounds and photodecomposition of hydrogen peroxide due to the low absorption at this wavelength. Developed in recent decades xenon flashlamps (FLs) have several advantages over ML, such as high pulsed radiation power, which is 10^4 – 10^5 times higher than typical ML value, and continuous emission spectrum in the wavelength range from the envelope transmission (170 nm for quartz) to the near-infrared region. The non-selectivity property of the FL emission spectrum allows efficient use of photons for both photolytic reactions with various pollutants and the photochemical decomposition of hydrogen peroxide into hydroxyl radicals. Taking into account the proportionality of the photochemical reaction rate and the amount of the absorbed photons, greater decomposition efficiency using FLs instead of MLs could be achieved with identical radiation energy transferred to the solution. Moreover, FLs do not contain hazardous substances such as mercury, which makes the process environmentally friendly.

A relatively high (>95%) efficiency of photo-oxidation of an SDS solution with an initial concentration of 100 mg L^{-1} using UV/ H_2O_2 AOPs technology with a xenon flashlamp as a source of UV radiation was shown in [12,13]. Additionally, the prior studies have demonstrated that the efficiency of the UV/ H_2O_2 process slightly increases in an alkaline medium, while a decrease in the rate of SDS decomposition is observed providing that $[HCO_3^-]/[SDS] > 140$.

Due to the reduced interaction probability of SDS molecules and short-lived radicals, the photodegradation process is susceptible to the influence of limiting factors at low contaminant concentrations (10–50 TLV). At the same time, these concentrations are likely to appear in industrial wastewater and at the final stages of water purification. Therefore, based on the obtained results with an initial SDS concentration of 100 mg L^{-1} , it was decided that this research would be focused on low concentration solutions.

This paper aims to investigate the UV/ H_2O_2 method features for the purification of water from SDS in low concentrations. Additionally, the main parameters and patterns of the photochemical process with an FL as a source of high-intensity pulsed ultraviolet radiation of continuous spectrum are determined.

2. Materials and methods

A xenon flashlamp with 120 mm arc length and 5 mm inner diameter operated in a discharge circuit with an average electrical power of 200 W and a frequency of 3.3 Hz was used as a radiation source. The spectral energy distribution of the lamp was recorded by means of an AvaSpec-ULS2048 spectrometer (Avantes, The Netherlands) using the procedure described in depth in [14]. The photon fluence, that is, the number of photons per unit of the solution surface, was determined through the use of uranyl oxalate actinometry [15].

The experimental setup is shown in Fig. 1. Samples with a volume of 100 mL were irradiated in a 104 mm internal diameter Petri dish located at a distance of 207 mm from the lamp axis. A set of opaque diaphragms that limit the lamp radiating area was designed to evaluate the effect of photon fluence on the efficiency of the process. Cooling air was blown to decrease the heat effect on the rate of the reactions. Additionally, the inner surfaces of the safety cover were painted black to minimize reflection and scattering.

Solutions of SDS (USP, Panreac, Spain) were prepared in distilled water at room temperature immediately before the experiments. All other reagents used during the experiments were of analytical grade.

The electronic absorption spectra were measured with a Varian Cary 50 Scan spectrophotometer (Varian, USA). The pH values of the solutions were controlled on an Expert-pH device (Econix, Russia). The concentration of SDS was determined by means of the extraction-photometric method with methylene blue [16] and the concentration of hydrogen peroxide was evaluated by the formation of the peroxide complex $[TiO \cdot H_2O_2]^{2+}$ [17].

3. Results and discussion

Fig. 2 shows the dependence of the molar attenuation coefficient of the oxidant (H_2O_2) and the pollutant (SDS) in a neutral medium (pH 6.7) against the wavelength, as well as the spectral distribution of photons emitted by the FL per pulse. The absorption range of H_2O_2 and SDS overlaps with the emission range of the selected radiation source, which suggests the possibility of chemical transformations initiated by absorbed photons.

