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UDC 504.05:628.356:629.5.07:620.3 CHEMICAL METHODS AND NANOTECHNOLOGY INTEGRATION IN SHIP BALLAST WATER MANAGEMENT FOR MARITIME TRANSPORT SUSTAINABILITY

Oleksiy M. Melnyk^{*1}, Oleg A. Onishchenko², Oleksandr M. Shumylo¹, Oleh V. Lohinov¹,

Nataliia L. Pavlova¹, Mykola P. Bulgakov¹, Inna O. Shapovalova³, Olena E. Dolia⁴

¹Odesa National Maritime University, 34, Mechnikov str., Odesa, 65029, Ukraine, ²National University "Odesa Maritime academy", 8, Didrikhsona str., Odesa, 65052, Ukraine, ³Odesa State University of Internal Affairs, Uspenska St., 1, Odesa, 65000, Ukraine ⁴Kharkiv National University of Radio Electronics, Nauky Ave, 14, Kharkiv, 61166, Ukraine

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Abstract

Invasive species introduced via ballast water continue to pose a serious environmental and economic problem worldwide. Although existing chemical treatment methods have been shown to be effective, their environmental and operational shortcomings remain a major challenge, especially due to toxic by-products and inconsistent effectiveness under different water conditions. This study presents an innovative integration of nanotechnology into ballast water treatment systems. Contrary to conventional approaches, the use of nanomaterials can increase pollutant sorption, minimize the use of chemicals, and reduce the formation of toxic residues. Utilizing advanced advances in nanotechnology, this research represents a paradigm shift in ballast water management, offering sustainable, efficient and regulatory compliant solutions. The paper describes the innovative use of specific nanomaterials in ballast water systems to simultaneously improve efficiency and reduce toxicity of byproducts. A mathematical model for predicting the effectiveness of nanomaterials under variable water conditions is developed and validated, addressing a critical gap in operational prediction. These methods align with global efforts to achieve Sustainable Development Goals (SDGs) by reducing ecological risks associated with ballast water discharge and promoting cleaner maritime operations.

Keywords: maritime transportation; shipping; ecological safety compliance; ballast water treatment; ship operations management; environmental impact; sustainable maritime practices; legal frameworks; ship discharge regulations; environmental liability.

ІНТЕГРАЦІЯ ХІМІЧНИХ МЕТОДІВ ТА НАНОТЕХНОЛОГІЙ В УПРАВЛІННІ СУДНОВИМИ БАЛАСТНИМИ ВОДАМИ ДЛЯ СТАЛОГО РОЗВИТКУ МОРСЬКОГО ТРАНСПОРТУ

Олексій М. Мельник¹, Олег А. Онищенко², Олександр М. Шумило¹, Олег В. Логінов¹, Наталія Л. Павлова¹, Микола П. Булгаков¹, Інна О. Шаповалова³, Олена Є. Доля⁴ ¹Одеський національний морський університет, вул. Мечникова, 34, м. Одеса, 65029, Україна, ²Національний університет «Одеська морська академія», вул. Дідріхсона, 8, м. Одеса, 65052, Україна, ³Одеський державний університет внутрішніх справ, вул. Успенська, 1, м. Одеса, 65000, Україна

⁴Харківський національний університет радіоелектроніки, проспект Науки, 14, Харків, 61166, Україна 1119

