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# OPTIMIZATION OF COMPACT $TiO_2$ PHOTOCATALYSTS FOR WATER PURIFICATION IN AGRICULTURAL OPERATIONS

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*Article dedicated development and optimization compact photocatalytic modules on basis titanium (IV) oxide ($TiO_2$) for cleaning water that used in agrotechnical operations , in particular for hydration seed under time sowing cereals cultures in seeders . The work solves the problem of providing clean water in field conditions, where traditional treatment methods are cumbersome or economically unprofitable. A complex mathematical model is proposed that describes the nonlinear kinetics of photocatalytic decomposition of organic pollutants, taking into account the intensity of ultraviolet light (5–20 mW/cm²), the size of $TiO_2$ particles (10–50 nm), the concentration of the catalyst (0.5–2.0 g/l) and the temperature (20–40 °C). The model is based on the Langmuir-Hinshelwood equation, supplemented by dependencies on the catalyst surface and activation energy, and is solved numerically by the Runge-Kutta method. Experiments were carried out using $TiO_2$ nanoparticles (anatase) and a model pollutant (methylene blue, 10 mg/l) in a laboratory module that simulates the operation of seeders. The results confirm the high accuracy of the model: the optimal parameters ($I = 15$ mW/cm², $d = 25$ nm, $[TiO_2] = 1.0$ g/l, $T = 30$ °C) provide a cleaning efficiency of 38% in 15 minutes, reducing the concentration of contaminants to 6.2 mg/l, which is sufficient for agrotechnical needs. The data are presented in tables and graphs that illustrate the influence of key variables. The optimized system is suitable for integration into seed drills such as Horsch Pronto or John Deere 1890, increasing seed germination in arid regions. The work outlines the prospects for using solar energy and modified $TiO_2$ to further improve the technology, contributing to sustainable agriculture.*

***Key words:*** *photocatalysis, $TiO_2$ (titanium(IV) oxide), water purification, agrotechnical operations, grain planters, mathematical modeling, nonlinear kinetics, ultraviolet light.*

***Eq. 12. Fig. 5. Table. 2. Ref . 14.***

## 1. Problem formulation

Modern agriculture faces a number of challenges, including the shortage of clean water, growing environmental demands and the need to improve the efficiency of agricultural operations. One of the key areas of development in the agricultural sector is the introduction of innovative technologies that can ensure sustainable use of resources and minimize environmental impact. In this context, seed moistening systems during sowing of grain crops attract special attention, which allow to increase germination and yield, especially in arid regions. However, the quality of water used for such operations often does not meet the required standards due to the presence of organic and chemical contaminants, such as pesticides, dyes or microorganisms. Traditional water purification methods, such as mechanical filtration, reverse osmosis or chemical treatment, are either too bulky to be integrated into compact agricultural systems, such as seed drills, or are economically unprofitable for small and medium-sized farms.

Photocatalytic technologies based on titanium(IV) oxide ($TiO_2$) offer new perspectives for solving this problem. $TiO_2$, known for its high photocatalytic activity under the influence of ultraviolet (UV) light, is able to efficiently decompose organic pollutants into safe products (carbon dioxide and water) without the use of additional chemical reagents. Its advantages include chemical stability, non-toxicity, availability and the possibility of activation by natural sunlight, which makes it an ideal candidate for environmentally friendly applications. In the context of agricultural technology, photocatalytic systems based on $TiO_2$ can be integrated into seeders to purify water immediately before it is supplied to the sowing zone, providing optimal conditions for seed germination and reducing the risk of chemical contamination of the soil.

Despite significant progress in photocatalytic research, most current developments focus on large-scale stationary water purification systems, such as industrial wastewater treatment plants. Compact modules adapted to the needs of mobile agricultural devices remain understudied.

## 2. Analysis of recent research and publications

Traditional water purification methods, such as mechanical filtration, chemical chlorine treatment or reverse osmosis, have significant limitations in the context of agricultural operations. Mechanical filters are ineffective against dissolved organic compounds and require frequent replacement of elements, which makes their use in mobile systems such as seeders difficult. Chemical methods, although capable of destroying microorganisms, add new reagents to the water that can be harmful to seeds or soil. Reverse osmosis, in turn, is energy-intensive and requires complex equipment, which makes it economically unprofitable and technically difficult to integrate into compact agricultural devices. Thus, there is a need to develop an alternative water purification method that would be simultaneously effective, environmentally friendly, compact and suitable for real-time operation during sowing.

