

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering



Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

Dr. Elmina Gadirova (Ed.)

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Prof. Javier Gonzalez-Argote (Ed.)

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Preface

The idea for Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering was born from a simple observation: the most pressing problems in energy and environmental engineering do not respect disciplinary boundaries. Addressing water pollution cannot rely solely on chemistry or solely on process engineering. Designing resilient, low-carbon energy systems cannot be achieved through materials innovation alone or through software alone. Meaningful progress requires that we bring these worlds together.

As editors, working across universities, research centers, and industries in different countries, we repeatedly encountered research projects that were technically excellent yet isolated: a new nanomaterial with remarkable catalytic properties that remained disconnected from real-world treatment systems; an elegant AI model that lacked robust physical grounding or suitable data; or a promising sustainable technology that had not been evaluated within a broader systems perspective. We envisioned a volume that would connect these efforts, showing how advanced materials, intelligent algorithms, and sustainable engineering principles can reinforce one another when thoughtfully integrated.

The chapters collected in this book reflect that ambition. Contributions on toxic pollutant monitoring and remediation demonstrate how analytical chemistry, environmental engineering, and materials science converge in the study and treatment of contaminated waters and ecosystems. Studies on underground water purification and dissolved gases show how biochemical processes, hydrodynamics, and cavitation-based technologies can be combined to remove iron, manganese, ammonium, and phenolic compounds with high efficiency. Work on nanostructured materials and photocatalytic systems illustrates the power of TiO_2 nanoparticles and related materials to transform persistent organic pollutants under controlled conditions, while also opening pathways for scalable, low-footprint treatment solutions.

Complementing these material and process innovations, chapters devoted to AI and digital technologies reveal how intelligent tools are reshaping the landscape of engineering practice. Authors explore AI in structural and construction engineering, show how data-driven models can support design, diagnostics, and maintenance of critical infrastructure, and discuss AI- and IoT-enabled approaches for manufacturing, healthcare, and energy systems. These contributions underscore the importance of robust data, domain knowledge, and interdisciplinary collaboration in ensuring that AI applications are not only powerful, but also safe, transparent, and aligned with sustainability goals.

This volume also bears witness to a rich international collaboration. The authors come from a broad array of regions and institutions, and they work in contexts that range from heavily industrialized urban environments to sensitive marine and coastal ecosystems. Their perspectives are diverse, but they share a common concern: building technologies that support human development while minimizing environmental harm. It is our hope that readers will find in these pages not only technical knowledge, but also inspiration to pursue similarly collaborative and cross-disciplinary projects.

We would like to express our sincere gratitude to all the contributing authors and reviewers, whose dedication and expertise made this book possible. We also thank the institutions and laboratories that supported the experimental and theoretical work compiled here, and the publishing team for their professionalism throughout the editorial process.

We invite readers—whether they come from materials science, environmental engineering, energy systems, computer science, or industry—to approach this book with curiosity and an openness to dialogue across fields. If this volume helps foster new collaborations, sparks innovative research ideas, or informs more sustainable engineering decisions, it will have fulfilled its purpose.

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Dr. Vugar Abdullayev
Prof. Javier Gonzalez-Argote
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Editors

Abstract

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering brings together cutting-edge research and applied studies at the intersection of materials science, intelligent systems, and sustainable engineering. The chapters explore how advanced materials—such as nanomaterials, smart and functional materials, carbon-based structures, and novel composites—can enhance the efficiency, safety, and resilience of energy and environmental systems. In parallel, the volume examines the growing role of artificial intelligence, data analytics, and automation in optimizing industrial processes, monitoring pollution, supporting decision-making, and enabling predictive maintenance across infrastructure and manufacturing.

Contributions range from experimental studies on water and wastewater treatment, pollution monitoring, and remediation, to the design of energy-efficient processes, AI-driven structural and civil engineering solutions, and sustainable resource management strategies. By linking fundamental advances in materials and intelligent technologies with real-world challenges in energy and environmental engineering, this book offers an integrated perspective for researchers, practitioners, and graduate students seeking to develop cleaner, smarter, and more sustainable technological systems.

Keywords: Advanced Materials; Artificial Intelligence; Sustainable Technologies; Energy Engineering; Environmental Engineering.

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Part I

Environmental Chemistry and Marine/Water Safety



Chapter 01

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Analysis of Toxic Substances in Seawater

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ABSTRACT

Environmental monitoring was conducted in two distinct regions of Caspian Sea. Hovsan is located on the coast of the southern Absheron Peninsula. Bilgah is located in the north of the Absheron Peninsula, on the coast of the Caspian Sea. Water samples were collected from the Hovsan and Bilgah areas and subsequently analyzed. Quantitative analyses were performed using the Agilent 6890N/5975 GC-MSD method. A total of 15 polycyclic aromatic hydrocarbons (PAHs) and 11 phenolic compounds were identified. The analysis revealed that the concentrations of organic toxic compounds in the water samples exceeded permissible limits. When comparing both areas, water samples taken from the Hovsan area were considered more polluted. Additionally, the physical-chemical parameters of the water samples from both Hovsan and Bilgah were determined.

Keywords: PAHs; Organic Compounds; Gas Chromatography; Environmental Monitoring; Seawater.

INTRODUCTION

It is very important to know the degree of pollution of seawater in the beach areas of the Caspian Sea. Since the Hovsan and Bilgah areas are beach areas, the increased level of water pollution in these areas is more dangerous. Pollution of sea water with polycyclic aromatic hydrocarbons is also a source of danger from the beach point of view; the increased risk of skin cancer is the most important of these factors.

The Caspian Sea is currently exposed to both pyrogenic and petrogenic pollution. On the other hand, against the backdrop of global warming, the decrease in the water level of the Caspian Sea is accompanied by an increase in the degree of water pollution and salinity. As a result, the aquatic ecosystem of the Caspian Sea is facing severe ecological pollution. Consequently, the Caspian National Park and beach areas are also affected by pollution. Seasonal ecological monitoring is conducted in these areas every year to assess the pollution levels of the seawater. Factors such as temperature, precipitation, and the discharge of other rivers and water flows into the sea significantly influence the degree of pollution. Considering the discharge of wastewater from the Oil Refinery located in the Baku area into the Caspian Sea, it is evident how severe the anthropogenic impacts are. As a result, the flora and fauna of the sea are seriously damaged. A clear example of this is the destruction and depletion of numerous fish species. Although the wastewater from the refinery is partially treated before being released into the sea, toxic

heavy metals and organic toxic substances still remain in the industrial effluent. Taking this into account, ecological monitoring has been carried out in the Caspian Sea. For the purpose of environmental ecological assessment, monitoring was conducted on water samples taken from two areas near the Caspian Sea; the chemical composition of seawater from the Bilgah and Hovsan regions was determined. Primarily, polycyclic aromatic hydrocarbons and phenolic compounds were analyzed in the oil-contaminated wastewater.

Organic compounds, such as polycyclic aromatic hydrocarbons (PAHs), present a global environmental challenge due to their potential to cause inflammation and skin cancer. There are two primary anthropogenic sources of hydrocarbons: petrogenic and pyrogenic sources. Petrogenic sources encompass crude oil and petroleum-derived hydrocarbon compounds, while pyrogenic sources arise from the incomplete combustion of organic materials such as oil, wood, and coal.⁽¹⁾

The Caspian Sea represents a highly sensitive ecosystem. Over recent decades, the condition of its ecosystems, particularly in the northeastern part of the sea, has significantly deteriorated due to both anthropogenic and biochemical factors. Observations in recent years indicate that the waters of the Caspian Sea, especially along the coast of the national park, are increasingly polluted by oil and sewage. The rapid industrialization and urbanization in the Caspian region over the past several decades, along with the associated rise in hydrocarbons, are major concerns for the area.

Offshore production, accidental oil spills, industrial waste, wastewater, and riverine discharges are considered the primary sources of anthropogenic hydrocarbons in the marine environment.^(2,3) It is widely believed that industrial activities are the predominant source of oil pollution in the Caspian Sea. On average, approximately 2,342 million m³ of industrial waste is discharged into the Caspian Sea annually, which contains around 122,5 thousand tons of oil, 1,1 thousand tons of phenols, and 9,9 thousand tons of organic chemical products. In the northwestern part of the South Caspian, the total hydrocarbon content is relatively low, ranging from 32 to 54,2 µg/g. In areas near oil fields, phenol concentrations are recorded at 0,002-0,003 µg/g.⁽⁴⁾

According to recent literature, it is reported that approximately 6 million tons of oil and oil products are discharged into the world's oceans every year.⁽⁵⁾ Pyrogenic and petrogenic pollution, along with contamination from ballast water and other sources, contributes to the pollution of shared water bodies.⁽⁶⁾ These segments of the hydrosphere function as dynamic systems, which over time leads to the reduction and depletion of freshwater supplies.^(7,8) Pollution of water and sediment is evident throughout the Absheron Peninsula and in Baku, with the majority (approximately 90 %) of the pollution entering the Caspian Sea through river runoff.⁽⁹⁾ The sources of seawater contamination by toxic organic compounds are well-known, but it is critical to implement stringent measures to prevent further pollution. This is particularly important as both PAHs and phenolic compounds pose significant risks to the flora and fauna of aquatic ecosystems.^(10,11)

Experimental Part

The article examines the chemical analysis of seawater collected from two locations of the Caspian Sea for environmental protection purposes. Water samples were obtained from two sites using the "12 L Niskin" sampler at a depth of 0,5 meters below the sea surface, specifically from the Bilgah and Hovsan areas. Chromatographic analyses were conducted using a gas

chromatograph with a flame ionization detector (GC-FID 6890, Agilent, USA), equipped with a ZB-1 column (Phenomenex, USA). Helium was utilized as the carrier gas in the analysis. The identification of organic toxic substances in the seawater samples from the Bilgah and Hovsan areas was supported by the Caspian Ecology Laboratory. Ultimately, 15 polycyclic aromatic hydrocarbons (PAHs) and 11 phenolic compounds were analyzed in the water samples.

RESULTS AND DISCUSSION

The problem of water pollution in the world is currently one of the most pressing issues. Azerbaijan is also facing the same problem in this regard. Therefore, since it is an oil country, the problem of pollution of the Caspian Sea is always relevant. Pollution of sea water against the background of pyrogenic and petrogenic pollution is also very dangerous for the flora and fauna of that ecosystem. On the other hand, since beach zones have been created on many coasts of the Caspian Sea due to the development of tourism, it is very important that sea waters are clean. In this regard, since the Bilgah and Hovsan areas of the Caspian Sea are also beach areas, ecological monitoring was mainly carried out in these analyses.

The concentration of PAHs in the analyzed water samples is presented in Table 1 below. The chromatograms obtained are illustrated in figures 1 and 2. The maximum permissible concentration for polycyclic aromatic hydrocarbons (PAHs) is 0,01 $\mu\text{g/L}$. The results indicated that the measured PAH levels in many cases exceeded this regulatory limit.

Table 1. Amount of the PAHs in the water samples taken from Hovsan and Bilgah		
PAHs, μgL^{-1} $\mu\text{gL}^{-1} = \text{mgkg}^{-1}$ (or 0,001 gL^{-1})	Hovsan	Bilgah
Naphthalene	0,19	0,01
Achenthylene	<0,01	<0,01
Acenaften	0,01	0,02
Fluoren	0,07	0,02
Fenantren	0,17	0,03
Anthracene	0,01	0,02
Fluoranten	0,01	0,01
Piren	0,01	0,00
Benz (a) anthracene	0,01	0,00
Chrizen	0,01	0,01
Benz (b + j + k) fluorantene	0,03	0,02
Benz (a) pyrene	0,01	0,01
Inden (1,2,3-cd) pyrene	0,01	0,01
Benz (ghi) perilen	0,01	0,01
Dibenz (ah) antracen	0,01	0,01

Based on the analysis, 15 PAHs were identified in the water samples, and it is important to note that the standard permissible concentration for PAHs is 0,01 $\mu\text{g/L}$. Table 1 illustrates that certain PAHs were present in concentrations significantly higher than the allowable limit. Among these, naphthalene was identified as the most hazardous. The amount of naphthalene in the water sample from Hovsan was higher than in the sample from Bilgah; however, in both cases,

the concentration exceeded the permissible limit.

The amount of naphthalene in the seawater sample extracted from Hovsan was approximately 19 times higher than in the sample taken from Bilgah.⁽¹²⁾ Naphthalene is considered highly dangerous, as it can significantly impact erythrocytes in humans, potentially leading to their destruction. According to the International Agency for Research on Cancer (IARC), naphthalene is classified as a carcinogenic substance for both humans and animals. Scientists have placed naphthalene among the most toxic substances, often referring to it as a “chemical substance that causes death.” This compound can enter the body through the respiratory system, where it exerts a carcinogenic effect. Fluorene, while a toxic organic substance, has not been found to possess the carcinogenic properties of naphthalene. Phenanthrene, a polycyclic aromatic hydrocarbon consisting of three fused benzene rings, is often found in cigarette smoke and has irritating properties that can cause the skin to become sensitive to light. Phenanthrene appears as a blue fluorescent white powder. Research conducted in the United States first identified phenanthrene as a substance associated with genetic mutations caused by exposure to smoking. This toxic compound is known to induce mutations that may lead to cancer.⁽¹³⁾

The results presented in the table indicate that the concentration of polycyclic aromatic hydrocarbons (PAHs) in the seawater samples from Hovsan was exceptionally high. Both pyrogenic and petrogenic pollutants play a significant role in this contamination.⁽¹⁴⁾

Abundance

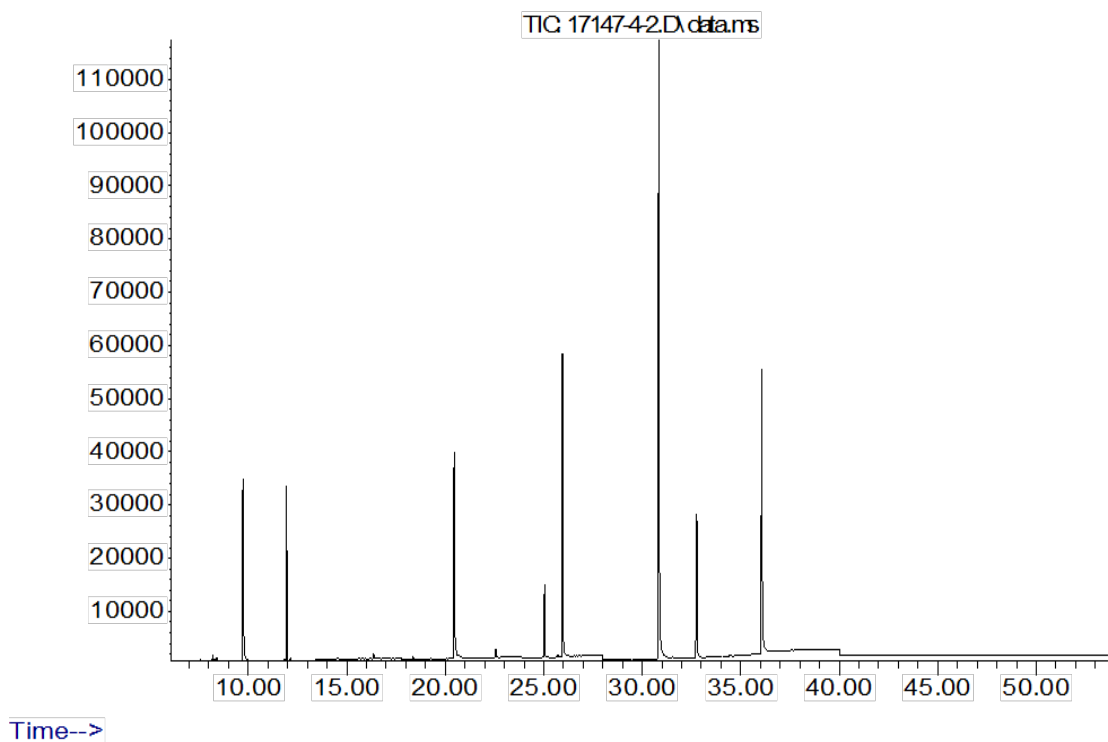


Figure 1. GC-MSD analysis of sea water sample taken from Hovsan (for PAHs)

Abundance

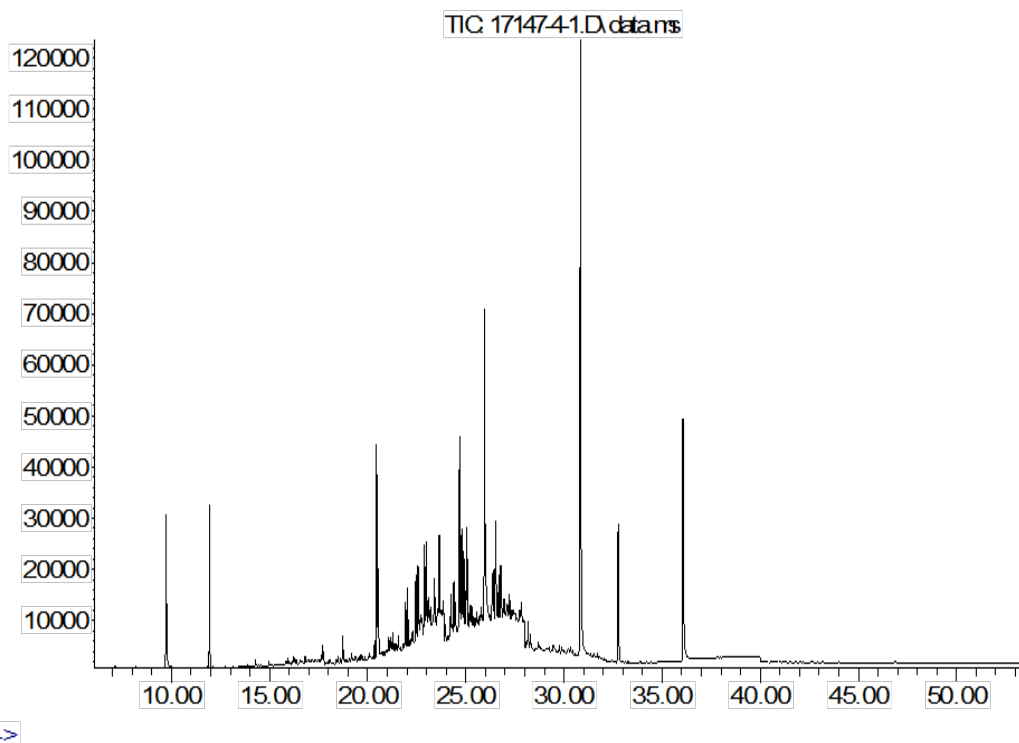


Figure 2. GC-MSD analysis of seawater sample taken from Bilgah (for PAHs)

Phenol and its derivatives, such as polycyclic aromatic hydrocarbons (PAHs), are considered hazardous to aquatic ecosystems. Lethal effects are observed when the concentration of phenol reaches 1 g/L, while concentrations below 0,5 g/L generally have no significant harmful effects. However, at a phenol concentration of 0,2 mg/L, the water begins to develop an unpleasant taste. The concentration of phenolic compounds in the analyzed water samples is presented in table 2.