A $C_{12}H_{25}OSO_3Na$ molecule does not contain chromophore groups and, therefore, weakly absorbs near and middle ultraviolet radiation. The undertaken experiments demonstrated that direct photolysis is ineffective for the decomposition of low concentrations of SDS. This statement was additionally confirmed in [18], where a xenon arc lamp was used as a source of solar radiation simulation. However, it was noticed that the SDS decomposition rate slightly increases in a neutral medium, while in an acidic medium the absorption of the solution increases due to the hydrolysis and the formation of dodecanol molecules.

Preliminary experiments have demonstrated that the presence of hydrogen peroxide in an SDS solution isolated from UV radiation does not cause SDS decomposition within 7 d.

It is known that the primary process of UV absorption by hydrogen peroxide induces dissociation with the formation of two hydroxyl radicals [19]. Moreover, the

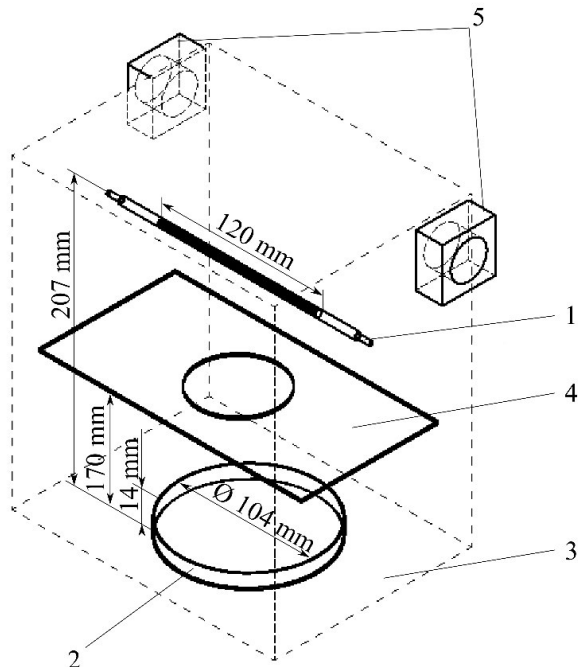


Fig. 1. Experimental setup. 1 – Xenon flashlamp, 2 – petri dish, 3 – safety cover, 4 – opaque diaphragm, 5 – air ventilation system.

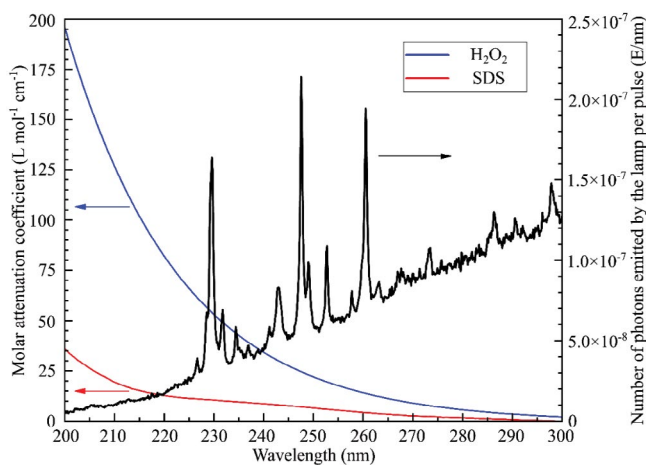


Fig. 2. Wavelength dependence of H₂O₂ and SDS molar attenuation coefficient and spectral distribution of photons emitted by the FL per pulse.

photodecomposition in the absence of acceptors occurs in two distinct ways [20]. First, a chain mechanism of H₂O₂ decomposition (initiated by hydroperoxide radicals) is observed at relatively low photon fluxes and the quantum yield of H₂O₂ removal can be significantly greater than one. Second, a non-chain mechanism occurs at high photon fluxes (high concentrations of radicals suppress the propagation of a chain reaction) and the quantum yield for the formation of hydroxyl radicals is 1.11 ± 0.07 in the wavelength range from 205 to 280 nm.

The kinetic dependences comparison of the individual SDS and hydrogen peroxide decomposition under

irradiation with the FL is presented in Fig. 3, as well as the effect on the process of their simultaneous presence in the solution. The photodegradation rate of SDS and H₂O₂ is relatively low and constant in the initial decomposition region.