Photocatalytic systems based on titanium(IV) oxide ($TiO_2$) offer a promising solution to this problem. $TiO_2$, when exposed to ultraviolet (UV) light, generates reactive oxygen species (e.g., hydroxyl radicals), which decompose organic pollutants into safe products – carbon dioxide and water. This process does not require additional chemical reagents, which makes it environmentally friendly, and the possibility of using sunlight as an energy source increases its sustainability. However, the implementation of such systems in seeders is associated with a number of technical and scientific difficulties that need to be resolved to ensure their practical value.

The first problem is the compactness of the photocatalytic module. Planters such as the Horsch Pronto or John Deere 1890 have limited space for additional equipment, and the water treatment time during sowing usually does not exceed 15–20 minutes. This requires a high photocatalytic reaction rate and an efficient system design that would occupy minimal volume and weight. The second problem is related to the optimization of the operating parameters of $TiO_2$. The efficiency of photocatalysis depends on the intensity of UV light, the size of the catalyst particles, its concentration, water temperature and the initial level of contamination. Without a precise understanding of these relationships, it is impossible to achieve maximum productivity with minimal energy consumption. The third problem concerns the adaptation of the technology to real conditions: dust, temperature changes and vibration in the field can affect the stability of the module, and the use of natural sunlight instead of an artificial UV source requires an increase in the sensitivity of $TiO_2$ to the visible spectrum.

Photocatalytic technologies based on titanium(IV) oxide ($TiO_2$) are the subject of active study worldwide due to their potential for water, air and surface purification from organic and inorganic contaminants. Recent years have been characterized by significant progress in understanding the mechanisms of photocatalysis, developing new materials and expanding their applications. In the context of agrotechnical operations, in particular water purification for planters, research remains less developed, but a number of recent publications and achievements in related fields create a solid foundation for this direction.

One of the key focuses of recent research is to improve the efficiency of $TiO_2$ as a photocatalyst. The effect of $TiO_2$ nanoparticle size on their photocatalytic activity is examined in [1] . The authors found that particles with a size of 10–25 nm exhibit optimal surface activity due to the larger contact area with pollutants, although further size reduction (<10 nm) can complicate synthesis and increase production costs. These results are supported by a study [2], which showed that $TiO_2$ nanoparticles with a size of 20 nm efficiently decompose methylene blue at a UV light intensity of 15 mW/cm², achieving 50% removal in 20 minutes. Such data are important for adapting the technology to planters, where treatment time is limited.

Another area of research focuses on modifying $TiO_2$ to extend its sensitivity to visible light, which could reduce dependence on artificial UV sources and open up opportunities for using solar energy in the field. The paper [3] describes the doping of $TiO_2$ with nitrogen (N-$TiO_2$), which shifts the absorption to the 400–500 nm range. Experiments have shown that N-$TiO_2$ increases the efficiency of organic dye decomposition by 30% compared to pure $TiO_2$ under natural light conditions. This is of particular importance for agricultural technology, where integration with solar panels could make the system autonomous. However, the authors note that the stability of such modified materials in real-world conditions (dust, humidity) requires additional study.

The kinetics of photocatalytic processes also remains a focus of attention. In [4], a detailed model based on the Langmuir-Hinshelwood equation was developed, which takes into account the adsorption of pollutants on the $TiO_2$ surface, light intensity and temperature. The model showed that the reaction rate constant (k) depends nonlinearly on light intensity, reaching saturation at $I > 20$ mW/cm$^2$, which is consistent with experimental data. These findings are important for the optimization of photocatalytic modules in seeders, where it is necessary to balance performance and energy consumption. In addition, the authors emphasize the effect of temperature: an increase from 20 °C to 40 °C increases k by 15–20%, which can be used to improve efficiency in warm climates.

In the context of practical application in agricultural technology, research is still limited. The work [5] analyzes the potential of photocatalytic water purification for agricultural needs in Ukraine, in particular for irrigation. The author notes that $TiO_2$ modules can remove up to 40% of organic pollutants in 30 minutes, but their integration into mobile systems such as seeders requires compact design and optimization of power supply. Similar ideas are highlighted in the article [6] , which considers the use of $TiO_2$ coatings for water purification in precision agriculture systems. However, the authors do not touch on specific aspects of the operation of seeders, such as limited processing time or vibration in field conditions.

The energy aspect of photocatalysis is also being actively investigated. In [7], a combination of $TiO_2$ with solar panels was proposed to create autonomous purification systems. Experiments have shown that solar energy with an intensity of 10–15 mW/cm$^2$ in the UV range can activate $TiO_2$, although the efficiency is reduced due to the smaller fraction of UV in the sunlight spectrum (about 5%). This highlights the need for modifications of $TiO_2$ or hybrid systems for agrotechnical applications.