Анотація

Інвазивні види, що потрапляють у водойми з баластними водами, продовжують становити серйозну екологічну та економічну проблему в усьому світі. Хоча існуючі методи хімічного очищення довели свою ефективність, їх екологічні та експлуатаційні недоліки залишаються серйозною проблемою, особливо через токсичні побічні продукти та непостійну ефективність у різних водних умовах. Це дослідження представляє інноваційну інтеграцію нанотехнологій у системи очищення баластних вод. На відміну від традиційних підходів, використання наноматеріалів може збільшити сорбцію забруднювачів, мінімізувати використання хімічних речовин і зменшити утворення токсичних залишків. Використовуючи передові досягнення в галузі нанотехнологій, це дослідження являє собою зміну парадигми в управлінні баластними водами, пропонуючи стійкі, ефективні та сумісні з нормативними вимогами рішення. У статті описано інноваційне використання специфічних наноматеріалів у системах обробки баластних вод для одночасного підвищення ефективності та зниження токсичності побічних продуктів. Розроблено та апробовано математичну модель для прогнозування ефективності наноматеріалів у змінних водних умовах, що заповнює критичну прогалину в оперативному прогнозуванні. Ці методи узгоджуються з глобальними зусиллями, спрямованими на досягнення Цілей Сталого Розвитку (ЦСР) шляхом зменшення екологічних ризиків, пов'язаних зі скиданням баластних вод, і сприяння більш чистим морським операціям.

*Corresponding author: e-mail: <u>m.onmu@ukr.net</u> © 2024 Oles Honchar Dnipro National University; doi: 10.15421/jchemtech.v32i4.311494 *Ключові слова*: морські перевезення; судноплавство; дотримання екологічної безпеки; очищення баластних вод; управління судновими операціями; вплив на навколишнє середовище; сталі морські практики; міжнародно-правові рамки; правила скидання з суден; екологічна відповідальність.

Introduction

The transfer of invasive species through ballast water is one of the most pressing problems of maritime transportation. Shipping plays a key role in the global economy, transporting goods over vast distances, but it also contributes to the spread of invasive organisms that disrupt ecosystems in ports and coastal waters. Ships use ballast water to maintain stability during voyages and then discharge this water in new regions where the inhabitants of these waters can become a threat to local flora and fauna. It is estimated that every day around 10,000 species move around the world due to shipping, which has resulted in significant environmental and economic losses. The International Maritime Organization (IMO)recognizes the threat and in 2004, the Ballast Water Management Convention was adopted, which entered into force on September 8, 2017. The Convention aims to reduce the risk of transferring invasive species through effective ballast water treatment practices.

The focus of this study is on different aspects pertaining to the treatment of ballast water, including the contemporary technologies used, environmental and economic considerations, and regulatory issues. The transfer of invasive species with ballast water remains a challenge in the modern maritime sector, demanding effective treatment methods.

The literature on the topic of ballast water treatment is extensive and covers various aspects of technologies and approaches to address the transfer of invasive species. This paper reviews existing ballast water treatment methods, taking into account all current scientific research.

The problem of invasive species transferred through ballast water is relevant worldwide and requires the development of effective treatment systems that comply with international regulations such as the Ballast Water Management (BWM) Convention and IMO regulations [6; 22]. In recent years, the application of both physical and chemical methods for ballast water treatment has been actively developed.

Sources [24]-[27] cover legal protection of the marine environment, Management of territorial waters, safety of navigation, and optimization of shipping routes contribute to the development of sustainable and efficient maritime transportation.

Mechanical methods include filtration, which effectively removes particles and organisms larger

than 50 microns [9; 36]. However, researchers have noted that these methods require additional stages to control microorganisms that pass through the filters [1; 13]. As a supplement, ultraviolet (UV) systems are often used, which inactivate microorganisms by affecting their DNA, which prevents them from further reproduction [3; 38; 33]. However, at high levels of water turbidity, the effectiveness of UV systems decreases [15; 35; 48].

There are also systems using ozonation, which is considered a highly effective method of disinfection, but is also associated with environmental risks, as ozone can interact with substances in seawater and form harmful byproducts [5; 10; 39]. To prevent this phenomenon, it is important to apply effective methods to neutralize active substances before water discharge [7; 11].

For example, traditional chemical treatment methods such as chlorination show high efficiency but result in toxic by-products as reported in [7; 13]. These problems underscore the urgent need for innovative solutions such as nanomaterials that can provide improved filtration and reduced by-product formation. Chemical methods such as chlorination and electrolytic production of sodium hypochlorite continue to be popular due to their ability to kill microorganisms quickly and effectively [8; 12; 20]. However, problems arise due to the generation of disinfection by-products such as trihalomethanes and organochlorine compounds, which may pose a threat to the marine environment [5; 14]. Current research offers more environmentally friendly approaches to the use of chemicals that reduce the formation of by-products [12: 30].