The obtained chromatograms are shown in figures 3 and 4. Table 2 presents the results of the analysis of phenolic compounds in two seawater samples. It is important to note that phenolic compounds are considered hazardous to aquatic ecosystems when their concentration exceeds 0,01 mg/L in seawater (and 0,001 mg/L in drinking water). Chlorinated phenol derivatives are even more dangerous than phenol itself, as they have a pungent odor. Even at a concentration of 0,001 mg/L, chlorinated phenol derivatives in seawater can have a negative impact. Excessive levels of phenol in water are detrimental to living organisms, causing severe health issues in aquatic life. Furthermore, through the food chain, phenolic contamination can pose a significant threat to human health.⁽¹⁵⁾

As shown in table 2, the concentration of phenol in the water sample taken from Hovsan was higher than in the sample from Bilgah. The standard permissible concentration for phenol is 0,01 µg/L; however, the amounts detected in both the Hovsan and Bilgah water samples exceeded this limit.

Table 2. Amount of the phenolic compounds in the water samples taken from Hovsan and Bilgah		
Phenol and its derivatives, $\mu\text{g L}^{-1}$ $1\ \mu\text{g L}^{-1} = \text{mg L}^{-1}(\text{or } 0,001\text{g L}^{-1})$	Hovsan	Bilgah
phenol	0,16	0,08
o-kresol	0,04	0,01
2-nitrophenol	0,12	0,02
2,4-dimetilfenol	0,13	0,03
2,4-dichlorophenol	0,04	0,04
2,6-dichlorophenol	0,08	0,06
4-chloro-3-metilphenol	0,06	0,04
2,4,5-trichlorophenol	0,10	0,06
2,4,6-trichlorophenol	0,10	0,06
2,3,4,6-tetrachlorophenol	0,07	0,07
pentachlorophenol	0,16	0,04

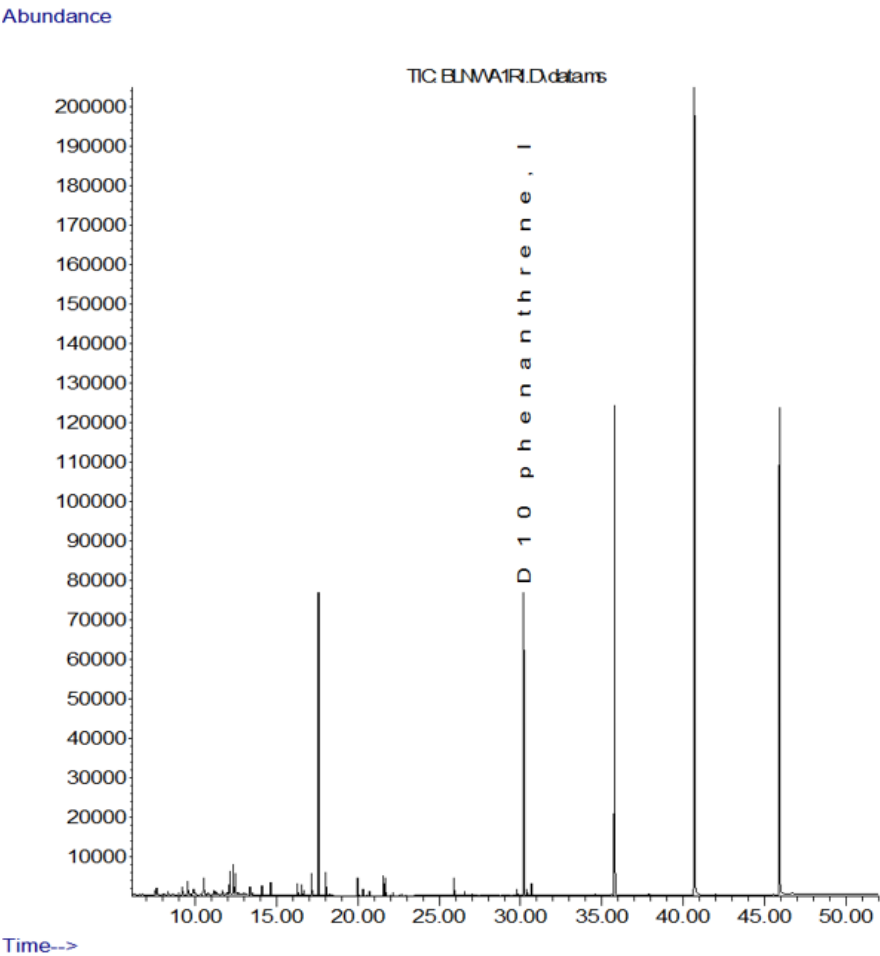


Figure 3. GC-MSD analysis of seawater sample taken from Hovsan (for phenolic compounds)

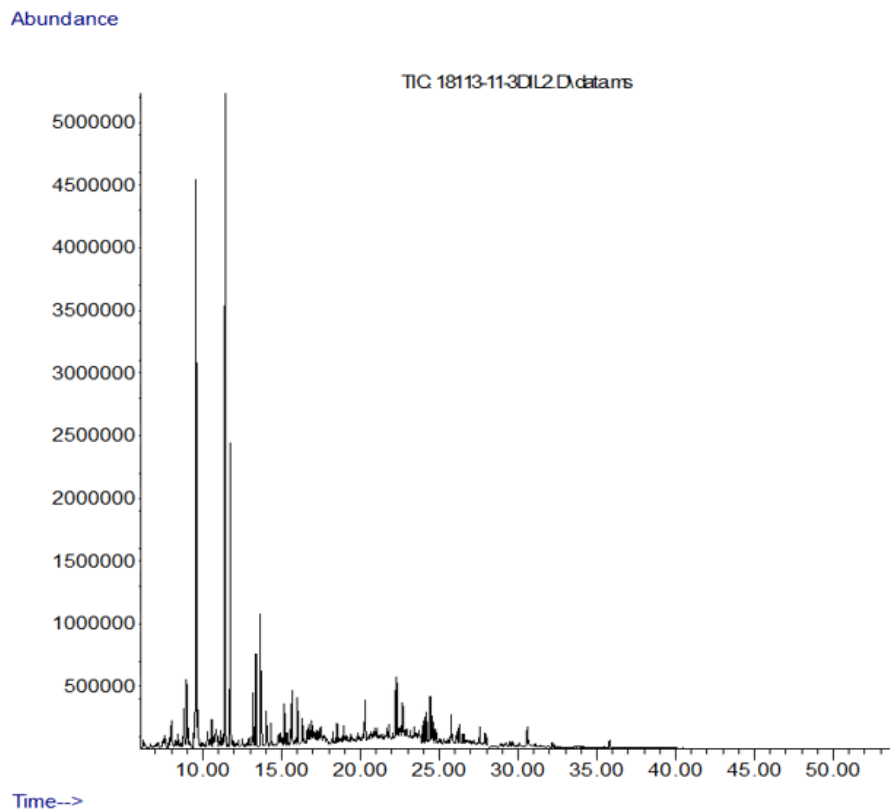
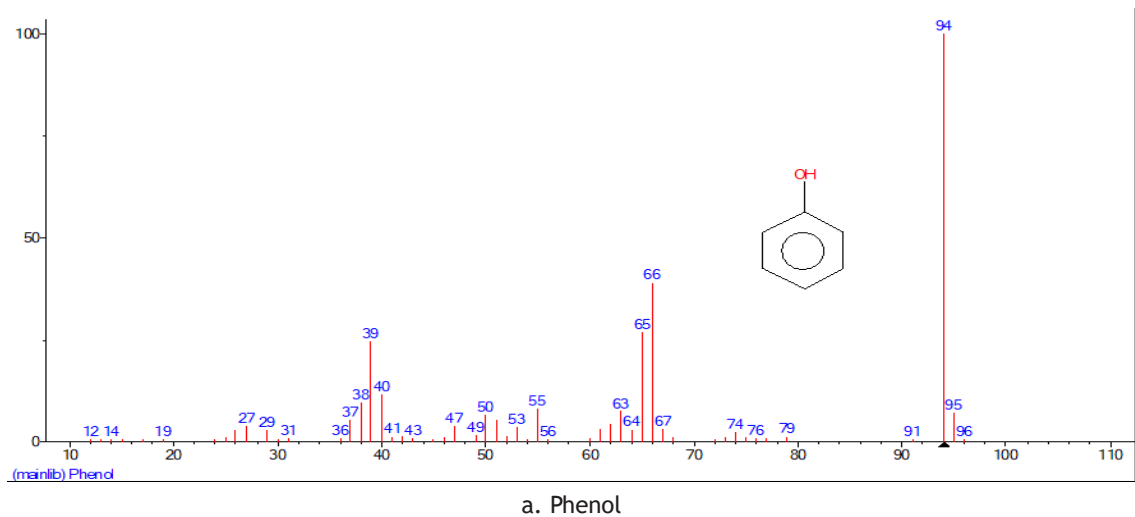
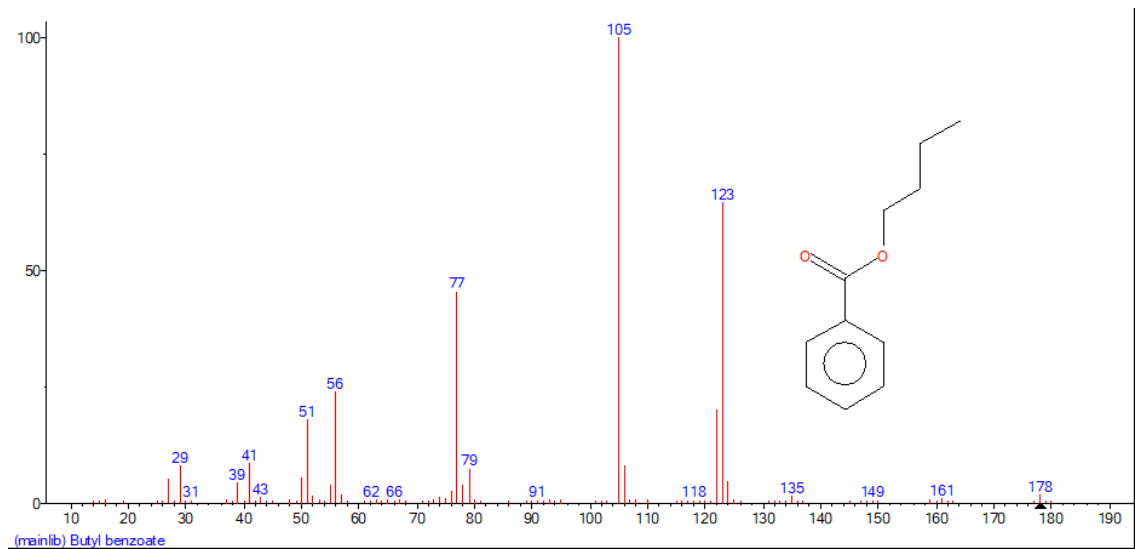


Figure 4. GC-MSD analysis of seawater sample taken from Bilgah (for phenolic compounds)

It should be noted that the content of toxic organic compounds in the water samples from both districts was above the permissible limits. Additional analyses were conducted on the water samples from Hovsan and Bilgah.





b. Butylbenzoat
Figure 5. Molecular spectra of some substances (a,b)

The molecular spectra (MS) of some of the substances obtained after the analysis process are shown below (figure 5 (a,b)). Molecular spectra provide information about the presence of substances in the analyzed sample based on their molecular mass.

Table 3 presents the physical and chemical characteristics of the analyzed water samples.

Table 3. Physical-chemical parameters of the water samples				
Areas	tem. °C	pH	salinity, %	Electrical conductivity mS/sm
Hovsan	26,1	8,7	10,8	18,2
Bilgah	26,8	8,0	10,7	18,4

Although the physicochemical parameters of the seawater samples are within the normal range, the pollution caused by toxic organic substances has exceeded the permissible limits. The primary objective of the environmental monitoring was to assess the content of seawater by conducting chemical analyses.

CONCLUSIONS

1. Environmental monitoring was conducted in two areas of Azerbaijan.
2. Water samples were collected from the Hovsan and Bilgah areas and analyzed.
3. The analysis of the water samples included 15 PAHs, 11 phenols, and their derivatives.
4. The amount of naphthalene in the water sample from Hovsan was higher than in the sample from Bilgah, likely due to the presence of nearby industrial facilities.
5. The concentration of phenol in the water sample from Hovsan was greater than in the sample from Bilgah.
6. Quantitative analyzes were performed by the Agilent 6890N/5975 GC-MSD method.
7. The physicochemical parameters of the water samples from Hovsan and Bilgah were determined.

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Chapter 02

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Use of Dissolved Gases and Their Radicals in Technologies for Purifying Natural Water

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ABSTRACT

The results of theoretical and experimental studies confirming the necessity and efficiency of using dissolved gases in biological and physicochemical technologies for purifying underground water from Fe^{2+} , Mn^{2+} , NH_4^+ , humic acids, and phenols have been presented. Optimal pH-Eh parameters of the environment and activators of the biochemical oxidation process of Fe^{2+} and Mn^{2+} cations have been determined. The efficiency of the destruction of the compounds difficult to oxidize (phenols, humic complexes) using the hydrodynamic cavitation process has been proven.

Keywords: Water Purification; Ferrobacteria; Dissolved Gases; Cavitation Flow.

INTRODUCTION

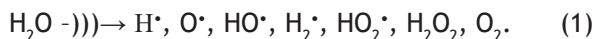
Water is one of the fundamental elements for ensuring life on the planet and a key component in the development of any civilization, including modern technogenic society. However, despite the rapid growth of modern megacities, industry, energy, and agriculture, the amount of available water remains practically unchanged and constitutes 200 000 km³. Meanwhile, over the past fifty years, humanity has invented more than 100 million new organic and inorganic substances that do not undergo natural degradation processes and affect human health. Despite natural protection, groundwater aquifers are also exposed to anthropogenic influence.^(1,2)

As a result, the development of new and the improvement of existing technologies based on a scientifically grounded and rational combination of already known and advanced biological and physicochemical purification methods is a relevant issue today.

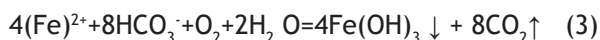
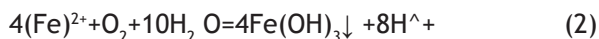
The main methods for removing contaminants from natural water include chemical, physicochemical, biological, and biochemical approaches, as well as technologies based on their combination.⁽²⁾

Many technologies use so-called dissolved gases: oxygen and its active forms, singlet oxygen, ozone, carbon dioxide, hydrogen peroxide, and nitrogen. The use of gases can be direct (introducing them into the system from an external source), indirect (producing gases within the system through biochemical reactions or via mechanical thermal decomposition of water molecules during hydrodynamic or acoustic cavitation), or combined.