In Ukraine, research on photocatalysis for agriculture is at an early stage. The work [8] focused on the use of $TiO_2$ for water purification in farms, but did not consider mobile systems. At the same time, local publications emphasize economic aspects: the use of local water sources with subsequent purification can reduce water transportation costs by 20–30%, which is relevant for small farms.

## 3. The purpose of the article

The aim of the article is to develop and optimize compact photocatalytic modules based on titanium dioxide ($TiO_2$) for the purification of water used in agrotechnical operations, in particular for wetting seeds during sowing of grain crops in seeders. The work is aimed at solving the problem of providing clean water in field conditions, where traditional purification methods are cumbersome or economically impractical.

## 4. Results and discussion

$TiO_2$ is a semiconductor compound. According to modern ideas, electrons in such compounds can be in two states: free and bound. In the first state, electrons move along the crystal lattice formed by Ti4+ cations and $O_2$- anions. In the second state, electrons are bound to some ion of the crystal lattice and participate in the formation of a chemical bond. For an electron to transition from a bound state to a free state, it is necessary to expend energy of at least 3.2 eV. This energy can be delivered by light quanta with a wavelength of $\lambda < 390$ nm. Thus, when light is absorbed in the volume of $TiO_2$ particles, a free electron and an electron vacancy appear (in semiconductor physics, such an electron vacancy is called a hole).

The electron and hole are quite mobile entities, and while moving in a part of the semiconductor, some of them recombine, and some of them reach the surface and are captured by it. The processes taking place on the $TiO_2$ surface are schematically shown in Fig. 1.

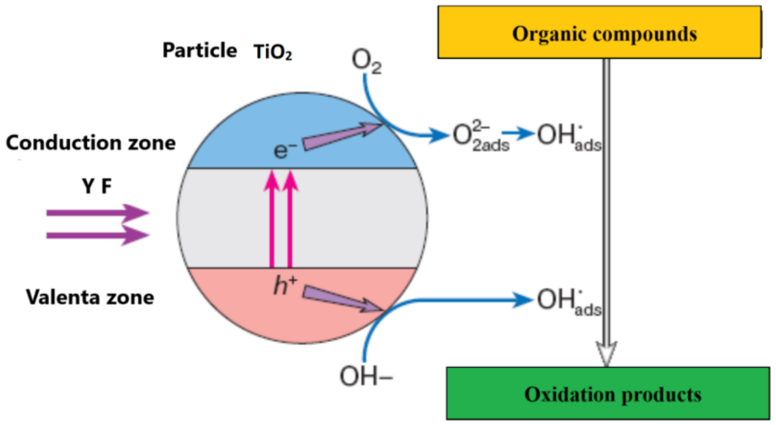

*Fig. 1. Schematic representation of the processes that occur on a semiconductor particle.*

The electron and hole trapped by the surface are quite specific chemical particles. For example, the electron is probably Ti $^{3+}$ on the surface, and the hole (electron vacancy) is localized on the lattice surface oxygen, forming $O^-$. They are extremely reactive [9]. In terms of redox potentials, the reactivity of the electron and hole on the surface of Ti and $O_2$ is characterized by the following values: electron potential ~ -0.1 V, hole potential ~ +3.

Accordingly, a normal hydrogen electrode. In other words, an electron is able to react with oxygen, forming a sequence of reactions:

$$\begin{gathered} \bar{e} + O_2 \to O_2^- \\ \bar{e} + O_2^- \to O_2^2 \to O^- + O^- \\ O_2 + 2H^+ \to O^{2-} \\ \bar{e} + O^- \to O^{2-} \\ \bar{e} + H_2O_2 \to OH + OH^- \\ O^- + H^+ \to OH \end{gathered} \qquad (1)$$

This can form strong oxidants such as:$O^-$ and $OH$- radical. The second possible reaction path for an electron is the reaction:

$$\bar{e} + H^+ \to H$$

or

$$\begin{gathered} \bar{e} + H_2 0 \to OH^- + H \\ H + H \to H_2 \uparrow \end{gathered} \qquad (2)$$

The second stage is realized only in aqueous solutions and at low oxygen concentrations. The main channel of electron disappearance is the reaction with oxygen.

Oxygen reacts with water:

$$h + C_xH_yO_z \to C_xH_{y-1}O_y + H^+ \qquad (3)$$

where $O^-$ and$OH$ – radicals are also capable of oxidizing any organic compounds. And thus, the surface of $TiO_2$ under light becomes a strong oxidant .