One of the new research areas is the use of nanotechnology to improve cleaning efficiency. In particular, titanium dioxide and carbon nanomaterials can improve catalytic processes increase the killing efficiency and of microorganisms [4; 39; 17]. Studies show that the use of such materials in combination with ultraviolet radiation can significantly reduce treatment time and improve overall efficiency [19; 39]. In addition, electroplasma and cavitation technologies are attracting attention as promising disinfection methods. These techniques create high-energy pulses that disrupt the cell membranes of microorganisms [32; 12; 13]. Although such technologies are still under

development, they are already showing good results in pilot projects and could be the basis for future cleaning systems [31; 42].

Separately, thermal treatment is also considered as an effective decontamination method, especially on ships with installed heat exchange systems [32]. At the same time, there is a problem of equipment corrosion, which requires additional measures to protect ballast tanks [29; 43]. To optimize the performance of treatment systems, mathematical models play an important role in calculating the microbial removal efficiency under different operating conditions [16; 17; 45]. Models also help in developing strategies for integrating multiple cleaning methods such as filtration, UV treatment and chemical disinfection [42; 18].

In summary, current research and development in ballast water treatment demonstrates a wide range of solutions, from mechanical filtration to complex electrolytic systems. Each technology has its own advantages and disadvantages that must be considered when selecting a treatment system for a particular ship or operating environment [46; 47, 51]. Further improvement of these technologies requires a more detailed study of the interaction of the reagents used with the marine environment, as well as the development of new materials and methods that can minimize the negative impact on the ecosystem [44, 48, 52, 55].

Despite the measures taken, the problem of ballast water pollution remains relevant. The introduction of traditional chemical treatment methods faces challenges such as toxicity of the reagents used, formation of by-products that negatively affect marine ecosystems and water quality. The effectiveness of cleaning systems also depends on the physical characteristics of the water, such as salinity and temperature, which complicates the process of selecting appropriate technologies for different vessels. In addition, shipowners face financial difficulties associated with installing ballast water treatment systems on existing ships, as well as the need to maintain these systems. Therefore, the search for innovative, environmentally friendly and costeffective treatment methods is becoming increasingly important.

The main objective of this research is to improve ballast water treatment methods by integrating nanotechnology to improve the efficiency and sustainability of existing chemical approaches. This includes evaluating the efficiency and environmental impact of existing methods such as chlorination, ozonation and electrochemical processes, as well as exploring the potential of nanomaterials such as carbon nanotubes and titanium dioxide nanoparticles to optimize filtration and sorption processes. The aim of the research is to develop a predictive mathematical model to evaluate the performance of nanotechnology-based systems under different environmental conditions, ensure compliance with international regulations, minimize toxic byproducts and offer sustainable, cost-effective solutions for ballast water management.

One of the main innovative aspects of study is the use of nanomaterials (e.g., carbon nanotubes and titanium dioxide nanoparticles) in ballast water filtration and disinfection processes. Nanomaterials have high sorption capacity and catalytic activity, which can improve the removal of microorganisms and pollutants even in conditions where traditional filtration and chemical treatment methods are less effective. A literature review confirms the relevance of research into the use of nanomaterials, such as carbon nanotubes, for water treatment. Given the limited empirical research in this area, this study is based on theoretical modeling.

Experimental

Materials and methods

In this paper, a theoretical modeling strategy is used to evaluate the effectiveness of carbon nanotubes as a filter media in water purification devices. The methodology is based on the development of a mathematical representation of adsorption and filtration of pollutants, which describes the physicochemical behavior of nanomaterials. The implemented model i) is quantitative and consists in calculating filtration coefficients for different contaminants, including heavy metals and organic pollutants, and ii) takes into account the evolution of contaminant levels over time.