High pressure and temperature inside the bubbles, formed during the cavitation process, lead to the disintegration of water molecules and the formation of radicals with high chemical activity:



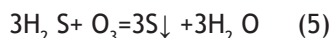
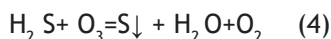
The most well-known application is the use of atmospheric oxygen for oxidizing Fe^{2+} cations in iron removal technologies based on simplified and deep aeration methods:



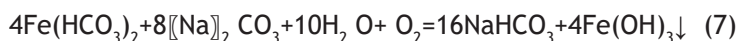
According to the given reactions, the oxidation of 1 mg of FeCO_3 produces 1,6 mg of free CO_2 while simultaneously reducing the total alkalinity of the water by 0,043 mmol/dm³, which leads to a decrease in water pH and inhibits oxidation and hydrolysis processes.

To remove organic iron compounds, water ozonation method can be applied. The ozone dose is set equal to the Fe^{2+} concentration. As a result, oxidation of organic and mineral compounds (Fe^{2+} , Mn^{2+}) occurs, followed by a change in their phase-dispersed state, namely converting them into insoluble hydroxides, which can then be removed through filtration³.

One of the significant advantages of ozone is its ability to oxidize hydrogen sulphide at pH 5,0 - 9,0:



When removing iron from acidic and slightly acidic underground water containing complex compounds, the use of alkaline reagents may be applicable:



The aim of this research is to analyse the effectiveness of dissolved gases in natural water purification technologies for removing Fe^{2+} , Mn^{2+} , NH_4^+ , humic acids, and phenols based on modern theory as well as our own experimental research.

METHOD

Experiment 1

The concentrations of Fe^{2+} and Mn^{2+} ions were measured according to established methods,^(3,4) using an experimental pilot installation (figure 1). Comparative researches were carried out concerning the determination of the efficiency of using iron bacteria in various conditions. The pilot experimental installation is composed from the capacity of rising water of 2000 ml volume, a reaction flask of 500 ml volume, a Kamovski pump, a flask with the changeable paper filter «blue line» and a ceramic filter, a magnetic mixer MM-5, a system of rubber hoses (figure 1). Into the outlet water capacity was added the calculated 0,1 n hydrochloric solution and iron (II) sulphate. A reaction flask was filled with 10 ml of sediment, with autotrophic bacteria

Gallionella (figure 2a), and depending on the experimental method, bacterial growth activators were added (table 1). All samples were taken in triplicate.

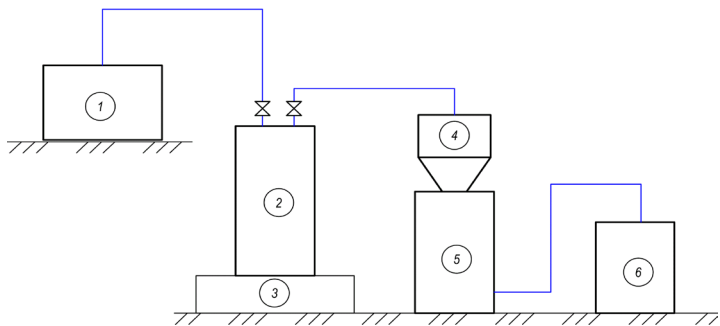


Figure 1. Scheme of experimental installation. 1 - outlet imitation solution capacity; 2 - reaction flask; 3 - magnetic mixer; 4 - hermetic ceramic filter; 5 - flask of filtrate collection; 6 - Kamovski pump

In a series of experiments on the oxidation of Mn^{2+} , a reaction flask was filled with 10 ml of sediment, with heterotrophic bacteria of the *Leptothrix* and *Crenothrix* genera (figure 2b).

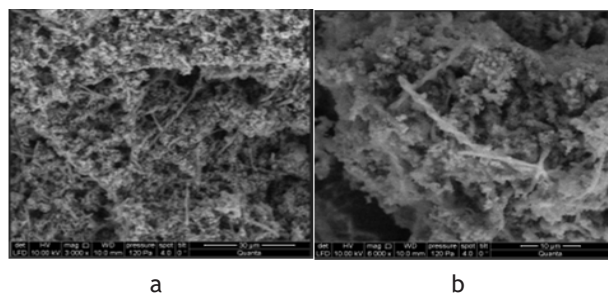


Figure 2. The electronic image of the matrix structures of *Gallionella* (a) and *Leptothrix* (b) from the sediment x 6000

Experiment 2

The pH values, concentrations of dissolved oxygen, phenols, and NH_4^+ were determined following the methods^(5,6,7,8) using an experimental installation (figure 3).

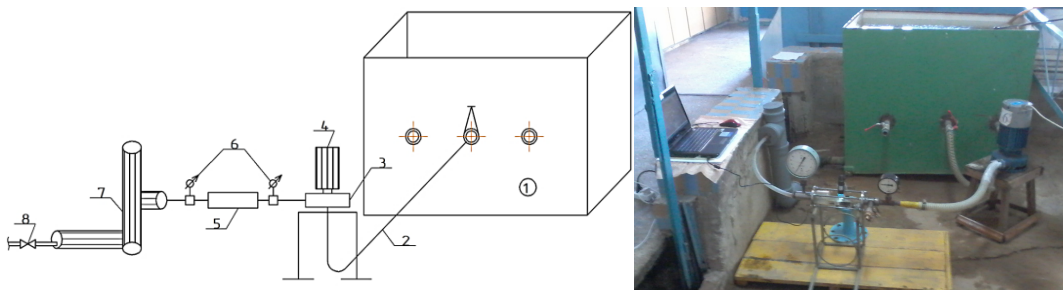


Figure 3. Experimental semi-production installation. a - the general scheme of the installation with the BC 1,1-18 pump; b - the installation with a multi-stage cavitator; 1 - a metal tank with a volume of 900 dm³ with a model solution; 2 - a suction pipe of the pump; 3 - a pump unit; 4 - an electric motor; 5 - a hydrodynamic cavitator; 6 - manometers; 7 - a contact camera; 8 - shut-off valve

The installation (figure 3a) worked as follows: the pump 3 to the hydrodynamic cavitator 5 fed the model solution from container 1. The water treated in the cavitator entered the contact chamber 7, where the process of oxidation of destructured organic compounds with reactive radicals took place. Sampling from the contact chamber was carried out after certain time periods (5, 30, 60, 90, 120 min). All samples were taken in triplicate. The selected samples were treated sequentially with solutions of aluminum hydroxochloride (20 mg/dm³) and nonionic flocculant. After the flake formation process took place, the treated model solution was filtered through a blue band paper filter.

RESULTS

Experiment 1

The water solution quality parameters (table 1) indicate that Fe²⁺ cations cannot be oxidized by chemical methods. Comparing the results of experiments № 1 and № 2 (table 1), it can be concluded that the kinetics of Fe²⁺ cation removal by iron bacteria, except for the initial period (0-5 minutes), were almost identical, differing by only 2-5 %.

The increased oxidative capacity of the system (experiment № 2) during the first five minutes is explained by the higher concentration of Fe²⁺ ions, which act as electron donors necessary for the respiration process of autotrophic Gallionella.⁽⁹⁾ In the experiments № 3-4, the system received an additional external source of inorganic carbon in the form of Na₂CO₃ solution, which allowed iron bacteria to build new cellular mass and significantly accelerated the biological oxidation of Fe²⁺ cations.^(9,10)

Table 1. The quality parameters of researched water with an increased content of cations Fe²⁺

№	Quality parameters of source water	Filtrate	Duration of contact, min				
			5	15	30	45	60
1	pH=6,0; Fe ²⁺ =31,0 mg/dm ³ ; O ₂ = 2,0 mg/dm ³ ; Hydro-carbonate alkalinity (HCA) 1,3 mmole/dm ³	Fe ²⁺ mg/dm ³	25	15	7	3,8	2
		E, %	19	51,6	77,4	87,7	93,5
2	pH=6,5; Fe ²⁺ =44,0 mg/dm ³ ; O ₂ = 1,0 mg/dm ³ ; HCA =1,3 mmole/dm ³	Fe ²⁺ mg/dm ³	27	19	12,5	6,3	2,3
		E, %	38,6	56,8	71,6	85,2	94,8
3	pH=6,0; Fe ²⁺ =45,0 mg/dm ³ ; O ₂ = 1,0 mg/dm ³ ; HCA =1,5 mmole/dm ³ ; Na ₂ CO ₃ = 40 mg/dm ³	Fe ²⁺ mg/dm ³	24	14,5	6,0	2,3	1,5
		E, %	46,7	67,8	86,7	95	96,7
4	pH=6,3; Fe ²⁺ =38,0 mg/dm ³ ; O ₂ = 1,7 mg/dm ³ ; HCA=2,7 mmole/dm ³ ; Na ₂ CO ₃ = 80 mg/dm ³	Fe ²⁺ mg/dm ³	13	7,8	3,8	0,8	0,1
		E, %	65,8	79,5	90	98	99,7

Note: *standard deviation values: Fe δ =±10 %; pH Δ =±0,05.

In a series of experiments on the oxidation of Mn²⁺ (table 2) cations by heterotrophic bacteria of the Leptothrix and Crenothrix genera, it was observed that without the addition of an external organic carbon source, the primary factors influencing the oxidation process were the pH and Eh values of the environment (experiments № 1, 3, 4, 5).

When 10 mg/dm³ of C₁₂H₂₂O₁₁ was added (experiments № 2-6), the intensification of Mn²⁺ cations oxidation was observed in the bacterial environment of Leptothrix and Crenothrix.

Table 2. The quality parameters of researched water with an increased content of cations Mn ²⁺											
№	Quality parameters of source water	Filtrate	Duration of contact, min								
			3	5	10	15	20	30	40	50	
1	CMn2+ = 3 mg/dm3; pH 6,3 Eh = 120 mV	Mn2+ mg/dm3	2,8	2,65	2,0	1,3	0,7	0,4	0,3	0,28	
		E, %	6,7	11,7	33,3	56,7	76,7	86,7	90,0	90,7	
2	CMn2+ = 3 mg/dm3; pH= 6,3; Eh = 120 mV; 10mg/dm3 C ₁₂ H ₂₂ O ₁₁	Mn2+ mg/dm3	1,5	1,0	0,9	0,7	0,6	0,3	0,15	0,15	
		E, %	50,0	66,7	70,0	76,7	80,0	90,0	95,0	95,0	
3	CMn2+ = 3 mg/dm3; pH 6,3 Eh = 150 mB	Mn2+ mg/dm3	2,8	2,6	1,6	0,7	0,45	0,2	0,2	0,2	
		E, %	6,7	13,3	46,7	76,7	85,0	93,3	93,3	93,3	
4	CMn2+ = 3 mg/dm3; pH 8,3 Eh = 150 mV	Mn2+ mg/dm3	1,4	0,75	0,3	0,2	0,2	0,2	-	-	
		E, %	53,3	75,0	90,0	93,3	93,3	93,3	-	-	
5	CMn2+ = 3, mg/dm3; pH 7,4 Eh = 80 mV	Mn2+ mg/dm3	-	2,0	1,7	1,6	1,5	1,4	1,3	1,2	
		E, %	-	33,3	46,9	50,0	53,1	56,3	59,4	62,5	
6	CMn2+ = 3,2 mg/dm3; pH 7,4; Eh = 80 mV; 10mg/dm3 C ₁₂ H ₂₂ O ₁₁	Mn2+ mg/dm3	-	1,12	0,96	0,9	0,75	0,5	0,4	0,3	
		E, %	-	65,0	70,0	71,8	76,5	84,4	87,5	90,6	
Note: *standard deviation values: Mn2+ δ=±10 %; pH Δ=±0,05; Eh Δ=±0,05											

Experiment 2

Table 3 presents the results of studies of the effectiveness of the destruction of phenols in an aqueous solution depending on the time of its stay in the pressure contact chamber (figure 3b).

The results showed that when a 3 % hydrogen peroxide solution was added to the cavitation range, an increase in the oxidation rate of phenols was observed. This effect is caused by the formation of an additional amount of hydroxyl radicals, which are formed during the decomposition of hydrogen peroxide in the void of cavitation: $H_2O_2 \leftrightarrow 2|OH^\bullet|$. A coagulant solution used to remove oxidized and colloidal compounds from the reaction zone in a timely manner.

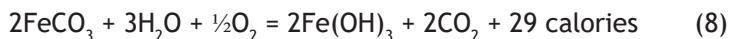
Table 3. The results of the research of phenol destruction in cavitation flow				
Tap water simulant quality parameters: C phenols 1,0 mg/dm ³ ; pH 6,5; t = 10,1°C				
Time of water hold-up in the pressure contact chamber, min.	5	15	30	60
Output, mg/dm ³	0,31	0,21	0,15	0,06
E%	69	79	85	92
While introducing 3 % solution of H_2O_2 in the cavitation area				
Output, mg/dm ³	0,17	0,12	0,088	0,015
E%	83	88	91	98,5

DISCUSSION

Experiment 1

According to the data of ⁽¹⁰⁾, the bacteria of Gallionella genus use the energy of the iron carbonate oxidation to assimilate carbon dioxide, which acts as a carbon source as per the

following equation:



This reaction is accompanied with the energy release in the amount of 125 g-cal per 1 g of the oxidized salt FeCO_3 . This is the energy used in the cells of *Gallionella* for all the work, required for the breakage of carbon (IV) oxide (CO_2) and the synthesis of organic matter in the cell.⁽¹⁰⁾

The process of enzymatic oxidation of Fe^{2+} ions occurs due to the transfer and integration of the electron into the breathing chain of the bacteria. The synthesis of 1g of the cellular biomass of the microorganism requires the enzymatic oxidation of 276 g of Fe^{2+} ions with the release of 500 g of ferric hydroxide, which, as a result of the biochemical transformation of $\text{Fe}^{3+} \rightarrow \gamma\text{FeOOH}$, creates the matrix structures of bio-minerals.

The mechanism of Mn^{2+} ion oxidation by the bacteria of *Leptothrix* genera occurs by the peroxide pathway and appears in the capsules and on the surface of the cellular wall:

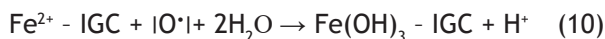


Hydrogen peroxide is a product of the bacterial metabolism of *Leptothrix* bacteria, formed during the oxidation of organic substances as electrons are transferred through the respiratory chain.

The oxidation of manganese by H_2O_2 occurs with the participation of catalase, which performs a peroxidase function. In this process, Mn^{2+} serves as an electron donor.

The physiological significance of Fe^{2+} and Mn^{2+} oxidation involving H_2O_2 is the detoxification of a harmful metabolic by-product.

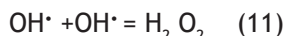
It was found out that while using the biological purification method, there is a possibility of removing ferrichumic complexes, ammonium nitrogen (to 1,5 mg/cdm) from the underground waters. In the molecular form, the oxidation of the ferric-humic complexes (IGC) by the activity products of the ferrobacteria from *Leptothrix*, *Crenothrix* genera can be shown by the following equation of the chemical reaction:



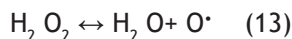
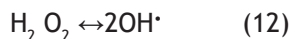
Experiment 2

Phenols destruction mechanism

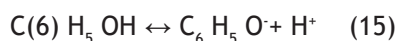
On the basis of the known free-radical mechanism of formation of $\text{OH}^\bullet$ radicals in the cavitation flow,⁽¹¹⁾ we have come up with a mechanism for the destruction of phenols followed by removal of the formed intermediates with the help of an electrolyte solution outside the reaction zone. According to ⁽¹¹⁾, as a result of the reaction, H_2O_2 can be formed as its intermediate products:



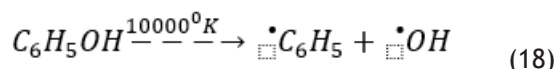
Under the effect of high cavitation pressure and temperatures, up to 5000 °C in the middle of the bubbles,⁽¹²⁾ at the time of their destruction, hydrogen peroxide dissociates under a radical mechanism:



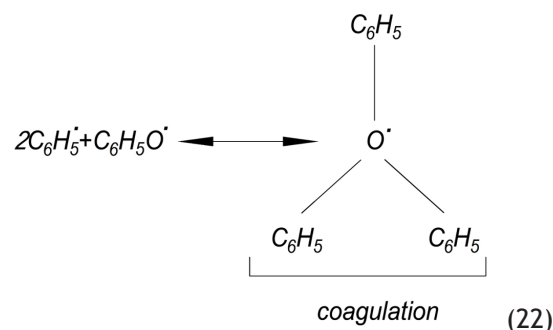
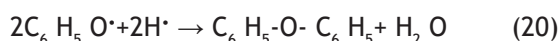
Phenols in water dissociate as acids:



Radical reactions take place in the cavitator:

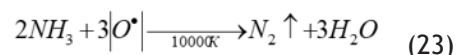


The recombination of radicals leads to the formation of a number of compounds:



The mechanism of removal of nitrogen and ammonium compounds

When cavitation bubbles are trapped under conditions of local high pressure (10 000 atm) and temperature (up to 10 000 K), the process of dissociation of hydrogen peroxide occurs by a radical mechanism (equations 12, 13) with subsequent oxidation of NH_3 and the formation of gaseous N_2 :



Thus, the application of HDC makes it possible to carry out the destruction of difficult-to-oxidize high-molecular organic and nitrogen-ammonium compounds with a change in their

phase-dispersed state and makes it possible to significantly facilitate the functioning of the next stages of the technological schemes of natural water treatment.