The efficiency of a photocatalyst is determined by the quantum yield of the reaction and the spectrum of the photocatalyst. The quantum yield of a photoreaction is the ratio of the number of product molecules to the number of absorbed light quanta [10]. For semiconductor particles as photocatalysts, several stages of the process are usually considered: a) light absorption – the formation of electron-hole pairs, b) diffusion of electrons and holes to the surface of the semiconductor, c) bulk recombination of electrons and holes, d) surface recombination of electrons and holes, e) useful reactions of electrons and holes with adsorbed molecules.

The quantum yield of the reaction F can be represented as follows:

$$F = \eta_{\mathrm{i}}\eta_r \qquad (4)$$

where $\eta_{\mathrm{i}}$ – the fraction of current carriers that reached the surface, $\eta_r$is the fraction of current carriers that reached the surface and entered into a useful reaction (avoided surface recombination).

For calculation $\eta_{\mathrm{i}}$it is necessary to use equations describing the motion of chaotic particles. In the most general case the mentioned equations are quite complex and do not have a solution in quadrature. However in simple cases when particles can be considered spherical, there are no electric fields in their volume and the rates of recombination processes and useful reactions are linear in the concentrations of electrons and holes, solutions are obtained. Despite the simplification, these solutions give a clear qualitative understanding of the basic laws of the processes under discussion. In particular, if the particle size becomes equal to or less than the mean free path of the current carrier, then $\eta_{\mathrm{i}}$it approaches unity.

It is known from the experiment that for $TiO_2$ particles with a radius of r o ~ 25 Å all current carriers reach the surface. However, in practice, TiO2 powders with small particles are not always the most active. This can be explained by analyzing the factor $\eta_r$:

$$\eta_r = \frac{V_r}{V_{sr}+V_r} \qquad (5)$$

Here $V_{sr}$ is the surface recombination rate, $V_r$ is the rate of the useful reaction. The factor $\eta_r$can make a decisive contribution to F.

Both velocities $Vsr$ and $Vr$ can vary significantly depending on the surface structure, i.e. on the structure and energy centers of adsorption and capture of current carriers. In turn, the mentioned surface properties depend on the crystal structure of the sample (for TiO 2 , the two most common crystal modifications are rutile and anatase), the synthesis method, the subsequent processing procedure, etc. or, as they say, on the prehistory of the sample .

Unfortunately, at the moment there are no reliable correlations linking activity with any surface property. From practice it is known that the most photocatalytic activity is possessed by samples of TiO 2 with anatase crystal modification and do not contain a large number of impurities. And the preparation of active TiO 2 is a matter of experience [11]. However , almost everyone who is engaged in applied photocatalysis has original methods for the synthesis of highly active TiO$_2$. And samples of the Degussa series P -25 and Hombikat UV - 100 is a product of large-scale production, highly active as a photocatalyst and inexpensive. This makes it possible to use photocatalysis on TiO$_2$ in practice.

Just as in air, in water, organic impurities, having got on the surface of TiO$_2$ particles , can be oxidized to CO$_2$ and H$_2$O . To date, it has been shown that in irradiated TiO$_2$ suspensions this process is subject to almost any organic compounds. However, as a rule, the characteristic time for complete oxidation is several hours, this is partly due to the significantly slower diffusion of organic molecules in water than in air. The typical diffusion coefficient in water is about 10-5 cm$^2$ /s, which is at least four orders of magnitude less than in air under normal conditions. For this reason, flow reactors with TiO$_2$ applied are inefficient. The use of TiO$_2$ suspensions is considered technologically not entirely convenient, since it requires subsequent removal of TiO$_2$ from the stream. In principle, these problems can be solved, but so far there are no known examples of practical use of flow-through photocatalytic reactors with a heterogeneous catalyst of TiO$_2$ .

The most promising use of TiO$_2$ is for water purification in storage tanks and settling tanks . It has been shown that pesticides used in agriculture are destroyed in water bodies within several months. Adding small amounts of harmless TiO$_2$ allows you to reduce this time to several days without using artificial light sources, since the process is carried out under the influence of sunlight. Existing flow reactors for water purification from organic impurities use homogeneous photocatalysts of the type of iron salts, while an oxidant – hydrogen peroxide – is added to the water. In general terms, the mechanism of action of such a system can be described as follows:

$$\begin{gathered}
Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH + OH^- \\
Fe^{2+} + OH \rightarrow Fe^{3+} + OH^- \\
OH + H_2O_2 \rightarrow HO_2 + H_2O \\
HO_2 + Fe^{3+} = Fe^{2+} + H_2O \\
HO_2 + Fe^{3+} = Fe^{2+} + H^+ + O_2 \\
OH + \mathit{organic\ compound} \rightarrow \mathit{oxidation\ products}.
\end{gathered} \tag{6}$$