The obtained experimental data were used to estimate the quantum yield of hydrogen peroxide photolysis by pulsed polychromatic radiation considering the first-order reaction and the assumption of an optically transparent medium. As a result, the averaged quantum yield was 0.55 ± 0.06 that defines the ratio of the number of decomposed H₂O₂ molecules to the number of absorbed photons in the range from 200 to 300 nm. This value correlates well with the literature data for monochromatic radiation sources [20,21].

The photochemical decomposition rate of hydrogen peroxide decreases in the presence of SDS in the irradiated solution due to the reaction of hydroxyl radicals with SDS which limits the chain mechanism of the H₂O₂ reaction. However, the presence of H₂O₂ drastically increases the decomposition rate of SDS itself, this is caused by the scavenging of the generated hydroxyl radicals. The data presented in Fig. 3 show that the use of H₂O₂ and an FL as a source of UV radiation allows achieving high (greater than 99%) degree of water purification at low initial concentrations of SDS.

The evolution of the concentrations of SDS and H₂O₂ against the photon fluence in the wavelength range from 200 to 300 nm is shown in Fig. 4. The irradiation time for all experimental points was constant and the photon fluence variation was performed by reducing the radiating surface area of the xenon flashlamp by means of diaphragms.

The decrease in the concentration of hydrogen peroxide only depends on the number of photons absorbed by the solution. The initial oxidation period, in which the influence of the reaction products is insignificant, was studied. The linear dependence of the concentrations of SDS and H₂O₂ from the photon fluence leads to the conclusion that the constant amount of H₂O₂ molecules is consumed in the photochemical decomposition process of an SDS molecule. Taking into account the slope of the straight lines in Fig. 4 and the molar concentrations of the reagents, it was found that the decomposition of one molecule of SDS expends about 20 molecules of H₂O₂.

As shown in Fig. 5, the kinetics of the photo-oxidative decomposition of SDS could be described by a pseudo-first-order reaction equation. The logarithm of the SDS removal rate is directly proportional to the irradiation time since the photon flux is constant, the medium is optically transparent and H₂O₂ concentration decreases slightly at the investigated exposure time.

The multiplicity and superposition of the absorption bands of the products resulting from the SDS photochemical decomposition, including the bands of the initial reagents, complicate the analysis of the reaction mechanism by means of the photometric method. However, applying nuclear magnetic resonance spectroscopy, various carbonyl compounds (for instance, formic, acetic acid, and propionic acids) were detected among the decomposition products after treatment of highly concentrated solutions of SDS (0.1 M) by hydroxyl radicals [22].

Based on the previous research and the conducted experiments, photochemical decomposition of SDS initiated by pulse UV radiation of continuous spectrum in the presence

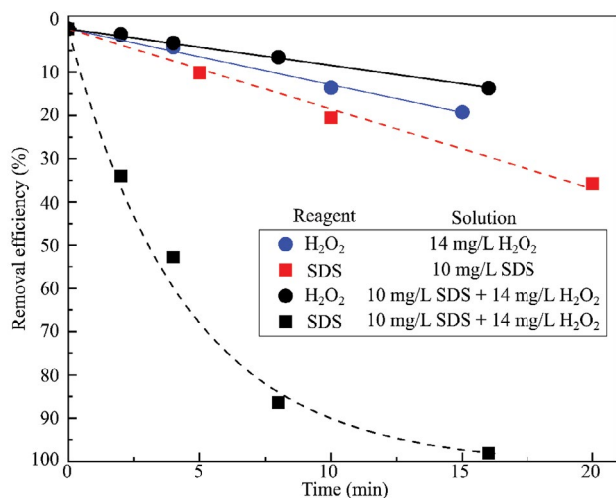


Fig. 3. Removal of SDS and H₂O₂ with their various combinations. The photon flux on the surface of the solution in the range from 200 to 300 nm is $5.3 \times 10^{-5} \text{ E m}^{-2} \text{ s}^{-1}$.