CONCLUSIONS

As a result of the above theoretical and experimental studies, the importance of using dissolved gases in biological and physicochemical technologies for purifying underground water from Fe^{2+} , Mn^{2+} , NH_4^+ , humic acids, and phenols has been proven. Optimal pH-Eh parameters of the environment and activators of the biochemical oxidation process of Fe^{2+} and Mn^{2+} cations have been obtained. The efficiency of the destruction and oxidation of the compounds difficult to oxidize (phenols, humic complexes) using the hydrodynamic cavitation process has been proven.

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Chapter 03

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Use of nano substances for environmental safety

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ABSTRACT

Purification of aquatic ecosystems using nanotechnological methods is one of the most important problems from an environmental point of view and for this purpose, environmentally friendly TiO_2 nanoparticles were used. TiO_2 nano particles have excellent catalytic properties in photochemical processes as they are also environmentally friendly. Chemical-physical properties of TiO_2 nanoparticles have been investigated. The main aims of this study are to investigate the photochemical degradation of phenol with TiO_2 nanoparticles in the nitrogen medium and nitrogen-free medium. Photochemical reactions were carried out in the presence of TiO_2 nanoparticles having the size of 10-30 nm. In this study, TiO_2 nanoparticles that have been used in photochemical reaction with phenol were synthesized by sol-gel method. TiO_2 nanoparticles were characterized by SEM and XRD-methods. Photochemical degradation of phenol was found to be better at $\text{pH} > 5$. Decomposition of 1 mgL^{-1} phenol was 99 % in the nitrogen-free medium. However, in the medium containing nitrogen, the decomposition of phenol decreased, the decomposition rate was determined 52 %. Quantitative analyzes were performed using high sensitivity Agilent 5975 mss detector equipped with an Agilent 6890N gas chromatograph. The process was carried out under the same conditions in the presence of the same amount of TiO_2 for 1 hour in the “Varian Cary 50” spectrophotometer. Was also studied the effect of the pH of the reaction medium on the course of the photochemical reaction. At the same time the adsorption properties of TiO_2 nanoparticles were studied. It has been found that TiO_2 nanoparticles have very poor adsorption capacity properties.

Keywords: Decomposition; Nano- TiO_2 ; XRD; SEM; GC-MSD.

INTRODUCTION

Currently, water pollution treatment is one of the widespread environmental problems in the world. It is essential to develop an efficient, economical, and environment-friendly process of wastewater treatment in order to allow the discharge of wastewater to the receiving environment. Phenol is known as a stubborn compound due to its toxicity and non-biodegradable properties, and is therefore difficult to treat.^(1,2) The treatment technologies of phenol in wastewater are based either on separation or destruction. The known separation techniques are steam distillation, extractions, adsorption, membrane pervaporation, and membrane-based solvent extractions, while destructive techniques include electrochemical oxidation, photocatalytic oxidation, chemical oxidation, and biochemical reduction. There is a lot of research on these techniques.⁽³⁾ Since nanotechnology is one of the rapidly evolving areas nowadays, purification methods based on nanoparticles for various purposes leads to new directions.

Many photochemical processes take place in the presence of TiO_2 nanoparticles.^(4,5,6,7) Decomposition of organics materials using TiO_2/Ce systems is widely discussed in the literature.

⁽⁸⁾ Such systems have a high level of active oxygen which leads to the rapid degradation of organic compounds. It is very useful because it is cheap, durable and most importantly, environmentally friendly. In many cases photochemical reactions have been carried out to remove toxic substances from the aquatic environment, mainly using TiO_2 in the form of anatase and mixed composites: for example, photocatalytic oxidation or mineralization of phenol in the presence of a Degussa P25- TiO_2 suspension (consisting of 80 % anatase and 20 % rutile phase). A vital piece of information is available in the literature on methods of depositing precious metals such as silver, gold, platinum on the TiO_2 surface. Heterogeneous photocatalysis is a transferable oxidation process. Large-scale decomposition of pollutants in the air and water also occurs on the basis of this process.^(9,10,11) In addition, many doping systems and modifications are being developed to ensure that TiO_2 undergoes photochemical reactions in the visible field. TiO_2 systems with non-metals are of great interest: mainly alloyed with nitrogen and carbon. It is theoretically explained that the photocatalytic properties of TiO_2 ⁽¹²⁾ based on doping with carbon and nitrogen atoms can increase from the UV radiation field to the visible portion of spectrum. Systems doped with a nitrogen atom are very common in the literature, and thus air purification is carried out.⁽¹³⁾

Nitrogen is alloyed with TiO_2 by various methods. For example; The TiO_2/N system modified with Ar/N_2 has very good photocatalytic activity in the visible field.⁽¹⁴⁾ Since titanium dioxide is structurally resistant to UV radiation, it is also important to obtain nanoparticles based on it and apply it in various fields. Both anatase and rutile forms of TiO_2 nanoparticles are important for chemical processes. The anatase form of TiO_2 is metastable and converts to rutile when heated. The permissible amount of TiO_2 in an aqueous medium is 0,7-16,0 mgL^{-1} . In this regard it is effective to use small amounts of nanoparticles. The behavior of nanoparticles in water depends on pH. Taking into account the above we can say that nano technological methods are the most modern methods of water purification from toxic compounds. The most effective of them was the purification of wastewater from phenol, an organic toxic substance based on the $\text{GO}/\text{Al}_2\text{O}_3$ composite by 99,9 %.⁽¹⁵⁾

The main aims of this study are to investigate the photochemical degradation of phenol with TiO_2 nanoparticles in the nitrogen and nitrogen-free medium to determine of adsorption properties of TiO_2 nanoparticles.

Experimental Part

TiO_2 nanoparticles have been investigated in order to carry out photochemical reactions. TiO_2 nanoparticles were synthesized by the sol-gel method. In the system TiO_2+Ph (phenol) the process took place only in the UV-radiation area. For the this system it was taken 0,05 gr TiO_2 equally distributed in the water of 10 mL. Then 5 ml of obtained mixture has been added to 20 mL of the 1 mgL^{-1} phenol solution. In this system the decomposition of phenol was 99 %.

For the $\text{TiO}_2+\text{Ph}/\text{N}$ system was taken 0,05 g $\text{TiO}_2+0,05$ g N compound: ethyl-3,3,5,5-tetracyano-2-hydroxy-2-methyl-4,6-diphenylcyclohexane carboxylate ($\text{C}_{26}\text{H}_{22}\text{N}_4\text{O}_3$). Their solution has been equally distributed in the water of 10 mL. In the $\text{Ph}+\text{TiO}_2/\text{N}$ system the process took place in the UV-Vis area. As it is mentioned above TiO_2 nanoparticles are not toxic and gets excited by UV radiation; this contributes to the reaction process. Complete mixing of TiO_2 nanoparticles in the participation of UV radiation has been carried out in advance for their equal distribution in the water. 5 mL of obtained mixture has been added to 20 mL 1 mgL^{-1} phenol solution and then 0,05 g N-compound has been added. The viewed mixture has been subject to photochemical dissociation for 60 minutes. All quantitative analyzes were performed on Agilent 6890N /5975 device. The device has a very high sensitivity. After photolysis process the dependence of the

solution's absorption coefficient on wavelength has been measured in UV "Varian Cary 50" spectrophotometer. Although the decomposition of phenol occurs in a lower yield compared to Ph+TiO₂ system it has been found that the photochemical process extends from the UV area to the Visible area. In the Ph+TiO₂/N system the decomposition of phenol was less than 52 %.

X-ray structure of the C₂₆H₂₂N₄O₃-ethyl-3,3,5,5-tetracyano-2-hydroxy-2-methyl-4,6-diphenylcyclohexane carboxylate obtained for the first time by us «Bruker APEX II CCD » (T = 100K, λMoKα - radiation, graphite monochromator, φ- and ω-scanning, 2θmax = 56°) was analyzed in the diffractometer and the following structure was obtained. The obtained carboxylate consists of white crystals.⁽¹⁶⁾

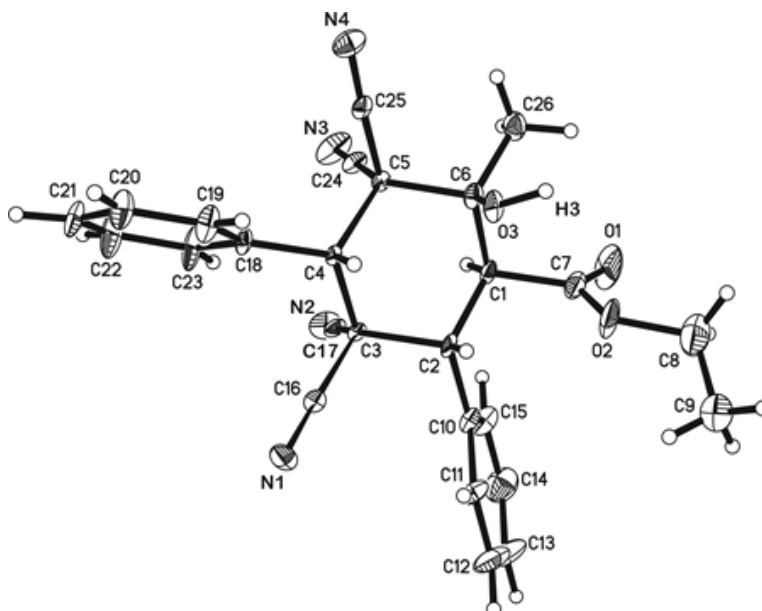


Figure 1. Structure of the C₂₆H₂₂N₄O₃-ethyl-3,3,5,5-tetracyano-2-hydroxy-2-methyl-4,6-diphenylcyclohexane carboxylate

RESULTS AND DISCUSSION

TiO₂ nanostructures are synthesized by the sol-gel method. It was obtained by the hydrolysis of titanium IV isopropoxide. This process usually proceeds through hydrolysis of titanium (IV) isopropoxide followed by condensation of formed Ti(OH)₄. The high rate of hydrolysis contributes to the formation of Ti(OH)₄ which interrupts the development of the chain Ti-O-Ti. The presence of a large number of Ti-OH groups and the low development of a three-dimensional polymer structure leads to a low particles packing 1 mgL⁻¹ of phenol solution was used during the process. The purity and crystalline properties of the TiO₂ nanoparticles were investigated by powder X-ray diffraction (XRD) method. Figure 2 shows the XRD patterns of the synthesized TiO₂ nanoparticles. XRD peaks were well defined and corresponded to TiO₂ at rutile phase. X-ray structure analysis graphs of the studied nanocomposite materials were recorded on the Rigaku Mini Flex 600spowder diffractometer. Its features are given below:

X-ray tube with copper anode (Cu-Kα radiation, 30 kV and mA) was used to draw the diffraction specters at room temperature. At 2θ = 20° -80° with discrete growth mode these specters were obtained as Δ2θ = 0,05° and the exposure time was τ = 5 seconds (figure 2).

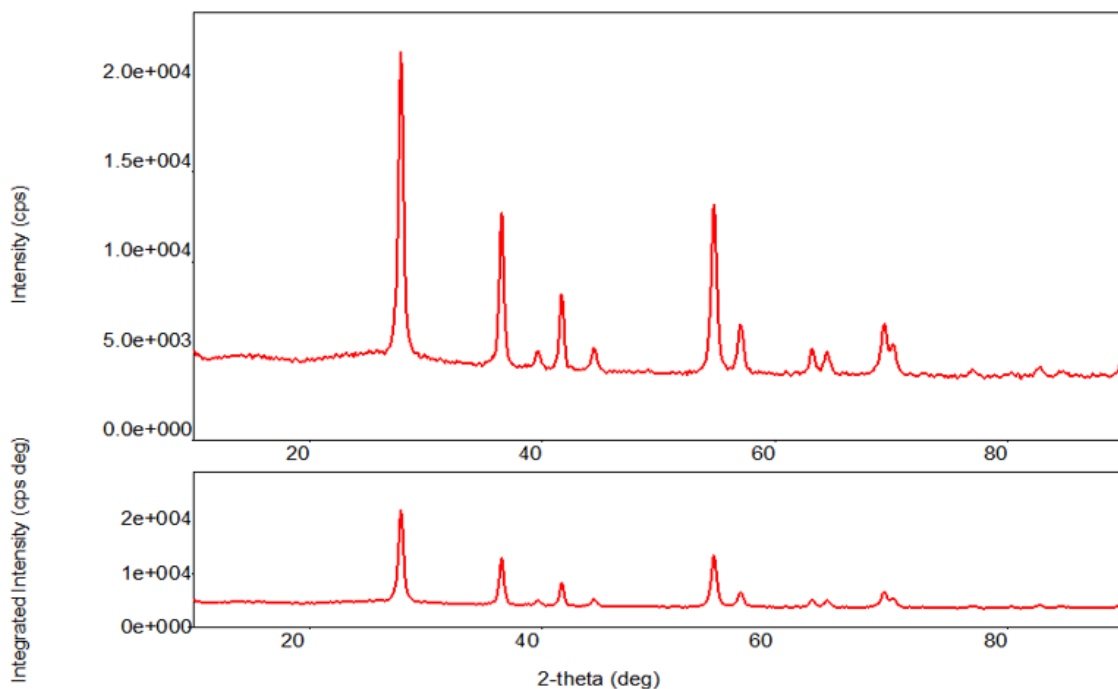


Figure 2. XRD patterns of the rutile phase TiO_2 nanoparticles

Figure 3 show the SEM patterns of the synthesized TiO_2 nanoparticles. Based on the SEM analysis of TiO_2 the nanoparticles were 10-30 nm in size.

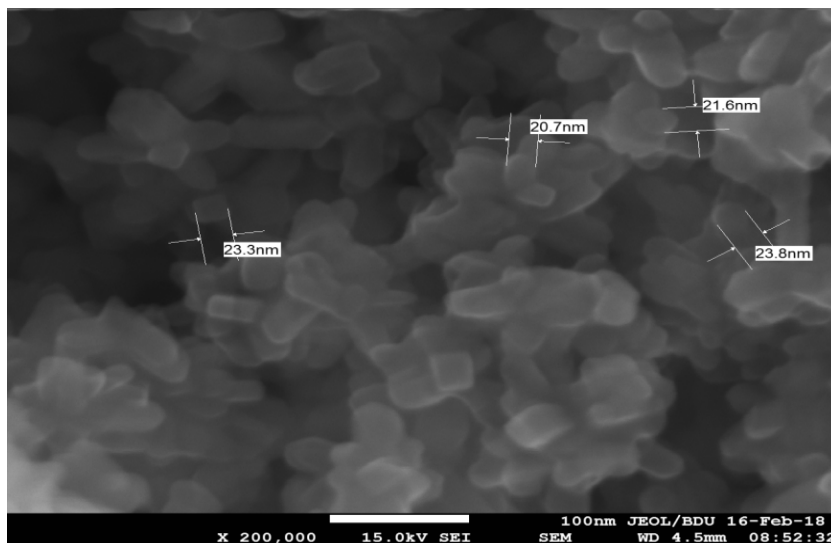


Figure 3. SEM patterns of the rutile phase TiO_2 nanoparticles

As can be seen from figure 4 the highest peaks for TiO_2 were obtained at 300-350 nm wavelengths after UV irradiation of TiO_2 nanoparticles. Starting from this wavelength (350 nm) the emission of the UV spectrum increases sharply in the figure 4.