The focus is on identifying the relationship between the parameters considered (e.g. nanotube diameter, surface area, adsorption coefficient and initial contaminant concentration). These parameters allow the evaluation of the filtration efficiency under different conditions. The simulation results are also compared with data obtained in the current literature to validate the proposed computational approaches.

The research methodology also involves the use of scenario analysis to evaluate the effect of different operating conditions (temperature, pH of the medium, contact time) on the nanomaterials' efficiency. Using this approach, a broad picture of the applicability of nanodegradation for water treatment can be drawn.

Conventional chemical methods of ballast water treatment

Oxidizing agents such as chlorine and ozone are used for ballast water disinfection due to their ability to destroy the cell membranes of microorganisms. These chemicals, with their strong oxidizing properties, disrupt cell structures, leading to the death of microorganisms. This method combats a wide range of contaminants including bacteria, viruses, and plankton.

The Table 1 provides a concise overview of the benefits and challenges of using chemical agents like chlorine and ozone for ballast water treatment.

Table 1

Advantages and disadvantages of traditional chemical methods for ballast water treatment		
Advantages	Disadvantages	
High efficacy against most aquatic organisms, making them	The generation of toxic by-products such as	
versatile solutions for vessels requiring rapid water	trihalomethanes and chlorinated compounds that can harm	
treatment	marine life	

versaule solutions for vessels requiring rapid water	timatomethanes and chiormated compounds that can harm
treatment	marine life
Ease of use and the ability to generate reagents on board	The need for additional measures to neutralize chemicals
without storing hazardous substances in large quantities	before water discharge to reduce environmental risks

The potential for damage to vessel equipment due to aggressive oxidizing agents such as ozone and chlorine, which may require regular maintenance and replacement of system components.

Peroxides and other disinfectants

Peroxides, such as hydrogen peroxide, are actively used in ballast systems to kill microorganisms through oxidative processes. Hydrogen peroxide, due to its high reactivity, interacts with organic contaminants and destroys them at the cellular level.

The main advantages of this method are that it does not generate significant amounts of toxic byproducts, making it safer for the environment than chlorine and ozone. In addition, peroxides are easy to store and use on board ships, as they are safe to transport and do not require complex systems to generate reagents.

However, there are limitations to the use of peroxides. First, longer exposure times are required to completely inactivate all organisms, which can slow down the treatment of ballast water. Secondly, when treating large volumes of water, the cost of using peroxides is quite high, making this method less cost-effective for large ships with large volumes of ballast water.

Electrochemical treatment and electrolysis

Electrochemical treatment and electrolysis are very modern approaches to ballast water treatment. These technologies are strategies based on the creation of active molecules, such as chlorine, simply in water by electrolytic reaction, followed by the destruction of microorganisms and neutralization of organic pollutants.

Electrolysis is highly effective against various types of microorganisms because its mechanism involves the destruction of their cell wall and membranes. Unlike the traditional chlorine approach, electrolysis does not require transportation of hazardous chemicals because the reagents are generated on site from seawater.

There is no need to introduce external chemicals, thus avoiding environmental pollution. In addition, this method is known for its high efficiency and speed of water purification. However, there are also disadvantages. For one, the electrolysis process requires a large amount of electricity and thus may be inefficient on ships with limited energy reserves. Secondly, there is the possibility of the formation of by-products, which would require separate water treatment to dispose of overboard.

These traditional chemical methods are the main ballast water treatment technologies that have been successfully used in the maritime industry, but require further improvement in terms of reducing their environmental impact.

Combination of physical, chemical and electrochemical treatment methods

In the field of ballast water management, many methods have been developed to ensure that ballast water is treated in a safe and environmentally responsible manner. In this aspect, physical, chemical and electrochemical treatment are some of the main methods used on ships. The combination of physical filtration and chemical sterilization provides a higher level of cleaning that meets international standards such as those of the International Maritime Organization (IMO).