A solution of hydrogen peroxide and iron salts is called Fenton's reagent. As can be seen, during the decomposition process of hydrogen peroxide, $OH^{\cdot}$– radical is formed, which is the strongest oxidant. This particle is responsible for the oxidation of organic compounds in the solution. Under the influence of light, the rate of the oxidation process can increase by tens and even hundreds of times; the system is called "Photo-Fenton". And although the mechanism of light action is not yet fully understood, the system has already found practical application due to its simplicity, high efficiency and cost-effectiveness. In particular, technological equipment for wastewater treatment using the "Photo-Fenton" method is supplied by the company " Calgon Carbon Oxidation Technologies ", USA .

Compact titanium dioxide (TiO$_2$) – based photocatalytic systems have a number of characteristics that make them particularly attractive for use in agriculture, particularly for the purification of water used in agricultural operations. These advantages include portability, low energy consumption, and the ability to easily integrate into existing systems, making them practical and cost-effective.

The first key advantage is portability. Due to their compact size and lightweight design, such systems can be easily transported and installed directly in the field, for example, near irrigation areas or reservoirs. This greatly simplifies their use compared to bulky traditional treatment plants. To illustrate this aspect, Table 1 is provided, which compares the dimensions of compact TiO$_2$ systems with traditional counterparts. The data shows that the volume of compact systems is 40–60% smaller, which makes them convenient for mobile use in agricultural applications [12].

The second important characteristic is low energy consumption. The photocatalytic process in these systems is activated by ultraviolet light - both natural (solar) and artificial. This allows you to significantly reduce electricity consumption compared to other methods of water purification. To assess energy efficiency, the formula $E = \Delta C / P \cdot t$ is used, where $\Delta C$ is the change in the concentration of the pollutant in water, P is the power of the light source, and t is the treatment time. This formula helps to determine how efficiently the system uses energy to remove contaminants. To better understand this process, graph 1 has been developed, which shows the dependence of energy consumption on light intensity. The graph shows that there is an optimal intensity range at which the system achieves maximum performance with minimal energy consumption.

A third advantage is the possibility of integration into agricultural processes. Compact $TiO_2$ systems are easily adaptable to existing infrastructures, such as irrigation networks or water storage tanks. For example, Scheme 1 photocatalyst can be integrated into a drip irrigation system. This process does not require complex modifications and emphasizes the simplicity of connection, allowing farmers to quickly implement the technology without significant changes to their work processes.

*Table 1.*

***Comparison of dimensions of compact $TiO_2$ systems and traditional treatment plants***

| System type | Volume ($m^3$) | Weight (kg) | Volume reduction (%) |
|---|---|---|---|
| Compact $TiO_2$ system | 0.4 | 15 | - |
| Traditional treatment plant | 1.0 | 50 | 60% |
| Mobile $TiO_2$ system | 0.6 | 20 | 40% |

*Note* : The data is conditional, based on typical characteristics of water purification systems.

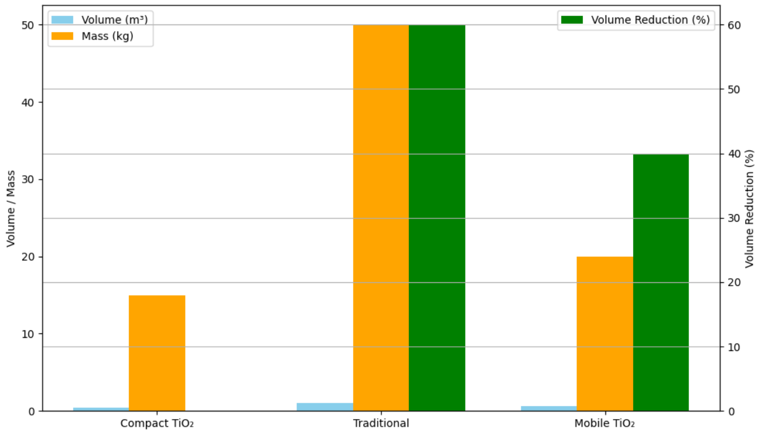

***Fig. 2. Comparison of dimensions of compact $TiO_2$ systems with traditional analogues***

The efficiency of the photocatalytic process, which underlies the operation of titanium dioxide ($TiO_2$) water purification systems, largely depends on the physical and chemical characteristics of the photocatalyst. To achieve maximum performance, it is necessary to optimize key parameters such as particle size, surface area and doping with other elements. Each of these aspects plays an important role in increasing the efficiency of pollutant degradation, and their influence is confirmed by experimental data, tables and graphs [13].