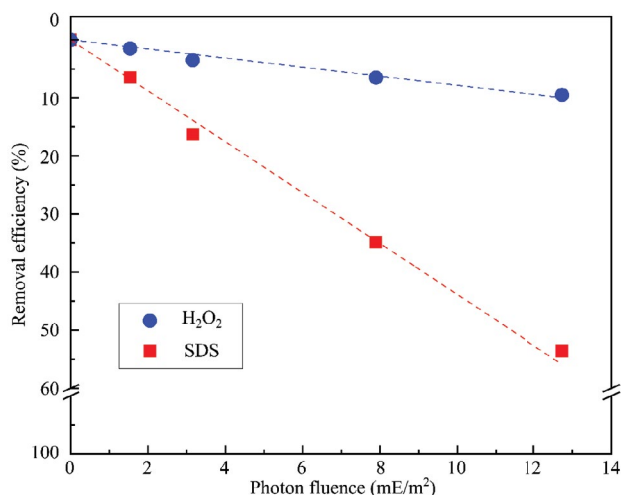


Fig. 4. Effect of the photon fluence in the wavelength range from 200 to 300 nm on the removal of SDS and H₂O₂. Experimental conditions: 10 mg L⁻¹ SDS; 14 mg L⁻¹ H₂O₂; 4 min of irradiation.

of hydrogen peroxide can be described by a number of fundamental processes [12,22,23]. Primarily, photodecomposition of hydrogen peroxide molecules occurs with the hydroxyl radicals formation with a quantum yield of 0.55 ± 0.06 for irradiation in the wavelength range from 200 to 300 nm:



The generated highly reactive radical interacts with the dodecyl sulfate ion in a way that hydrogen atom detaches from the hydrocarbon chain of SDS and the organic radical forms (with a reaction rate constant of $8.2 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ [24]):

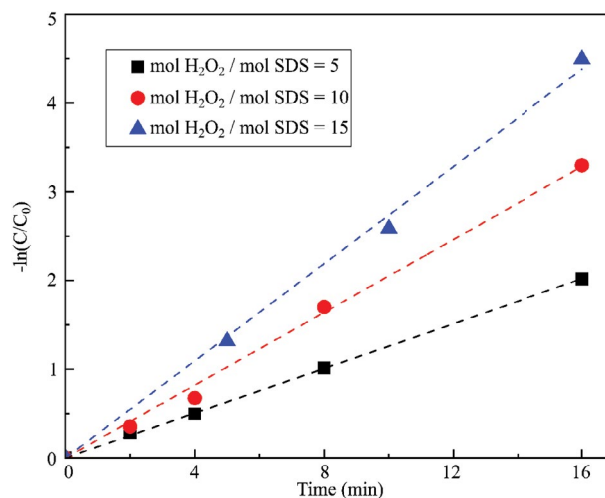
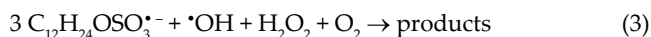


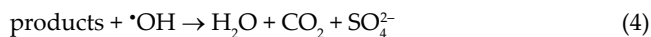
Fig. 5. Semilogarithmic anamorphosis of photodecomposition of SDS with an initial concentration of $3.5 \times 10^{-5} \text{ M}$ for various molar ratios of H₂O₂ and SDS initial concentrations. The photon flux on the surface of the solution in the range from 200 to 300 nm is $5.3 \times 10^{-5} \text{ E m}^{-2} \text{ s}^{-1}$.

Further chemical transformations of SDS are associated with the occurrence of numerous and complex redox reactions involving both the initial reagents and the intermediate products. If an aqueous solution is aerated, additional reactions with oxygen molecules and the formation of peroxide radicals are expected. This multistage process could be expressed by the following simplified scheme:



As a result of photochemical transformations of SDS, the sulfate group is eliminated and surface-active properties are lost. Hydroxyl radicals react with the hydrocarbon chain of SDS and, apparently, the insertion of the carbonyl groups occurs chaotically [22].