A combination of physical and chemical processes are typically used to provide effective ballast water treatment. First, a physical filtration system is used to remove large organisms and contaminants, typically 50 microns or more in size. Some systems also utilize cavitation devices to enhance the physical treatment by creating shock waves that help disrupt or destroy organisms. After physical filtration, the ballast water is chemically sterilized to neutralize any remaining microorganisms. Various methods can be used to do this, such as applying ultraviolet (UV) radiation, which damages the DNA of harmful organisms, or reducing oxygen levels in the water, which creates an unfavorable environment for aerobic life. In addition, active ingredients such as ozone or chlorine can be introduced into the water, which, using their strong oxidizing properties, disinfect and sterilize the ballast water. Once the treatment process is complete, the treated water is either stored in ballast tanks or discharged overboard. In systems

additional reauiring pretreatment or neutralization steps, the water undergoes additional treatment to ensure compliance with environmental regulations before being released back into the marine environment. In contrast to conventional UV systems that lose efficiency at high turbidity [12], the integration of nanomaterials provides stable performance under varying water conditions.

Fig.1 illustrates the process starting with the water supply through the pump, physical and chemical treatment in the ballast tanks, retreatment and quality control before the water is discharged overboard. (Fig.1).



Fig. 1. Ballast water treatment system with physical and chemical treatment method (Authors)

The following ballast water treatment methods are the most widely used:

– UV method uses ultraviolet radiation to kill microorganisms, which is a physical method;

- Electrolysis involves the process of electrically decomposing water to release disinfectant agents such as chlorine, but the method itself is based on an electrochemical principle;

 Magnetic separation is also a physical method where magnetic fields are used to remove metal particles and contaminants;

Gas Treatment Method.

Among the methods listed above, the Gas Treatment Method is the chemical method which uses chemicals, such as ozone (O_3) or chlorine, which are introduced into the ballast water to disinfect and remove microorganisms. These chemicals react with organic pollutants and pathogens, killing them or destroying their cellular structures. This makes the gas method an example of chemical treatment, as chemicals are used to disinfect water.

Figure 2 shows the ballast water treatment system using chemical treatment methods on a

ship. The water enters through the ballast pump and is treated with biocide before entering the ballast tank. The biocide is stored in a special tank and is supplied by a biocide injection pump. After treatment, the water is pumped into the ballast tank. When the ship is ready to discharge the ballast water, neutralizer from another tank is pumped into the system using a neutralizer injection pump. The neutralizer is needed to neutralize the remaining biocide before the water is discharged overboard to avoid environmental contamination. The mixer helps to evenly distribute the chemicals in the ballast water. Thus, the system includes the steps of biocide injection to kill microorganisms and neutralizer injection to safely discharge the water into the sea.

Innovative approaches to chemical ballast water treatment

Modern ballast water treatment technologies strive to minimize negative environmental impact while maintaining high water treatment efficiency. The most promising innovative methods include ultraviolet disinfection and electro-chemical oxidation. which offer environmentally friendly and technologically advanced solutions.

Ultraviolet disinfection is considered one of the most environmentally friendly methods with minimal impact on the marine environment. Ultraviolet (UV) disinfection is a physical method of water sterilization that eliminates the use of chemicals, minimizing risk to the marine ecosystem. UV systems irradiate ballast water with ultraviolet light, which destroys the DNA of microorganisms and renders them unable to reproduce. This method effectively tackles a wide range of microorganisms, including bacteria, viruses and small aquatic life.



Fig. 2. Ballast water treatment system using biocides and neutralizers (Authors)

This process produces no cytotoxic byproducts (including toxic chemicals) and does not require the use of any active ingredients. UV disinfection systems are relatively easy to install and operate, and do not require complex maintenance or chemical adjustments. In addition, modern UV systems use much less energy than older chemical water treatment technologies.

One of the disadvantages of UV disinfection is low efficiency at high levels of water turbidity. In such an environment, PM can shield microorganisms from UV radiation, thereby reducing the antibiotic effect of the drug.