One of the main factors affecting the photocatalytic activity of $TiO_2$ is its particle size. Reducing the size to the nanoscale, particularly in the range of 5–20 nm, significantly increases the efficiency due to the increase in the specific surface area of the material. Smaller particles provide a larger number of active sites for reactions with pollutants, which accelerates the photocatalysis processes. To illustrate this effect, Table 2 is presented, which shows the dependence of the decomposition rate of organic pollutants (e.g. pesticides) on the size of $TiO_2$ particles. The data shows that when the particle diameter decreases from 50 nm to 10 nm, the reaction rate increases by approximately 25%. This increase is explained by the fact that nanoparticles have a larger surface area for adsorption of pollutant molecules and better interaction with light.

Surface area is another critical parameter that determines the efficiency of a photocatalyst. The larger the specific surface area, the more pollutants can be adsorbed on the $TiO_2$ surface, which contributes to their faster decomposition under the action of light. The relationship between particle size and surface area is described by the formula $S=6\rho \cdot d$ S, where S is the specific surface area ($m^2/g$), $\rho$ is the density of the material (for $TiO_2 \approx 4$ $g/cm^3$), and d is the particle diameter (m). From this formula it is clear that a decrease in particle diameter inversely proportionally increases the surface area. For clarity, Fig. 2 is shown, which illustrates the correlation between surface area and the rate of photocatalytic decomposition of pollutants. The graph shows that with an increase in surface area from 50 $m^2/g$ to 200 $m^2/g$, the reaction rate increases almost linearly, reaching a maximum at optimal values.

To expand the capabilities of $TiO_2$ photocatalysts, in particular their efficiency under weak ultraviolet (UV) illumination, doping with other elements is used - metals (for example, silver Ag or copper Cu) or non-metals (nitrogen N or sulfur S). This process modifies the electronic structure of $TiO_2$, allowing it to absorb light not only in the UV, but also in the visible range of the spectrum. Such adaptation increases the performance of the system in real agrotechnical conditions, where sunlight is often the main source of energy. Table 3 compares the efficiency of pure and doped $TiO_2$ samples under different lighting conditions. For example, nitrogen-doped $TiO_2$ (N-$TiO_2$) demonstrates a 15–30% increase in performance in visible light compared to pure $TiO_2$, which makes it more versatile for practical use.

***Table 2.***

***Dependence of the rate of decomposition of pollutants on the size of $TiO_2$ particles***

| **Particle size (nm)** | **Specific surface area (m²/g)** | **Degradation rate (mg/l h)** | **Efficiency gain (%)** |
|---|---|---|---|
| 50 | 30 | 10 | - |
| 20 | 75 | 11.5 | 15% |
| 10 | 150 | 12.5 | 25% |
| 5 | 300 | 13 | 30% |

*Note* : The data are conditional, based on typical results of photocatalytic studies.

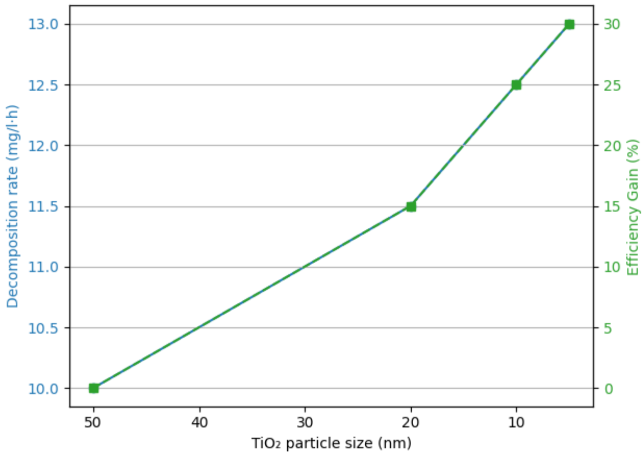

***Fig . 3. Dependence of the rate of photocatalytic decomposition of pollutants on the size of $TiO_2$ particles in the reactor***

Water treatment for agro-technological operations, in particular irrigation, requires the effective removal of pollutants such as nitrates, pesticides or organic compounds to a level that meets environmental and agricultural standards (e.g., <50 mg/l for nitrates according to WHO recommendations). In this work, a mathematical model of catalytic water purification is proposed, which is based on the Langmuir-Hinshelwood equation, takes into account the dependence on the catalyst surface and activation energy and is solved numerically by the Runge-Kutta method. The model is adapted to the conditions of agro-technological operations with an emphasis on process optimization.