The destruction of products leads to the formation of sulfate ion, carbon dioxide, and water molecules. However, this process requires significant time and energy consumption:



According to the photochemistry laws, the amount of a reacted substance is proportional to the number of absorbed photons. Therefore, taking into account the Beer–Lambert–Bouguer law and the low absorption capability of the solution ($\epsilon Cl \ll 1$), the equation for the photodegradation rate (r) of an irradiated substance can be expressed as follows:

$$r = \text{const} \cdot I_0 \cdot (1 - e^{-\epsilon Cl}) = k_{\text{eff}} C \quad (5)$$

where $k_{\text{eff}} = \text{const} I_0 \epsilon l$ is the effective reaction rate constant (min^{-1}), C is the concentration of the analyzed substance (mol L^{-1}), ϵ is the molar attenuation coefficient ($\text{L mol}^{-1} \text{ cm}^{-1}$), l is the solution layer thickness (cm), I_0 is the photon fluence (E m^{-2}).

The first order of the Eq. (5) is supported by the experimental data that was obtained using direct photolysis of SDS and H_2O_2 (Fig. 3).

The pseudo-first-order reaction parameters, such as the process rate constant (k_{eff}) and the time required to reduce the SDS concentration by half ($t_{1/2}$), were calculated to compare the efficiency of photo-oxidative decomposition of SDS and to clarify the influence of the $[\text{H}_2\text{O}_2]/[\text{SDS}]$ molar ratio on its efficiency. These parameters are general and take into account the influence of kinetic and radiation effects, as well as the specific setup design and the experimental conditions. The values of the parameters are given in Table 1.

As can be noted, k_{eff} substantially increases with the increment of H_2O_2 content addition in the solution while $t_{1/2}$ significantly decreases. Thus, the rate of the SDS photodecomposition process mainly depends on $[\text{H}_2\text{O}_2]/[\text{SDS}]$. This parameter determines the speed of the fundamental reactions of the oxidation process initiation Eqs. (1) and (2) that directly affects the speed of the entire photo-oxidative process as described by Eqs. (1)–(4).

Electrical energy per order (E_{EO}) was calculated to estimate the efficiency of the photochemical decomposition of SDS (Table 1). The E_{EO} value represents the energy input required to reduce the concentration of a target contaminant in a unit volume by order of magnitude. This parameter is a figure of merit to evaluate the energy requisition of UV-based AOP technologies [25]. Although the experiments were carried out in stationary conditions during this study, the value of E_{EO} is of cardinal importance for assessing the energy efficiency of the technology. However, E_{EO} depends on a significant number of additional factors and should be treated carefully for the comparison with the results obtained using other experimental setups.

As can be seen from the data presented in Table 1, the direct photolysis of SDS is an inefficient method. In the presence of H_2O_2 , the E_{EO} value is reduced by 5–10 times. Additionally, due to the relatively low cost of H_2O_2 and low reagent consumption, the total cost of the purification technology does not rise significantly.

4. Conclusion

Ultraviolet radiation initiates the decomposition of SDS in an aqueous solution. Due to the low absorption of UV by SDS, direct photolysis has been proven to be an inefficient method for water purification from SDS. Furthermore, high electrical energy consumption makes this technology unpromising for industrial applicability.

Table 1
Parameters of the pseudo-first-order reaction and electrical energy per order for different molar ratios

Process	$[\text{H}_2\text{O}_2]/[\text{SDS}]^a$	k_{eff} (min ⁻¹)	$t_{1/2}$ (min)	E_{EO} (kWh m ⁻³)
UV	0	0.02	31.2	>50
UV/ H_2O_2	5	0.13	5.5	11.3
UV/ H_2O_2	10	0.20	3.4	7.5
UV/ H_2O_2	15	0.27	2.6	5.7

^aInitial concentration of SDS is 3.5×10^{-5} mol L⁻¹.

The results of the conducted analysis show that the efficiency of SDS decomposition significantly increases when using the combined effect of high-intensity UV radiation from a xenon flashlamp and hydrogen peroxide. The decomposition rate increases significantly and, at the same time, the electrical energy per order becomes less than 6 kWh m⁻³ with $[\text{H}_2\text{O}_2]/[\text{SDS}]$ molar ratio growth that is sufficient enough for further detailed process optimization and technology approbation in photochemical reactors. The further reduction of energy consumption for the UV/ H_2O_2 method is possible in several ways: the selection of optimal process parameters (pH and reagent concentrations), an increase in the efficiency of the radiation source in the spectral range from 200 to 300 nm and the addition of catalysts.

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