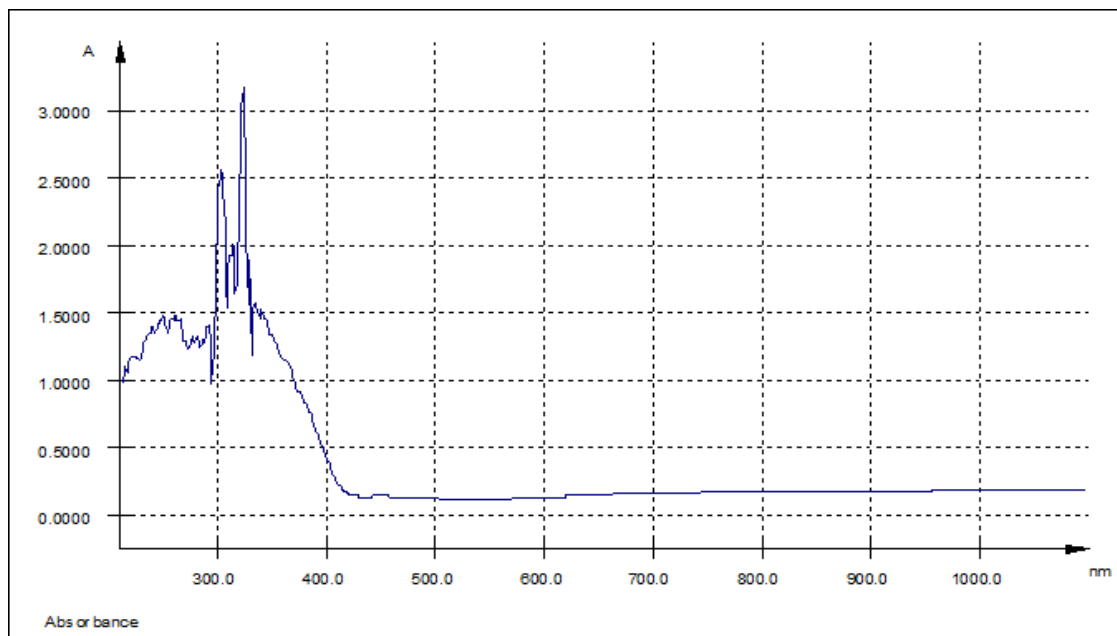


Figure 4. Light absorption of TiO_2 nanoparticles

The process of decomposition of phenol in the presence of UV in the system $\text{Ph} + \text{TiO}_2$ is shown below (figure 5).

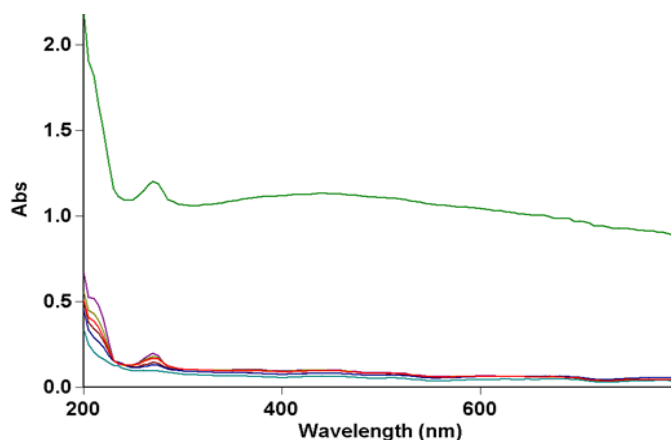


Figure 5. Photochemical decomposition of the $\text{Ph} + \text{TiO}_2$ in the presence of UV

As shown in figure 5 for the 1 mgL^{-1} $\text{Ph} + \text{TiO}_2$ system the characteristic wavelengths (270 nm) for phenol are not observed in the last (blue) curve compared to the other curves. This is due to the lack of or insufficient quantity of phenol after photolysis (sensitivity of the device) in the solution. The sample was then analysed in a gas chromatographic mass detector for more sensitive and accurate analysis. Amount of phenol has dropped from 1 mg to 10 μg . This means that 99 % of phenol has degraded.⁽¹⁷⁾

It may be noted that TiO_2 nanoparticles has very good photo dissociation together in

combinations with N atom. The matter is that we have considered more appropriate to use TiO_2 nanoparticles as the works done by us have been carried out in the participation of UV radiation, since TiO_2 nanoparticles gets excited only during UV radiation ($\lambda < 387 \text{ nm}$) it has only 5 % excitement in the Visible area. Furthermore TiO_2 is chemically sustainable it is obtained in soft condition that's easily seen in the viewed case and the most important is that it is considered ecologically clean. In addition the photochemical reaction in the $\text{Ph} + \text{TiO}_2/\text{N}$ system was considered. The reaction range ranged from the UV radiation range to 400-600 nm in the visible area (figure 6). In the $\text{Ph} + \text{TiO}_2/\text{N}$ system photolysis process has been done in UV radiation device; the dependence of absorption coefficient on the wavelength has been determined by "Varian Cary 50" device the concentration of phenol remained in the solution after photochemical reaction has been determined.

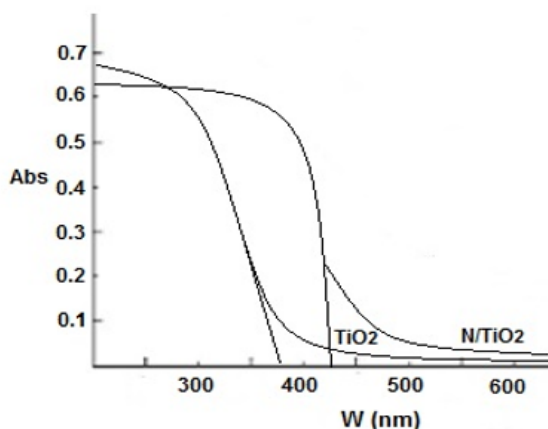


Figure 6. The dependence of the absorption coefficient on the wavelength for $\text{Ph} + \text{TiO}_2$ and $\text{Ph} + \text{TiO}_2/\text{N}$ systems

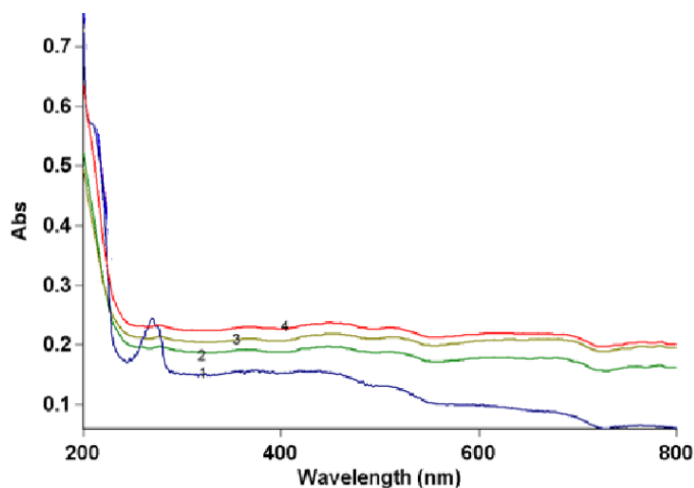


Figure 7. Photochemical decomposition of the $\text{Ph} + \text{TiO}_2/\text{N}$ in the presence of UV

1. Curve before irradiation.
2. Curve obtained at the 20th minute of the photocatalytic process.
3. Curve obtained at the 40 th minute of the photocatalytic process.
4. Curve obtained at the 60th minute of the photocatalytic process.

As can be seen in figure 7 for the Ph +TiO₂ system (1) the light absorption of the solution was intense in the UV irradiation area up to 400 nm while the light absorption of the Ph+TiO₂/N system (2,3,4) covered the area after 400 nm. The transition in the UV-Vis areas occurs with the transition of the adsorption wavelength dependence curve to the area after 400 nm in the presence of N-retaining substance.

The effect of pH on the photochemical reaction was also studied in the process. pH was determined by taking samples from the reaction solution at different times of the photochemical process. It has been determined that photochemical decomposition occurs at best in an acidic area: pH>5 (figure 8).

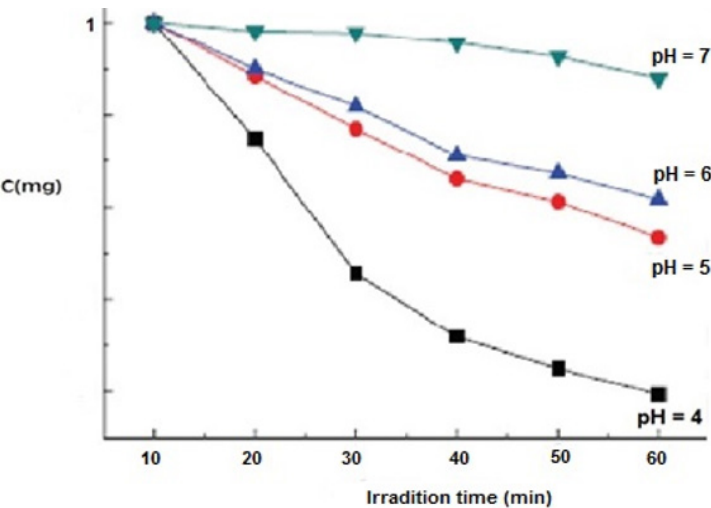


Figure 8. Effect of the pH of the reaction medium on the course of the photochemical reaction

Abundance

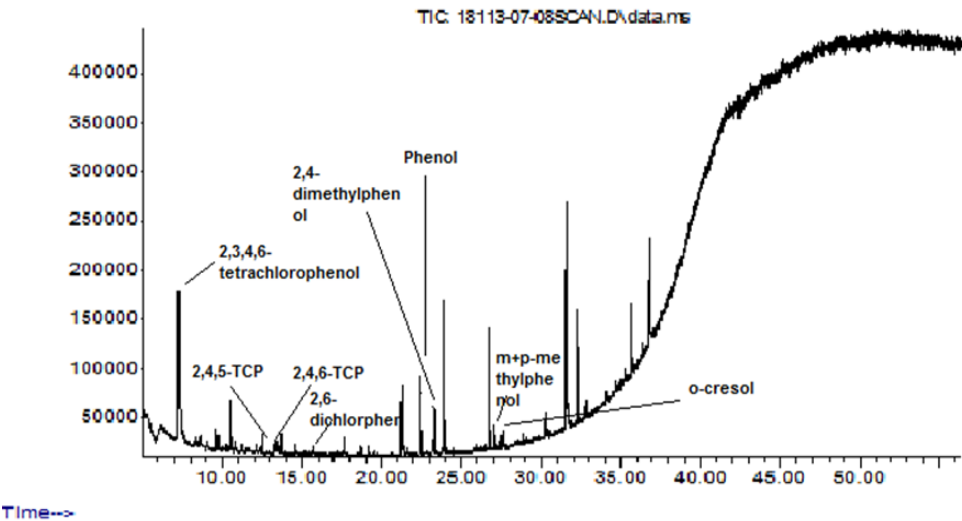


Figure 9. GC-MSD analysis of the Ph+TiO₂ solution after photochemical decomposition

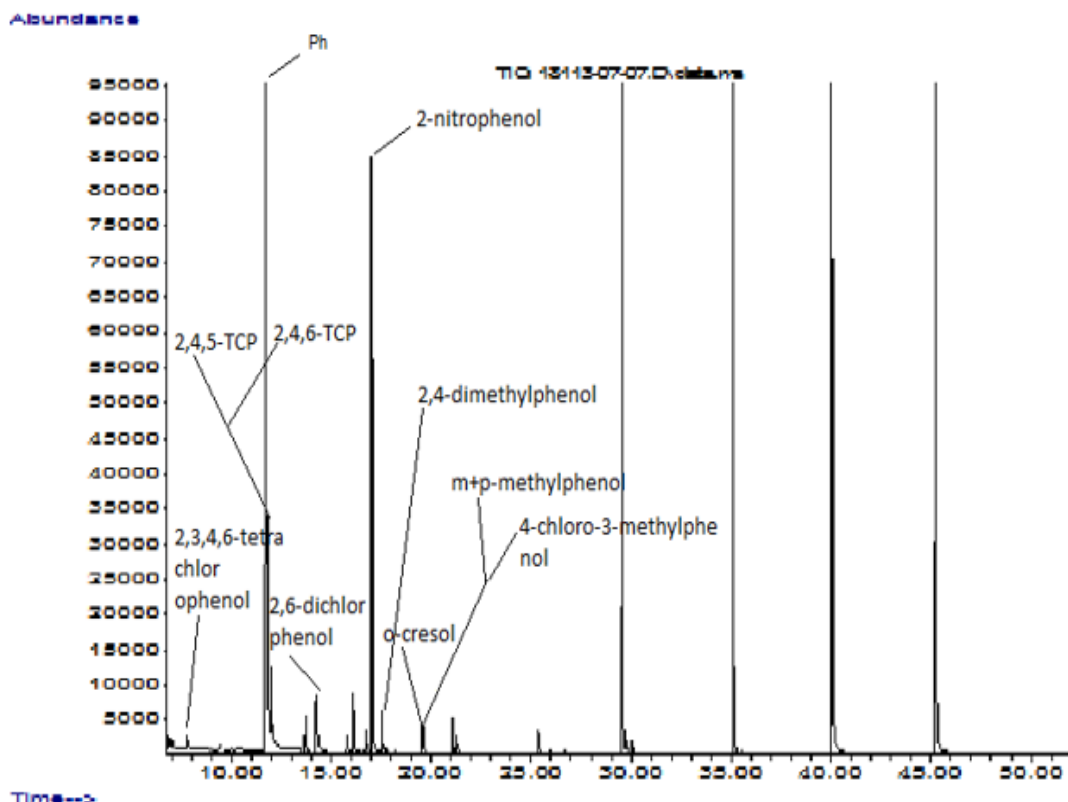


Figure 10. GC-MSD analysis of the Ph+ TiO₂/N solution after photochemical decomposition

In the systems Ph+TiO₂ (figure 8) and Ph+ TiO₂/N (figure 9) a quantitative analysis of treated samples after photolysis were carried out on a 6890N GC-MSD gas chromatograph with an Agilent 5975 high-performance mass-selective detector manufactured by Agilent Technologies (USA).

Also it was studied the adsorption process in the presence of TiO₂ nanoparticles which was carried out at room temperature (25 °C) for 2 hours. The process was monitored on a “Varian Cary 50” instrument. It was found that the adsorption process was very weak. This suggests that TiO₂ is a very poor adsorbent despite the fact that it is a good photo catalytic reagent. It should be noted that the TiO₂ nanoparticles belonged to the rutile phase. The process was monitored on a “Varian Cary 50” spectrophotometer. During the 2-hour process solution samples were taken and peaks were observed in the phenol-specific region of 270 nm every time (figure 10). This suggests that the adsorption process was absent. It is possible that the adsorption did not take place due to chemisorption. This can be said according to the Langmuir-Hinshelwood (LH) hypothesis.

Thus the work on the photochemical decomposition of phenol from wastewater in the presence of TiO₂ nanoparticles was studied and a high percentage of photochemical decomposition of phenol was achieved but as an adsorbent TiO₂ had a weak property. In conclusion it should be noted that in our time wastewater treatment by nanotechnological methods is one of the most developed and modern areas therefore work in this direction will continue in the future.

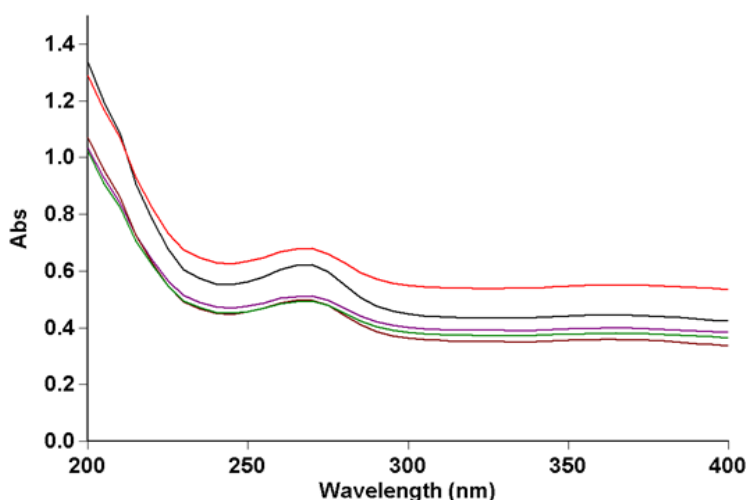


Figure 10. Comparison of phenol adsorption curves in the presence of TiO_2

CONCLUSIONS

1. The article deals with the decomposition of phenol in the $\text{Ph}+\text{TiO}_2$ and $\text{Ph}+\text{TiO}_2/\text{N}$ systems.
2. For the first time, a new synthesized organic matter: $\text{C}_{26}\text{H}_{22}\text{N}_4\text{O}_3$ containing nitrogen was used in the photochemical process.
3. In the $\text{Ph}+\text{TiO}_2$ system, the decomposition of phenol was 99 % and the decomposition of phenol in the $\text{Ph}+\text{TiO}_2/\text{N}$ system was 52 %.
4. The purpose of using a nitrogenous substance was to carry out a photochemical reaction in the visible area in the presence of TiO_2 nanoparticles in the UV area of radiation. This increases the practical significance of the process.
5. XRD and SEM analyzes of the TiO_2 nanoparticles were carried out.
6. The sizes of TiO_2 nanoparticles used ranged from 10 to 30 nm.
7. Decomposition of 1 mg/L phenol was carried out for 1 hour. In this case, the influence of the pH of the medium on the course of the reaction was determined.
8. The photochemical process was monitored on a “Varian Cary 50” spectrophotometer.
9. Quantitative analyzes were performed using an Agilent 6980N/5975 GC/MSD.
10. It was studied that TiO_2 nanoparticles have a very poor adsorption capacity.

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AUTHORSHIP CONTRIBUTION

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Data curation: Elmina Gadirova, S.R. Hajiyeva.

Formal analysis: Elmina Gadirova, S.R. Hajiyeva.