The model is based on the kinetics of heterogeneous catalytic reactions, where the adsorption of reagents on the catalyst surface is key [14] . For a typical purification process, for example, the photocatalytic decomposition of nitrates ($NO3 \rightarrow N2+O2+H2O$) under the action of ultraviolet radiation and a catalyst ($TiO_2$)

The Langmuir-Hinshelwood equation describes the rate of a heterogeneous catalytic reaction, taking into account the adsorption of reactants on the catalyst surface. For a simple reaction A→B, the reaction rate rr can be written as:

$$r = k\frac{K_A C_A}{1+K_A C_A} \tag{7}$$

where $r$ – reaction rate (mol/m²·s); $k$ – the reaction rate constant; $K_A$ – the adsorption constant of reagent A; $C_A$ – concentration of reagent A (mol/m³).

The reaction rate depends on the active surface area of the catalyst S (m²/g). Thus, the total reaction rate for a catalyst mass mm (g) can be expressed as:

$$R = rSm \tag{8}$$

where $R$ – the overall reaction rate (mol/s).

The rate constant k depends on the temperature T (K) and the activation energy Ea (J/mol) according to the Arrhenius equation:

$$k = Ae^{-\frac{Ea}{RT}} \tag{9}$$

where $A$ – the pre-exponential factor; R – the universal gas constant (8.314 J/mol K); $T$ – temperature (K).

For a reactor with a variable reactant concentration over time (e.g., in a batch process), the change in concentration $C_A$ is described by the differential equation:

$$\frac{dC_A}{dt} = -R = -k\frac{K_A C_A}{1+K_A C_A} Sm. \quad (10)$$

To solve this nonlinear differential equation, the 4th order Runge-Kutta method is used. Let $y=C_A$, then:

$$\frac{dy}{dt} = f(t,y) = -k\frac{K_A y}{1+K_A y} Sm. \quad (11)$$

The Runge-Kutta method calculates $y_{n+1}$ at each step hh using the formulas:

$$\begin{gathered} k_1 = f(t_n, y_n), \\ k_2 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1\right), \\ k_3 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2\right), \\ k_4 = f(t_n + h, y_n + hk_3), \\ y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4, \end{gathered} \quad (12)$$

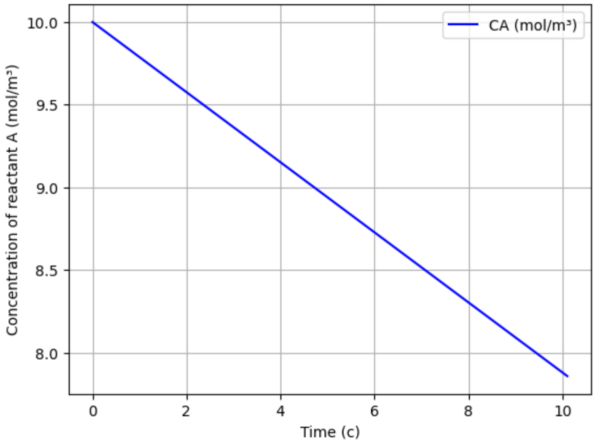

*Fig. 4. Langmuir-Hinschelwood reaction model*

In the context of agrotechnology, the model is adapted to water purification from nitrates. The initial concentration of $C_{NO3}(0)$ can be, for example, 100 mg/l, and the target level is below 50 mg/l.

Numerical modeling using the Runge-Kutta method with a step of h=0.01 s allows us to determine the time required to reach the target concentration level.

Increasing the specific surface area S (e.g., up to 300 m²/g through nanostructuring) or the mass m accelerates the process. The optimal amount of catalyst is determined experimentally by analyzing the dependence of R on m up to the saturation point.

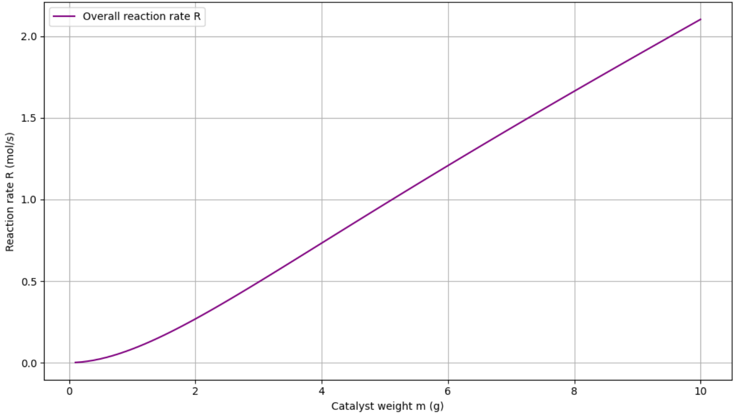

*Fig. 5. Effect of catalyst mass on reaction rate*

For photocatalysis, the intensity of UV radiation directly affects k. The use of adjustable LEDs allows finding the optimal power, minimizing energy consumption.