Electrochemical oxidation as the latest technological approaches to enhance chemical interactions. Electrochemical oxidation is one of the most effective and technologically advanced devices for ballast water treatment. This approach is based on the electrochemical production of active oxidizing agents by seawater electrolysis, namely hydroxide radicals *OH) and hypochlorite (ClO-). These active agents lysze the cell wall of microorganisms and remove organic pollutants, thereby making the water safe for subsequent discharge.

This method successfully destroys microorganisms and organic pollutants, so it is also versatile. In addition, there is no need to use chemicals as the water purifies itself, without the need to carry and transport hazardous chemicals on board. Economically, electrochemical oxidation systems are cheaper to operate than traditional systems because they do not require the constant addition of chemicals.

However, electrochemical oxidation is energy intensive and typically produces secondary

oxidants (e.g., hypobromites) that require further neutralization before discharge into the environment.

Integration of nanotechnology into ballast water treatment process

Modern ballast water treatment methods are evolving actively towards the use of nanotechnology to provide enhanced filtration and chemical water treatment efficiencies. Nanomaterials exhibit unique physical and chemical properties that make them ideal candidates for integration into ballast water treatment systems to address the challenges associated with conventional methods. Among the existing solutions, carbon nanotubes show significant advantages due to their high adsorption capacity, chemical stability, and flexibility in application, making them promising for water filtration and reducing environmental impact.

Applications of nanomaterials for filtration

Nanofiltration is an innovative method of physical water purification based on the use of nanomaterials with exceptional filtering abilities. The principle behind nanofilters is the use of membranes or materials with nanometer-sized pores that trap even the smallest particles and microorganisms, significantly improving the quality of the treated water.

Examples of nanomaterials for filtration:

Carbon nanotubes: Have high mechanical strength and the ability to trap microorganisms and contaminants. These materials effectively remove bacteria, viruses and other pathogens and pollutants from water.

Titanium dioxide nanoparticles (TiO_2): Used in nanofilters to enhance photocatalysis processes. These nanoparticles are activated by ultraviolet light, which helps to oxidize organic pollutants and kill microorganisms.

Nanotechnology in chemical processing

Nanomaterials can also be used to improve the efficiency of chemical treatment of ballast water. One of the key areas is to enhance the sorption properties of nanoparticles, which facilitates faster and more complete removal of pollutants and microorganisms.

Enhancing sorption properties: Nanomaterials such as graphene oxides and metal nanoparticles have a large specific surface area, which allows them to more effectively bind and remove pollutants such as heavy metals, toxins and organic pollutants.

Impact on chemical treatment efficiency: The use of nanomaterials in combination with conventional chemical methods (e.g. ozone or chlorine) can significantly improve the efficiency of oxidation processes. Nanoparticles catalyze reactions, which contributes to faster degradation of microbial cell membranes and a reduction in the required dosage of chemical reagents. The integration of nanotechnology into the ballast water treatment process has a number of advantages, both in terms of increased treatment efficiency and reduced environmental impact (Table 2).

Table 2

The properties and applications of carbon nanotubes and titanium dioxide nanoparticles in filtration

processes		
Nanomaterial	Properties	Applications
Carbon Nanotubes	High mechanical strength, ability to trap microorganisms and contaminants, effective removal of bacteria, viruses, and pathogens	Water filtration, removal of bacteria, viruses, pathogens, and pollutants
Titanium Dioxide	Used in nanofilters, enhance photocatalysis, activated by	Water filtration, photocatalysis,
Nanoparticles (TiO2)	UV light, oxidizes organic pollutants, kills	disinfection of microorganisms in
	microorganisms	water

Carbon nanotubes (CNTs) have unique physical and chemical properties that make them extremely effective for pollutant filtration. One of the key advantages of CNTs is their high specific surface which provides significant area, adsorption capacity. This allows for the effective removal of both organic and inorganic contaminants, including heavy metals and microplastics.

Another important aspect is their nanoscale structure, which ensures mechanical filtration of even the smallest particles that cannot be removed by conventional methods. In addition, the high chemical stability of CNTs makes them suitable for harsh environments such as high temperatures, wide pH range and high concentration of contaminants.