Drafting - original draft: Elmina Gadirova, S.R. Hajiyeva.

Writing - proofreading and editing: Elmina Gadirova, S.R. Hajiyeva.



Chapter 04

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Using nanoparticles to protect aquatic ecosystems

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ABSTRACT

Recently, the use of modern chemical methods for the protection of aquatic ecosystems has become very important. These methods are used to remove certain toxic organic substances. Using nanotechnology, a method has been developed to clean the aquatic ecosystem from toxic phenol. The main objectives of this study are: (1) to study the photochemical degradation of phenol by TiO₂ nanoparticles in nitrogenous and nitrogen-free media; (2) to determine the adsorption properties of rutile phase TiO₂ nanoparticles. Many photochemical reactions have been carried out in the presence of TiO₂ nanoparticles of 10-32 nm size. In this study, TiO₂ nanoparticles used in the photochemical reaction with phenol were synthesized by sol-gel method. TiO₂ nanoparticles were characterized by SEM and XRD. The adsorption properties of TiO₂ nanoparticles were also studied.

Keywords: Degradation; Phenol; Nano-TiO₂; XRD; SEM.

INTRODUCTION

Phenol is a toxic, persistent compound that is difficult to degrade.^(1,2) Degradation of organics using TiO₂/Ce systems has been widely reported in the literature.⁽³⁾ They are in great demand, economical and most importantly environmentally friendly.^(4,5) Currently, research on wastewater treatment is of great importance worldwide.⁽⁶⁾ Therefore, it is important to develop efficient, economical and environmentally friendly methods to ensure that wastewater is discharged to the receiving environment at phenol concentration values that meet regulatory standards. Wastewater treatment technologies for phenol are based on either separation or destruction. Well-known separation methods include steam distillation, extraction, adsorption, membrane pervaporation and membrane solvent extraction, while destructive methods include electrochemical oxidation, photocatalytic oxidation, chemical oxidation and biochemical reduction. Many studies have been conducted on these methods. Since nanotechnology is currently one of the rapidly developing fields, nanoparticle-based cleaning methods for various purposes are important. It is worth mentioning that recently Fe+H₂O₂ systems have been used for the purification of phenol from wastewater.⁽⁷⁾ In this context, studies based on TiO₂ are still relevant today. Many photochemical processes occur in the presence of TiO₂ nanoparticles.^(8,9,10,11,12,13) In particular, many photochemical reactions have been carried out using TiO₂ in the form of anatase and mixed composites for the removal of toxic substances from the aquatic environment: for example, photocatalytic oxidation or mineralization of phenol in the presence of Degussa P25-TiO₂ suspension (80 % anatase and 20 % rutile phase). There is considerable information in the literature about the deposition of precious metals such as silver, gold and platinum on the TiO₂ surface. Heterogeneous photocatalysis is a portable oxidative process. On the basis of this process, large-scale degradation of pollutants in air and water also takes place.⁽¹⁴⁾ In addition, many alloy systems and modifications are being developed to enable

photochemical reactions of TiO_2 in the visible region. Non-metallic TiO_2 systems are of great interest: especially alloyed with nitrogen and carbon. It has been theoretically described⁽¹⁵⁾ that the photocatalytic properties of TiO_2 can be enhanced from the UV region to the visible region of the spectrum due to doping with carbon and nitrogen atoms. In the literature, systems doped with nitrogen atoms are very common and thus air purification is realized.⁽¹⁶⁾

METHOD

TiO_2 nanoparticles were synthesized by sol-gel method and obtained by hydrolysis of titanium (IV) isopropoxide. In the TiO_2 +phenol (Ph) (1) system, the process was carried out only in the UV region, while in the TiO_2 +nitrogen+phenol (Ph) (2) process in nitrogen-containing medium, the process was carried out in the UV and visible region. For system (1), 0,05 g of TiO_2 was taken and evenly distributed in 10 ml of water. Then 5 ml of the mixture was added to 20 ml of phenol solution with a concentration of 1 mg/l.

For system (2), 0,05 g of TiO_2 was taken and evenly distributed in 10 ml of water. Then, 5 ml of the resulting mixture was added to 20 ml of phenol solution with a concentration of 1 mg/l followed by the addition of 0,05 g of nitrogenous compound. The mixture was subjected to photochemical decomposition for 60 min. The degradation of phenol was 60 %. All quantitative analyses were performed on a high precision Agilent 6890N/5975 instrument. After photolysis, the wavelength dependence of the absorption coefficient of the solution was measured on a Varian Cary 50 UV spectrophotometer. It was found that the photochemical process extends from the UV region to the visible region, although the degradation of phenol in system (2) occurs with a lower efficiency compared to system (1). Methyl 3-aminocrotonate ($\text{CH}_3\text{C}(\text{NH}_2)=\text{CHCOOCH}_3$) was taken as the nitrogen-containing component for the reaction.

The purity and crystalline properties of TiO_2 nanoparticles were investigated by powder X-ray diffraction (XRD).

RESULTS AND DISCUSSION

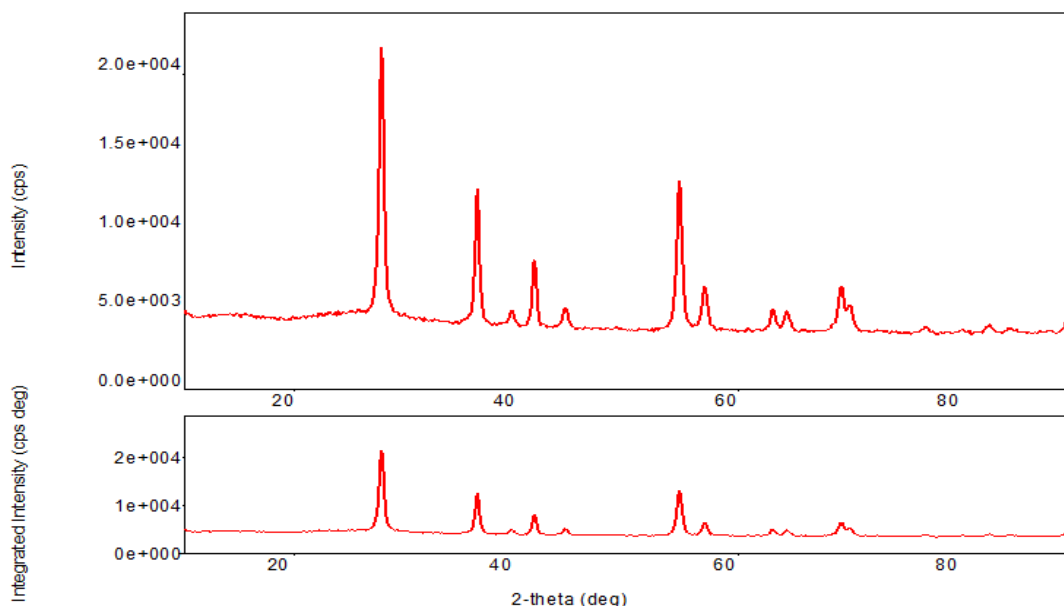


Figure 1. X-ray diffraction patterns of rutile phase TiO_2 nanoparticles

Figure 1 shows the X-ray diffraction patterns of the synthesized TiO_2 nanoparticles. The peaks are well defined and correspond to TiO_2 in the rutile phase. X-ray diffraction analysis plots of the investigated nanocomposite materials were recorded on a Rigaku Mini Flex 600 powder diffractometer. Their properties are given below: a copper anode X-ray tube (Cu-K α radiation, 30 kV and mA) was used to generate diffraction spectra at room temperature. These spectra were acquired at $2\theta = 20^\circ$ - 80° in discrete increment mode with $\Delta 2\theta = 0,05^\circ$ and exposure time $\tau = 5$ seconds (figure 1).

According to SEM analysis of TiO_2 , the size of the nanoparticles was 10-32 nm. Figure 2 shows SEM photographs of the synthesized TiO_2 nanoparticles.

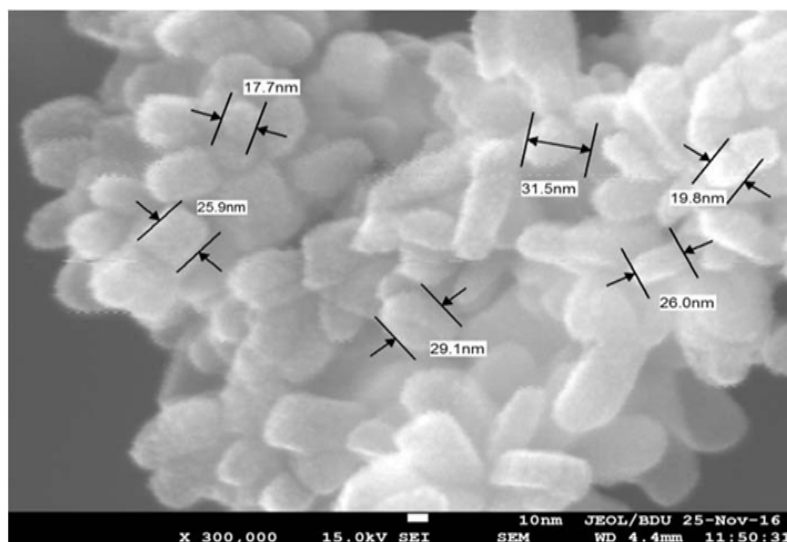
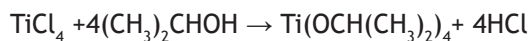


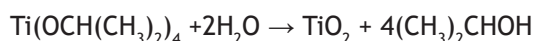
Figure 2. SEM analysis of rutile phase TiO_2 nanoparticles

TiO_2 nanoparticles used in the experiments were obtained by sol-gel method. The reaction proceeded with the formation of TiO_2 layers and a suspension solution was obtained. However, there are other ways to obtain TiO_2 ; for example, TiO_2 has also been obtained from white liquid isopropoxide- $\text{Ti}(\text{OCH}(\text{CH}_3)_2)_4$ under mild laboratory conditions. The general formula is $\text{C}_{12}\text{H}_{28}\text{O}_4\text{Ti}$.

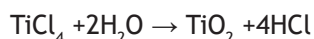
It is prepared by reaction of tetrachloride with isopropanol:



TiO_2 was obtained by reacting the resulting compound with water.

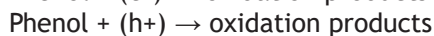
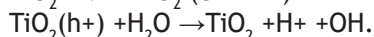


Since TiCl_4 is very soluble in water, TiO_2 was obtained from it and the reaction proceeded as follows:



This method is easy to use, but is not often used in the laboratory because TiCl_4 is toxic.

Therefore, organotitanium compounds are more often used to obtain small TiO_2 layers. It is believed that the oxidation of phenol under the influence of UV radiation in a medium containing TiO_2 nanoparticles occurs as follows:



In general, these types of photochemical processes are carried out in four stages:

1. Photolytic excitation.
2. Activation and displacement of oh groups.
3. Molecular displacement.
4. Fragmentation of the molecule.

The degradation process of phenol in the presence of UV radiation in the $\text{Ph}+\text{TiO}_2$ system is shown below (figure 3).

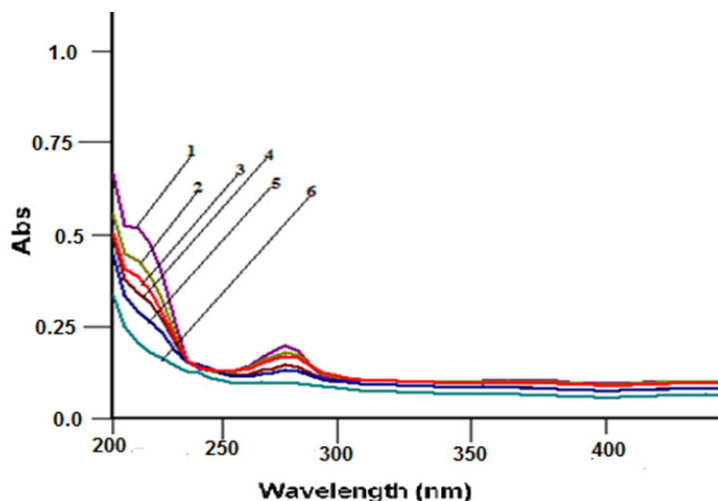


Figure 3. Photochemical decomposition of TiO_2 +phenol in the presence of UV radiation

Comparison of UV radiation curves obtained during photolysis for TiO_2 +phenol system: curve 1 - 10 min photolysis; curve 2 - 20 min photolysis; curve 3 - 30 min photolysis; curve 4 - 40 min photolysis; curve 5 - 50 min photolysis; curve 6 - 60 min photolysis.

As shown in figure 3, for the 1 mg/L phenol + TiO_2 system, the characteristic wavelengths of phenol (270 nm) are not observed in the last curve (curve 6) in contrast to the other curves. This is due to the absence or insufficient amount of phenol in the solution after photolysis. The sample was then analyzed in a gas chromatography mass detector for more sensitive and accurate analysis. The amount of phenol decreased from 1 mg to 10 μg . This means that 99 % of phenol is degraded.⁽¹⁷⁾

It can be noted that TiO_2 nanoparticles have very good photodissociation in combination with nitrogen atom. The point is that we considered it more convenient to use only the property of TiO_2 nanoparticles to be excited by ultraviolet radiation. Only 5 % of the nanoparticles are excited in

the visible region. In the system where the reaction extends from the UV radiation range to 400-600 nm in the visible region, a photochemical reaction in the phenol + TiO_2 + nitrogen compound (Ph + TiO_2/N) was considered (figure 4). Photolysis in the phenol + TiO_2/N system was carried out in the UV region; the wavelength dependence of the absorption coefficient was determined on a Varian Cary 50 instrument. Then, the concentration of phenol remaining in solution after the photochemical reaction was determined.

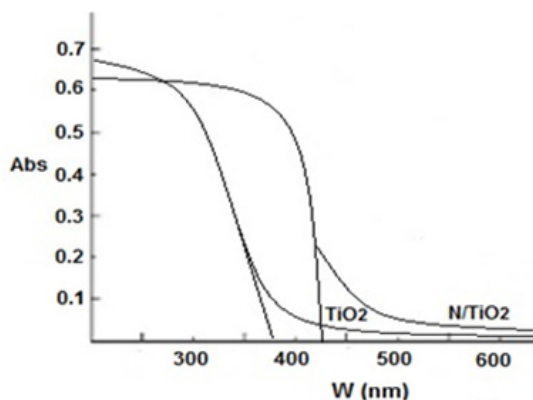


Figure 4. Wavelength dependence of absorption coefficient for phenol + TiO_2/N system For phenol + TiO_2/N system

Comparison of UV radiation curves obtained during photolysis for TiO_2 +phenol and TiO_2/N +phenol systems:

1. Photolysis curve for TiO_2 +phenol system.
2. Photolysis curve for TiO_2/N +phenol system.

As can be seen from figure 4, the photochemical decomposition of phenol in the presence of TiO_2 nanoparticles occurred in the UV region, i.e., in the region up to 400 nm (1). However, in the presence of N and TiO_2 , the process extended from the UV region to the visible region between 400 and 600 nm (2).

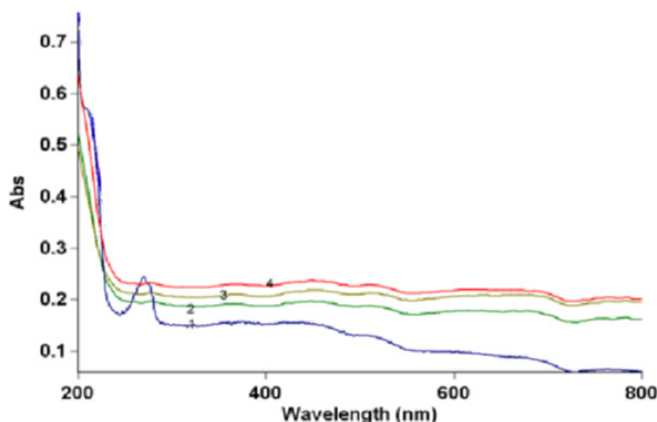


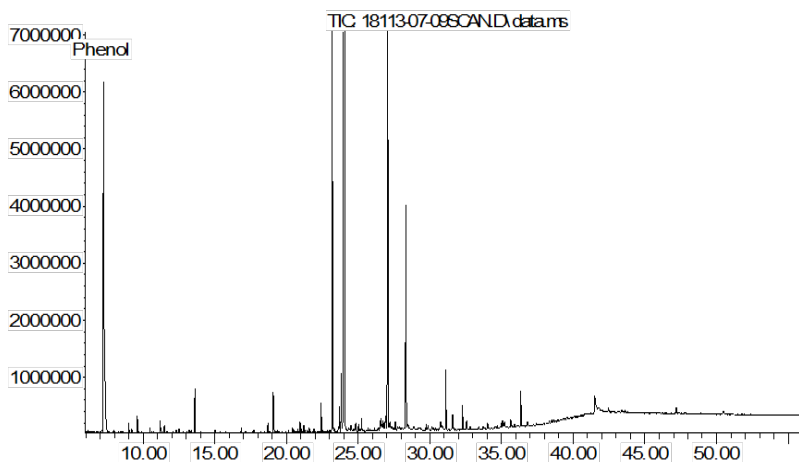
Figure 5. Photolysis for phenol+N/ TiO_2 system

1. Curve 1 - obtained before photolysis.

2. Curve 2 - obtained at 45 minutes of photolysis.
3. Curve 3 - obtained at 55 minutes of photolysis.
4. Curve 4 - obtained at 60 minutes of photolysis.