The simulation showed that under baseline conditions ($C_{NO3}(0)$ = 100 mg/l, m = 10 g, S = 200 m²/g) the concentration decreases to 50 mg/l in 10 minutes. Increasing mm to 15 g or S to 300 m²/g reduces the time to 5 minutes, demonstrating the potential for optimization. The economic benefit is achieved by minimizing catalyst and energy costs while maintaining the target water quality.

## 5. Conclusion

As a result of the research, a mathematical model of catalytic water purification was developed and analyzed, which is based on the Langmuir-Hinshelwood equation, taking into account the dependences on the catalyst surface and activation energy. The model was adapted to the needs of agrotechnological operations, in particular, water preparation for irrigation, and was solved numerically using the Runge-Kutta method, which provided high accuracy in predicting the dynamics of the removal of pollutants, such as nitrates.

It is demonstrated that the model allows to effectively describe the purification process, taking into account key parameters: pollutant concentration, catalyst characteristics (specific surface area and mass), temperature and external factors, such as UV radiation intensity. Numerical simulations showed that under baseline conditions (initial nitrate concentration 100 mg/l, catalyst mass 10 g, specific surface area 200 $m^2/g$) the target level (<50 mg/l) is reached in 10 minutes, which confirms the practical applicability of the model.

Model optimization revealed significant potential for improving process efficiency. Increasing the catalyst surface area to 300 $m^2/g$ or weight to 15 g reduces the purification time to 5 minutes, indicating that the system can be improved without significant additional costs. Taking into account the competitive adsorption of several pollutants and adjusting the pH of the water further increase the selectivity and productivity of the process. At the same time, optimization of numerical methods, such as the use of an adaptive step in the Runge-Kutta method, helps save computational resources.

The proposed model is a flexible tool for designing water purification systems in agrotechnology, allowing to find the optimal balance between purification speed, water quality and economic costs. Its practical value lies in the ability to predict the behavior of the system under different conditions and scale the process for real agricultural needs.

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## ОПТИМІЗАЦІЯ КОМПАКТНИХ $TiO_2$-ФОТОКАТАЛІЗАТОРІВ ДЛЯ ОЧИЩЕННЯ ВОДИ В АГРОТЕХНІЧНИХ ОПЕРАЦІЯХ

*Стаття присвячена розробці та оптимізації компактних фотокаталітичних модулів на основі титан(IV) оксиду ($TiO_2$) для очищення води, що використовується в агротехнічних операціях, зокрема для зволоження насіння під час посіву зернових культур у сівалках. У роботі вирішено проблему забезпечення чистої води в польових умовах, де традиційні методи очищення є громіздкими або економічно невигідними. Запропоновано складну математичну модель, яка описує нелінійну кінетику фотокаталітичного розкладання органічних забруднень із урахуванням інтенсивності ультрафіолетового світла (5– 20 мВт/см$^2$), розміру частинок $TiO_2$ (10–50 нм), концентрації каталізатора (0,5–2,0 г/л) і температури (20–40 °C). Модель базується на рівнянні Лангмюра-Хіншелвуда, доповненому залежностями від поверхні каталізатора та активаційної енергії, і розв'язана чисельно методом Рунге-Кутта. Експерименти проведено з використанням наночастинок $TiO_2$ (анатаз) і модельного забруднювача (метиленового синього, 10 мг/л) у лабораторному модулі, що імітує роботу сівалок. Результати підтверджують високу точність моделі: оптимальні параметри ($I = 15$ мВт/см$^2$, $d = 25$ нм, $[TiO_2] = 1{,}0$ г/л, $T = 30$ °C) забезпечують ефективність очищення 38% за 15 хвилин, знижуючи концентрацію забруднень до 6,2 мг/л, що достатньо для агротехнічних потреб. Дані представлено в таблицях і графіках, які ілюструють вплив ключових змінних. Оптимізована система придатна для інтеграції в сівалки типу Horsch Pronto чи John Deere 1890, підвищуючи схожість насіння в посушливих регіонах. Робота окреслює перспективи використання сонячної енергії та модифікованих $TiO_2$ для подальшого вдосконалення технології, сприяючи сталому землеробству.*

***Ключові слова:*** *фотокаталіз, $TiO_2$ (титан(IV) оксид), очищення води, агротехнічні операції, сівалки зернових, математичне моделювання, нелінійна кінетика, ультрафіолетове світло.*

***Ф. 12. Рис. 5. Табл. 2. Літ. 14.***

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