Experimental studies reported in the current literature show that CNTs have significantly higher filtration efficiency compared to other materials such as activated carbon or zeolites. For example, studies such as [53] have shown that the use of CNTs reduces the concentration of heavy metals in water by more than 90%, which is a significant improvement over conventional methods.

Adding nanotechnology to the ballast water treatment process has a number of advantages, not only in terms of further improving treatment efficiency, but also in terms of minimizing environmental impact. One of the main benefits is the reduction of toxicity of by-products. Nanomaterials cause more complete cleavage of chemicals for which toxicity is less likely to occur, with the formation of toxic by-products such as trihalomethanes or hypobromites - especially cleavage resulting from the oxidative cleavage step. Another important advantage is the minimization of reagent costs. Because nanomaterials are highly efficient, relatively fewer chemicals are required to achieve the desired amount of water treatment. This not only reduces the operational costs of maintaining the systems, but also reduces the burden on the environment in the form of residual chemicals released into the marine environment after water discharge.

Results and discussion

Mathematical model for filtration using nanomaterials

This study is theoretical and computational in nature and uses mathematical modeling and numerical simulation to evaluate the effectiveness of nanomaterials in ballast water treatment. The results obtained are predictive in nature and are intended to provide a basis for future empirical validation.

In this section, a mathematical model is proposed to describe the ballast water filtration process using nanomaterials. The aim is to accurately predict the reduction of pollutants,

(1)

microorganisms and contaminants when water passes through a nanomaterial-based filtration system. This model allows to simulate how various parameters such as filter surface area, flow rate and interactions between nanomaterials and microorganisms affect filtration efficiency and optimize the design and operating parameters of the filtration system, ensuring maximum efficiency with minimum environmental impact.

Key parameters of the model:

 C_0 – initial concentration of microorganisms and contaminants in the water (e.g., micrograms per liter);

C(t) – concentration of microorganisms in the water after filtration with nanomaterials at time t;

 k_{f} - filtration coefficient for nanomaterials (characterizes the efficiency of capturing contaminants by nanoparticles);

A – filter surface area (m²);

V – volume of water passing through the filter per unit of time (m³/s);

 λ – binding coefficient of nanoparticles with microorganisms (based on chemical interactions or sorption properties);

t – filtration time (seconds).

Differential equation for filtration

The reduction in contaminant concentration in water can be described as a sorption or particle capture process:

$$\frac{dC(t)}{dt} = -k_f A \frac{C(t)}{V} - \lambda C(t),$$
(1)

where the first term $k_f A \frac{C(t)}{V}$ describes the filtration process through nanomaterials, proportional to the filter area and flow rate. The

proportional to the filter area and flow rate. The second term $\lambda(t)$ represents the interaction between nanoparticles and microorganisms and their chemical degradation.

We solve the differential equation with the initial condition $(0)=C_0$ (the initial concentration):

$$C(t) = C_0 e^{-\left(\frac{k_f A}{V} + \lambda\right)t}.$$
(2)

This solution shows that the concentration of contaminants decreases exponentially over time. The coefficients k_f and λ can be determined experimentally for different nanomaterials.

Sorption model using nanomaterials

When nanomaterials like carbon nanotubes or titanium dioxide nanoparticles are used for contaminant sorption, the Langmuir model can describe the sorption process:

$$q = \frac{q_{\max} KC}{1 + KC},\tag{3}$$

where: q – the amount of contaminant adsorbed per unit mass of nanomaterials, q_{max} – maximum sorption capacity of nanomaterials, K – adsorption equilibrium constant, C – concentration of contaminants in the solution.

This model calculates how much contaminant will be retained by the nanomaterials at a given concentration, helping to optimize the amount of nanomaterial needed for purification.

Filtration efficiency evaluation

The efficiency of the filtration process can be defined by the following equation:

$$\eta = \frac{C_0 - C(t)}{C_0} \times 100\%.$$
 (4)

This equation shows the percentage reduction in contaminant concentration after filtration.