The light absorption for the phenol+TiO₂ system (1) is intense in the UV irradiation region up to 400 nm, while the light absorption of the phenol+N/TiO₂ system (2,3,4) covers the region after 400 nm. The transition from the UV region to the visible region occurs in the presence of N-containing material.

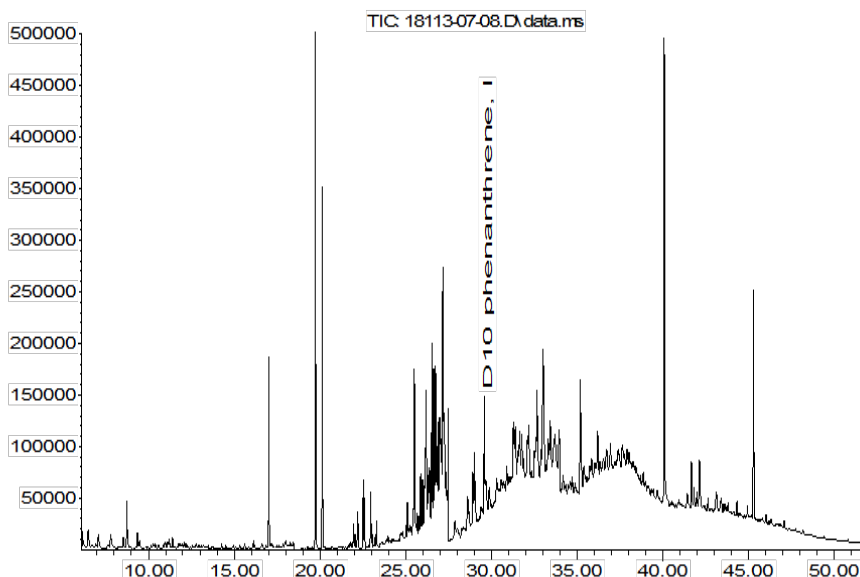
Abundance



Time-->

Figure 6. GC-MSD analysis of phenol+TiO₂ solution after photochemical decomposition

Abundance



Time-->

Figure 7. GC-MSD analysis of phenol+N/TiO₂ solution after photochemical decomposition

The adsorption process of phenol by TiO_2 nanoparticles was also studied. The process continued for 2 hours at room temperature. Long after the start of the process in the phenol+nano TiO_2 mixture: characteristic peaks of phenol (270 nm) were observed in the curves of 30, 60, 90 and 120 minutes, indicating that adsorption does not occur in the presence of these nanoparticles.

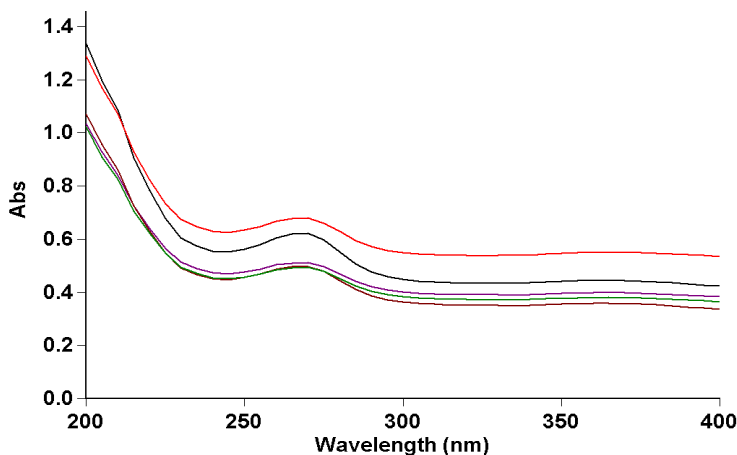


Figure 8. Comparison of curves obtained for phenol adsorption in the presence of TiO_2

Figure 8 shows the comparison of the curves obtained during the adsorption process (every 25 min). At this time, swelling was observed at the wavelength corresponding to phenol (240-270 nm) along the horizontal line.

CONCLUSIONS

1. This paper discusses the degradation of phenol in Ph+ TiO_2 (1) and Ph+N/ TiO_2 (2) systems.
2. In system (1), 99 % of degradation of phenol occurred under UV influence, whereas in the Ph+N/ TiO_2 system (2), 60 % of degradation of phenol occurred.
3. The purpose of using a nitrogenous agent was to carry out a photochemical reaction in the visible and UV radiation region in the presence of TiO_2 nanoparticles. This increases the practical importance of the process.
4. The sizes of TiO_2 nanoparticles used ranged from 10 to 32 nm.
5. The degradation of 1 mg/l phenol was carried out in 1 hour. At the same time, the influence of the pH of the medium on the course of the reaction was determined. The process was monitored on a Varian Cary 50 spectrophotometer.
6. XRF and SEM analyses of TiO_2 nanoparticles were performed.
7. Quantitative analyses were performed using an Agilent 6980N/5975 GC-MSD.
8. The adsorption process of phenol by TiO_2 nanoparticles was studied.

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CONFLICT OF INTEREST

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Part II

Oil, Gas, and Industrial

Environmental Challenges



Chapter 05

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Environmental problems arising from oil extraction

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ABSTRACT

The increase in air pollution and wastewater problems has recently been considered one of the serious factors in the pollution of the water ecosystem and the environment. These factors are related to anthropogenic factors rather than natural factors. In this regard, it is important to study the issue of wastewater and air pollution. In general, people's attitude towards waste, combating waste and treating it correctly, waste technology, general knowledge about waste and such educational information has been increasing recently. It is very significant to educate people in this direction. It is known that industrial wastewater contains a sufficient amount of oil products. Since Azerbaijan is an oil country, industrial wastewater collected in the technological facilities and commodity parks of the Oil Refinery is necessarily subjected to mechanical treatment. These waters are then fed into chemical and biological treatment plants. Finally, industrial wastewater is treated in biological treatment plants (50 thousand m³/day). Treatment is carried out in several stages. Thus, wastewater is fed into the first and second stage aeration tanks. Here, wastewater is treated close to the established standards and is subjected to biological treatment. Oil extraction on land and at sea leads to additional environmental problems. In particular, the ecosystem of the Caspian Sea is severely damaged: its flora and fauna are seriously polluted. For this purpose, the analysis composition was determined based on the extraction of crude oil from the largest oil fields, 28 May and Oil Rocks (Neft Dashlari).

Keywords: 28 May; Oil Rocks; Ecosystem; Waste Issue; Environment; Petrochemical Industry.

INTRODUCTION

As mentioned, during the operation of the chemical and petrochemical industries, quite a variety of gases enter the air. At this time, hydrocarbon mixtures of various compositions – C_xH_y , and then CO_2 , N_xO_y , SO_2 , etc., are released into the air, which causes serious problems.^(1,2) The gases released from the process are fed to an incinerator for combustion at a temperature of 800-850°C, and then (after combustion) the gases are discharged into the atmosphere through a smokestack at a temperature of 280°C.⁽³⁾ As a result of the processes that occur, not only the water layer but also the air layer is polluted. Oil products form an emulsion with water (oil sludge), seriously polluting water bodies. Phenolic compounds remaining in wastewater are a real source of danger for the living layer of the aquatic ecosystem. As a result, industrial wastewater generally creates serious problems in the environment.⁽⁴⁾ During the generation, storage, and processing of oil sludge, harmful substances are released into the atmosphere, and deep purification of industrial wastewater becomes difficult. Such waters cause serious environmental issues in all ecosystems: the atmosphere, hydrosphere, and lithosphere.

Due to the corrosion of steel technological equipment in the oil and gas and oil refining

industries, serious fires and explosions occur, which pollute the air, water, and soil ecosystems in those areas. It is precisely because of these environmental problems that the emergence of dangerous problems in oil and gas, oil refining, and petrochemical industries has been prevented as a result of the commissioning of new technological facilities over the past 50 years. In some cases, such issues cannot be avoided. In our modern era, important measures are constantly being taken to ensure safety in these industries in accordance with known environmental standards. In addition, measures are also being taken in the main directions of scientific and technical development to prevent processes that cause air pollution in oil production and oil refining enterprises. Improving and implementing automation is very important for conducting such processes and organizing environmental control.

Automatic control, which plays an important role in production management, environmental control, implementation of technological processes and preparation of economic reports, is currently gaining wide popularity. In such systems, the following requirements are mainly implemented:

1. Automation of technological operations in the process.
2. Regulation of energy carriers.
3. Automation of control over the release of harmful substances into the environment.
4. Automatic elimination of emergency situations.
5. Providing emergency warning in the event of a fire in production, as well as in the event of a dangerous or stressful situation.
6. Ensuring that technological equipment meets environmental and technical standards.

In our modern era, in connection with the development of scientific and technical progress, there are six main functions of automatic production control:

1. Regulation and regulation of processes.
2. Transmission and delivery of information.
3. Full organization of the protection system.
4. Regulation and improvement of the parameters of all technological processes.
5. Optimization of flexible modes, if necessary.
6. Organization of a system for obtaining and managing information that fully meets the production characteristics of the oil refining industry and meets the requirements.

The use of automation systems in the oil production and refining process, as well as the implementation of new facilities in accordance with modern technologies and, above all, the selection of environmentally optimal options, leads to a several-fold reduction in environmental problems arising in the oil refining process.

METHOD

The physical and chemical parameters of crude oil were carried out in the central laboratory of the Oil Refinery named H.Aliyev. Part of the analyses were carried out in the Caspian Ecological Laboratory. So compositional analysis of crude oils taken from 28 May and Oil Rocks was carried out on an Agilent 6890N GC-MSD gas chromatograph device.

RESULTS AND DISCUSSION

Recently, the oil refining industry has been highly valued economically in the world. During the extraction of oil as a raw material, gaseous hydrocarbons, in some cases hydrogen sulfide, SO₂ and other gases, as well as produced water are produced along with it. Mechanical impurities

contained in the oil: sand, clay, soil, salts, and then oily waters in the form of emulsions are also formed in the process. The produced water formed during the extraction of oil, as well as the presence of emulsions and mechanical impurities in the oil, cause environmental problems.

The process of cleaning oil from water is not easy. The cleaning process is complicated due to the fact that oil forms an emulsion with water. Despite the use of various adsorbents for this purpose, complete cleaning is not possible. There is a sufficient amount of scientific work on cleaning oil layers from water using industrially important adsorbents. We have also studied the sorption of oil collected on the water surface using bio-absorbents - oils of natural origin in laboratory conditions.⁽⁵⁾ However, the treatment of high-tonnage industrial wastewater by sorption is not efficient in terms of time and economic aspects.

During the purification of oil from water and mechanical impurities, the amount of oil in industrial wastewater containing a large amount of oil products is 1000-1500 mg/l. This leads to the formation of highly emulsified mixtures in the wastewater obtained during the initial purification of oil. Their separation and purification from water become major environmental problems.

When oil and oil products are cleaned of mechanical impurities, a large amount of impurities settles and accumulates at the bottom of oil storage tanks. Also, during the purification of oil from water, oil-sludge waste contained in industrial wastewater accumulates in the sewage system, at the bottom of treatment facilities and tanks. These substances are classified as class III hazardous substances. Since industrial waste is a third type of pollutant, it is considered moderately hazardous, but it is a source of serious danger to the living world.

Oil-sludge mixture is one of the main causes of environmental problems during the storage, purification, and transportation of oil as raw material. Thus, during the cleaning, storage, and processing of oil-sludge waste, a large amount of harmful substances are released into the atmosphere. At the same time, they become sources that create conditions for the pollution of water bodies and soil. Also, during the production of oil, its purification from water and mechanical impurities is carried out using special devices. A large amount of various hydrocarbons enters the atmosphere from the tanks where oil is stored during the day. Therefore, the use of special devices, furnaces, tanks, and separator devices for separation from gas is one of the main conditions during the production, storage, and purification processes of oil.

During the primary processing, extraction, purification, storage, and transportation of oil, harmful substances are continuously released into the environment. The release of gaseous substances C_xH_y (C_1-C_4) and liquid petroleum hydrocarbons into the atmosphere causes pollution of the air, water, and soil environment and the emergence of ecological problems. In particular, the problem of pollution of aquatic ecosystems occurs, the cleaning of which takes a long time.⁽⁶⁾

Even when the industrial wastewater obtained during the production, refining, and storage of oil is treated at the required level: in accordance with environmental standards, many harmful substances are contained in the water. The air is polluted when petroleum hydrocarbons, other organic compounds, hydrogen sulfide (H_2S) and substances harmful to the air layer are released into the atmosphere. In addition, water bodies are polluted as a result of the incomplete deep cleaning of other harmful substances contained in the water - oil emulsions, phenol and its derivatives, small-sized mechanical mixtures, oil sludge and other substances.

When oil and oil products prepared as commodity raw materials are loaded onto railway

platforms, seaports, and special ships, petroleum hydrocarbons evaporate and pollute the atmosphere. In many cases, during the transportation of oil and oil products under high pressure, large-diameter steel pipelines fail due to corrosion, which leads to long-term environmental problems as a result of their leakage into the soil and spillage into water bodies. Depending on the composition and properties of the soil, pollution occurs at depths of tens of meters. This, in turn, penetrates the upper and deeper layers of the soil, along with groundwater and surface rainwater, depending on the relief, causing its pollution. As a result, excessive damage and toxic effects occur to living organisms in water bodies and soil. These situations lead to the emergence of ecological issues, and the cleaning of ecosystems requires a long time. Classical methods are usually used for cleaning. Also, as a result of accidents during the transportation of oil products by water transport, railways, pipelines and special tankers, pollution of water bodies, soil and air occurs, and ecological problems arise from time to time.

As a result of the conducted research, it was determined that 5-10 % of harmful substances released into the atmosphere in tanks where oil is stored as raw material occur at oil filling platforms. For the shipment of oil products as export commodities in tanks by water, by rail and by auto-sterns, a large amount of volatile hydrocarbons enter the atmosphere at filling points. That is why, in the oil and oil refining industry, one of the main conditions is that the technological temperature is normal when filling raw materials and oil products from tanks to platforms. Since filling raw materials and oil products at very high temperatures is environmentally dangerous, it is normalized to carry out it at low temperatures. In addition, since it is very difficult to reduce the viscosity of products that require special heating, that is, transport at temperatures close to freezing point, additional heating is required when filling these oil products or high-paraffin oils. Only after this, their filling is carried out on platforms. Also, due to changes in meteorological conditions, the operating mode of production in oil product filling areas is changed. This is mainly applied in these areas to prevent the additional release of harmful substances and gaseous hydrocarbons into the atmosphere, that is, the creation of additional environmental problems. Regardless of the type, oil-contaminated waste is generated during the cleaning of areas contaminated with these products at oil and oil product filling points. Waste is usually in liquid form. After purification, waste mixtures of oil and oil products are returned to production. At this time, pollution of water, air, and soil is undeniable. That is why, as in other production areas, there should be an acceptable concentration limit (ACL) for harmful substances emitted into the air from filling platforms where oil and oil products are stored and transported as export commodities. For this, a regulatory and ecological technical document is being prepared. Reducing environmental issues during the primary and subsequent oil refining processes mainly depends on the improvement of technological equipment and processes. In the oil industry, the use of liquid fuels, which are the main energy carriers: fuel oil, solar oil, and natural gas, is important, as well as the organization of the efficient use of electricity.

Over the past 30-40 years, as in developed countries of the world, the volume of industrial wastewater of various compositions in oil production and petrochemical production areas has been reduced by millions of cubic meters per year and its discharge into the sea has been prevented, based on the operation of new technological facilities and the implementation of reconstruction and installation works in the oil industry of the Republic of Azerbaijan, as well as in the fields of oil production and petrochemical production. The amount of carbon and sulfur gases and nitrogen-containing compounds emitted into the atmosphere has been reduced tenfold. The processing of liquid and solid wastes, alkaline wastes, oil sludge, and the purification and neutralization of wastes of used slag (synthetic fertilizers made from oil waste) received in the oil and oil refining industry have been carried out.⁽⁷⁾

It is estimated that the productivity of vacuum distillate is two million tons/year. The following products are obtained during the processing of vacuum distillate according to the adopted technology:

- Obtaining high-octane components for gasoline fuel.
- Obtaining a catalytic cracking fraction purified with hydrogen (at 195-3500C).
- Obtaining a high-boiling fraction of the coking unit (above 4200C).
- Obtaining dry gas.