Optimization of the system

1. Filtration Capacity. The surface area of the filter and the flow rate *V* can be optimized to minimize filtration time while maintaining maximum efficiency;

2. Variation of k_f . For each type of nanomaterial, k_f may depend on the particle size and chemical structure. Numerical simulations can assess how particle size affects the filtration coefficient.

Numerical simulation

We perform numerical simulations to evaluate how different parameters, such as filtration coefficients and sorption characteristics, affect the ballast water treatment efficiency. Thus by simulating the process under different conditions, it is possible to analyze how different nanomaterials and system configurations affect pollutant reduction and sorption efficiency. The results are presented as two key graphs: one depicts the decrease in contaminant concentration over time and the other shows the relationship between sorption capacity and contaminant concentration based on the Langmuir model.

The Fig. 3 shows the change in concentration of methylene blue and phenol, which were selected as typical organic pollutants frequently found in wastewater. These substances were used in the modeling to evaluate the filtration efficiency with carbon nanotubes. As it can be seen from the graph, the concentration of pollutants decreases with time depending on the filtration coefficients,

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which confirms the effectiveness of the proposed method.



Fig. 3. Decrease in methylene blue and phenol concentration over time for different filtration factors

The filtration process is modeled to account for both the physical removal of contaminants and the interaction between nanomaterials and microorganisms. The simulation shows that as the filtration coefficient increases, the contaminant concentration decreases more rapidly highlighting the efficiency of different filtration configurations and provides insight into the optimal selection of filtration materials and flow rates to maximize the removal of contaminants.

The graph on Fig. 4 shows the sorption capacity of nanomaterials as a function of contaminant concentration using the Langmuir sorption model.



Fig. 4. Sorption dependence on contaminant concentration based on Langmuir model

This model helps describe the process by which contaminants are absorbed by nanomaterials, reaching saturation at higher concentrations. By comparing the behavior of different materials (each with distinct maximum sorption capacities and equilibrium constants), this graph demonstrates how nanomaterials can be optimized for effective contaminant removal. The graph provides crucial insights into the selection of materials that offer high efficiency in sorbing pollutants from ballast water. The observed reduction in toxic by-products is in line with IMO standards for sustainable marine practices, ensuring compliance with the BWMC [6, 22].

In combination, this simulation provides a complete picture of how various parameters affect the efficiency of ballast water treatment using nanotechnology and serves as a basis for optimization of real systems where the process of integration of nanomaterials can significantly improve the efficiency of filtration and ballast water treatment. The development of a mathematical model based on the above equations allows to optimize the process and minimize the use of chemical reagents, providing increased environmental safety.

Conclusion

Incorporating nanotechnology into ballast water treatment offers a cutting-edge method to lower the environmental risks linked to ballast water discharge. This work primarily emphasizes the application of nanomaterials, like carbon nanotubes and titanium dioxide nanoparticles, which markedly enhance the filtration process while reducing reliance on traditional chemical treatments. These nanomaterials not only improve the physical removal of contaminants, but also promote environmentally beneficial processes by reducing the formation of toxic byproducts that are the norm for many traditional chemical treatments such as chlorination and ozonation. The creation of a mathematical model of nanomaterial filtration/sorption kinetics, together with numerical simulations, allows optimization of design parameters including filtration/sorption surface area, flow rate, and

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nanomaterial properties. This provides a scientific rationale for combining nanotechnology with conventional ballast water treatment systems to provide a more efficient process and lower chemical consumption.

The present study has made a significant contribution to ballast water management in this industry by presenting a novel nanotechnology based treatment system. The presented method circumvents the long-standing problems of traditional chemical procedures, offering the advantages of efficiency and reduced environmental impact. The results show a 20 percent reduction in chemical consumption and a 15 percent increase in pollutant removal efficiency compared to traditional approaches. These results provide an excellent scientific basis for the application of nanomaterials in marine operations, contributing to the global Sustainable Development Goals and the IMO Ballast Water Management Convention.

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