During the implementation of the mentioned technological processes, environmental problems arise depending on the course of the reactions. During the distillation of oil, depending on the boiling point, the oil is separated into fractions, and the oil refining products consist of the following:

- Liquid and gaseous fuels.
- Solvents.
- Lubricating oils.
- Solid and semi-solid mixtures of hydrocarbons (paraffin, petroleum jelly, etc.).
- Naphthenic or petroleum acids, their derivatives (sulfonic acids, fatty acids).
- Various hydrocarbons (ethylene, propylene, benzene, toluene).

Before being refined, oil undergoes a preparation stage. The preparation process ends with the separation and dehydration of gases. Gas separation occurs by reducing the pressure and oil movement speed in the devices. At this time, gases are separated from the oil by desorption. Dehydration is carried out through long-term clarification. Fuel oil is considered an important raw material during the process. It plays the role of raw material in boiler fuels and recycling processes. Gas oil, oil fraction and tar are obtained from the vacuum distillation of fuel oil. The oil fraction serves as a raw material for obtaining lubricating oils, coke, and bitumen. The tar remaining on the ground is used in the production of asphalt mixtures and bitumen production. The distillation process takes place in two main stages:

1. Heating to a high temperature (boiling).
2. Separation of the products from each other.

The main equipment for heating is furnaces used to heat raw materials and intermediate products, as well as various heat exchangers. The separation of products by distillation of oil is carried out in rectification columns. At temperatures above 4500C, destructive changes occur in hydrocarbon molecules. Hydrocarbons with a large molecular mass are broken down into molecules with a smaller mass. This process is called cracking. During cracking, the following processes occur:

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The main equipment for heating is furnaces used to heat raw materials and intermediate

products, as well as various heat exchangers. The separation of products by distillation of oil is carried out in rectification columns. At temperatures above 450°C, destructive changes occur in hydrocarbon molecules. Hydrocarbons with a large molecular mass are broken down into molecules with a smaller mass. This process is called cracking. During cracking, the following processes occur:

1. Decompositions involving the cleavage of the C-C bond.
2. Dehydrogenation processes involving the cleavage of the C-H bond.
3. Isomerization processes.
4. Polymerization, cyclization, and other reactions.

The first two types of reactions are endothermic. The subsequent reactions are exothermic, and the starting materials for them are the products of the first two reactions. The decomposition of paraffin hydrocarbons occurs by a radical mechanism. The mechanism of their decomposition is determined by the bond energy between the carbon and hydrogen atoms in the primary hydrocarbons. Based on the bond energies, it can be noted that paraffin hydrocarbons are less thermally stable. These substances decompose at temperatures above 425-450°C, and the reactions under consideration occur by a chain mechanism.

Naphthenic hydrocarbons are more stable than paraffinic hydrocarbons. Therefore, they are destroyed at higher temperatures and dehydrogenated at temperatures above 500°C to form aromatic hydrocarbons. The unsaturated hydrocarbons formed during the initial reactions have a higher reactivity and easily undergo various transformations. The final product of the decomposition consists of low molecular weight saturated and unsaturated hydrocarbons. Naphthenic acids give crude oil its acidity. This quantity is measured in milligrams (mg) of potassium hydroxide required to neutralize one gram of oil. The acidity of crude oil is neutralized by adding NaOH.

Phenol and its compounds are observed in water only as a result of industrial effluents. The toxicity of phenol is due to the formation of stable chlorine-containing phenols during chlorination. These substances give water a special taste. Phenol and its compounds are found in high quantities in the spent solution after alkaline cleaning of oil. Since phenol is highly soluble in water, its purification is also very difficult. Therefore, it is more expedient to carry out the decomposition of phenol biologically. The speed and completeness of the process depends on the composition of the wastewater. When processing technological water containing 2,5 g/l of phenol, 95 % of phenol can be removed.

As we know, hydrocarbons constitute the main part of gas emissions in terms of quantity. The main method for cleaning gas emissions from organic substances is the combustion of the mixture at a temperature of 800-1000°C. The disadvantage of this method is associated with a large amount of fuel consumption and high material cost, which is economically disadvantageous. Recently, catalytic cleaning methods carried out at lower temperatures (600-700°C) have become widespread. These methods are based on the oxidation or reduction of organic substances in the gas mixture in the presence of a catalyst (e.g., platinum (Pt)). In this case, the catalysts should not be poisoned by sulfur compounds. These requirements are met by platinum catalysts, which accelerate various transformation reactions of organic substances in oxidizing and reducing environments. Therefore, platinum (Pt) is widely used. However, Pt is a very valuable metal. In this regard, other metal and non-metal oxides (Ni, Cu, Cr, Mn), which are cheaper than platinum metal, are also used.

A large amount of wastewater with various compositions is generated from the catalytic cracking process at the H. Aliyev Oil Refinery.^(8,9,10) The oil desalination unit provides its distillation. During the oil refining process, 0,3-0,5 % water containing 150-300 mg/l of salt enters the plants, the norm is 20-40 mg-eq/l of salt and 0,1-0,2 %. Therefore, before oil is refined, water and inorganic substances (salts) contained in it must be removed. In the desalination process, the oil is initially washed with soft water, as a result of which the salt content in the oil decreases from 300 to 10-20 mg/l, and the water content from 0,4 to 0,15-0,2 %. The wastewater is black due to the presence of colloidal particles and corrosion products. The volume of water used for desalination is 5-6 % of the total volume of refined oil.

Environmental problems also arise during the catalytic reforming process. Many reactions take place during this process:

- Conversion of olefins to alkanes.
- Desulfurization.
- Oxygen removal.
- Denitration-nitrogen removal.
- Separation of halogenated compounds.
- Metal separation.

Methods of neutralizing waste generated as a result of the processes taking place in the plant are one of the most important environmental issues. Light-colored gasoline, kerosene and diesel fractions (distillates) obtained during the primary processing of oil are subsequently subjected to many technological processes. When the gasoline fraction is obtained in the technological plant, it is passed through a NaOH solution. This method removes RSH, HCl, SO₂, H₂S, etc. substances from the gasoline composition, while free hydrogen sulfide and other harmful gases in its composition react with NaOH and turn into salts of NaCl, Na₂S, Na₂SO₃, etc. The salts obtained are generally discharged into the sewage system, where industrial wastewater is discharged. Na₂S is considered one of the most harmful substances in the composition of these salts. The salts formed in the production wastewater obtained during the initial cleaning and washing of the gasoline fraction from the alkaline solution are constantly discharged into water bodies, causing pollution with harmful Na₂S salt, which has a negative ecological impact on the fauna and flora of water bodies. Finally, the gasoline fraction undergoes technological processes to increase the octane number in accordance with the required standards and prepare a commodity product.

Since the late 1960s, alkaline wastes obtained as a result of production processes have been treated with sulfuric acid, during which naphthenic acids are obtained.



The obtained naphthenic acids are separated into fractions. These acids are used in the preparation of additives of particular importance in the petrochemical industry and other important chemical preparations for the national economy. During the purification of kerosene and diesel fractions with alkaline solutions, the organic compounds contained in these fractions are released into the atmosphere. At the same time, during technological processes, large volumes of oil waste and mixtures in the form of emulsions are obtained. As a result, environmental problems arise in the process of purification of industrial wastewater, which cause pollution of other water bodies.⁽¹¹⁾

Thus, during the technological processes carried out to obtain commodity products of

gasoline, kerosene and diesel fuels, in addition to the organic and other inorganic compounds contained in those fractions, during the combustion of fuels in technological processes, a large amount of C_xH_y , CO_2 , N_xO_y , H_2S , sulfur gases and other harmful compounds are also released into the atmosphere, these gases directly and indirectly participate in the greenhouse effect.⁽¹²⁾

Naphthenic acids account for 60-70 % of industrial waste. They contain phenolic compounds, RSH , H_2S , polycyclic aromatic hydrocarbons, Zn , Cd and other heavy metals. These compounds also cause serious problems from an ecological point of view.

In the oil refining industry, lubricating oils are obtained from fuel oil. The fuel oil fraction obtained from the primary processing of oil is heated again in technological furnaces and distilled in vacuum columns, and finally lubricating oils are obtained. Based on lubricating oils, primary oil distillates are subjected to technological operations and various branded commercial products are prepared. The fuel oil obtained in AVT units is distilled again in vacuum. In Azerbaijan, the production of various oil distillates by distillation of fuel oil in vacuum is carried out in special units. This process, in turn, causes extreme environmental problems. During these technological processes, a barometer-condenser system is used to create a vacuum in the columns. This requires a large amount of seawater. At this time, emulsion production wastewater containing a significant amount of a mixture of petroleum products is obtained. The purification of these waters is extremely difficult, and although some of these purified industrial wastewaters are reused in systems, they cause pollution of water sources and the air environment. One of the main reasons for the emergence of environmental problems during the production of oils in AVT facilities is the use of large amounts of liquid fuel oil in technological furnaces. During the combustion of fuel oil, harmful gases of various organic and inorganic origin are released into the atmosphere. These gases are of particular importance in the formation of greenhouse gases.

In AVT units, the fuel oil fraction is vacuum distilled. At this time, various brands of oil distillates are obtained - light, medium and heavy oil distillates. For the preparation of these oils as a full-fledged commodity product, the acid-alkali method, contact method and hydrogenation of oils are used. As a result, petroleum oils of various properties and qualities are obtained. Various wastes are obtained in the process, for example; acid tar, mineral oils. Acid tar is dark black, has a soft, sharp smell similar to sulfuric acid. Mineral oils contain toxic heavy metals and mainly polycyclic aromatic hydrocarbons.

Thus, the neutralization of industrial wastes such as acid tar and “processed gum,” which are formed during the aforementioned technological processes and cause significant environmental pollution, is carried out.⁽¹³⁾ Since 1970, the production of petroleum oils has been carried out. For this, the organic compounds contained in oil distillates and which negatively affect the quality of oils are cleaned, which also causes environmental problems.⁽¹⁴⁾

Since the early 1980s, the use of new technological facilities has prevented the discharge of acidic production waters obtained during the production of petroleum oils into the Caspian Sea. The amount of harmful substances emitted into the atmosphere has also been reduced by thousands of tons.

Currently, the process of hydrogen purification of oils is being carried out. In these facilities, mainly many petroleum oils are passed through technological furnaces and, using special reactor devices, catalysts and a hydrogen gas flow, the harmful substances contained in the oils, mainly sulfur compounds, are cleaned. The quality of the oils is brought to the required level. Certain

environmental problems also arise in these facilities. Thus, the formation of waste gases, mainly hydrogen sulfide, from the separation of harmful substances contained in oil distillates during the technological process leads to negative impacts on the environment.

In order to minimize environmental problems, waste gases are captured with ethanolamine in special devices, which prevents the direct release of hydrogen sulfide and other inorganic compounds into the air. Finally, these gas mixtures are burned in a production flare farm and completely neutralized. Using this method, the release of hydrogen sulfide and other harmful substances into the air during technological processes is prevented.

Since 2000, as a result of the commissioning of the new facility, the amount of both wastewater and gaseous harmful substances obtained during the production process has decreased tenfold compared to the old bitumen production. Due to the high amount of harmful substances obtained during bitumen production and the presence of some of them in the form of aerosols in the air, harmful substances cause pollution of the atmosphere, water, and soil ecosystem. The new bitumen facility is installed in accordance with European standards, and the waste obtained in gaseous form during the operation of the facility is neutralized in special furnaces and released into the atmosphere. Such gases are burned in special technological furnaces at a temperature of 800°C for neutralization. At the same time, gases that cannot be neutralized into the atmosphere are also released into the atmosphere.⁽¹⁵⁾ Based on the studies, the amount of harmful substances released into the atmosphere from the smoke pipe of that furnace was calculated (table 1).

Table 1. Annual TLV limit for harmful substances		
Name of the harmful substance	Amount of harmful substances produced t/year	LVD of the harmful substance in the working area (mg/m ³)
C _x H _y	28,032	300
H ₂ S	0,223	10
SO ₂	30,850	10
CO	17,291	20
NO ₂	0,257	2
NO	2,138	30
Toz	0,285	10
RSH	0109	-
C ₆ H ₅ OH	0,006	0,3

Even today, the bitumen production facility in Azerbaijan, despite meeting the most modern international standards, is one of the sources of environmental pollution. The accumulation of oil sludge (a mixture of oil, sand, clay, and soil) obtained during the treatment of industrial wastewater at the bottom of the treatment facilities and its subsequent treatment causes environmental problems. Thus, serious pollution of the soil and water ecosystem occurs during oil extraction.⁽¹⁶⁾ In particular, during oil extraction on land, soil degradation occurs. Unlike the less dynamic aquatic ecosystem, the soil is a slow-recovering system, requiring hundreds of years to recover. The organisms living in the aquatic ecosystem suffer serious damage. Despite the existence of various methods for wastewater treatment,⁽¹⁷⁾ these situations have serious consequences for flora and fauna, as global treatment is not implemented.

Table 2 shows some physicochemical parameters of crude oil taken from the two areas.

Table 2. Some physicochemical parameters of crude oil taken from different areas					
Types of oil	Chlorinated salts (mg/l)	Sulfur(%)	Tar(%)	Ash(%)	Paraffin(%)
Oil Rocks	39,2	0,21	13,40	0,0126	1,65
28 May	31,7	0,27	12,80	0,0207	1,27

We conducted chemical analysis of crude oil taken from some areas (table 3).^(18,19,20,21,22) Chromatographic analyses were performed to determine which organic hydrocarbons were present in the crude oil (figure 1, figure 2).

Table 3. Analysis of crude oil taken from two locations in the Oil Rocks				
Alkanes	Oil Rocks (I station)		Oil Rocks (II station)	
	Area	Ratio %	Area	Ratio %
nC 10	28518	1,02	27851	0,99
nC 11	27630	0,99	27647	0,98
nC 12	28438	1,02	28369	1,00
nC 13	27575	0,99	26380	0,93
nC 14	21991	0,79	21159	0,75
nC 15	17601	0,63	12477	0,44
nC 16	6091	0,22	5972	0,21
nC 17	5078	0,18	5190	0,18
Pristan	19617	0,70	18677	0,66
nC 18	2705	0,10	2673	0,09
Phytane	15656	0,56	15243	0,54
Total amount of hydrocarbons	2799090	100	2826610	100
Area ratio of isoprenoid hydrocarbons				
17/pristan	0,259		0,278	
18/phytane	0,173		0,175	
Pr/F	1,253		1,225	

Although crude oil is richer in alkanes and naphthenes (C_{10} - C_{18} alkanes), a certain amount of aromatic hydrocarbons is formed as a result of chemical transformations in the oil.^(22,23,24,25,26) Therefore, various processes in the Oil Refinery (OR) cause serious pollution of the environment: air and water.

Car engines running on petroleum fractions emit sulfur dioxide into the environment, polluting the atmosphere and thereby increasing greenhouse gases in the air. During the extraction of crude oil, as well as its combustion in chemical processes, some of the substances such as CO_2 , SO_2 , HCl , Cl_2 , H_2S , C_xH_y , NO_x are released into the air in the form of aerosols and spread widely in the air up to 100 km away, which ultimately leads to long-term environmental problems in

water, air and soil ecosystems.

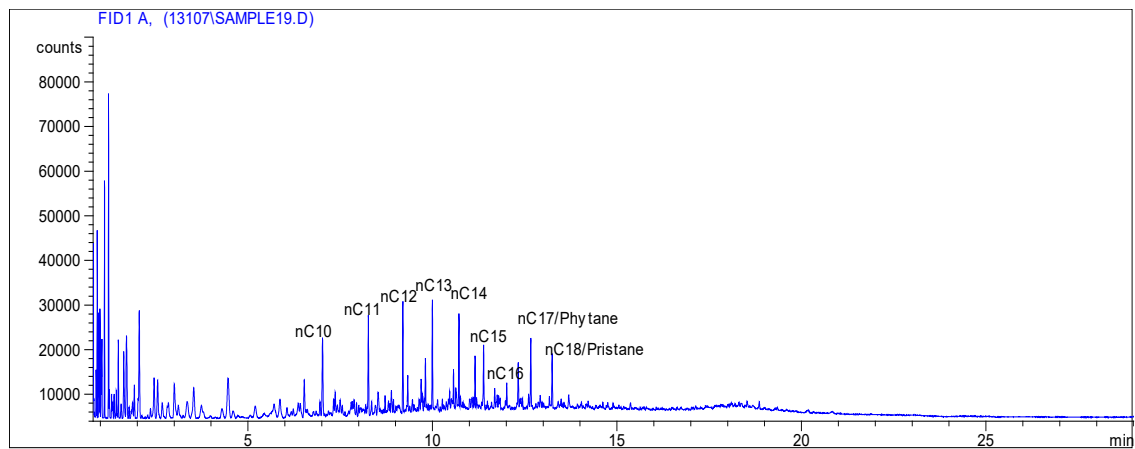


Figure 1. General view of the chromatogram of crude oil taken from Oil Rocks (Station I)

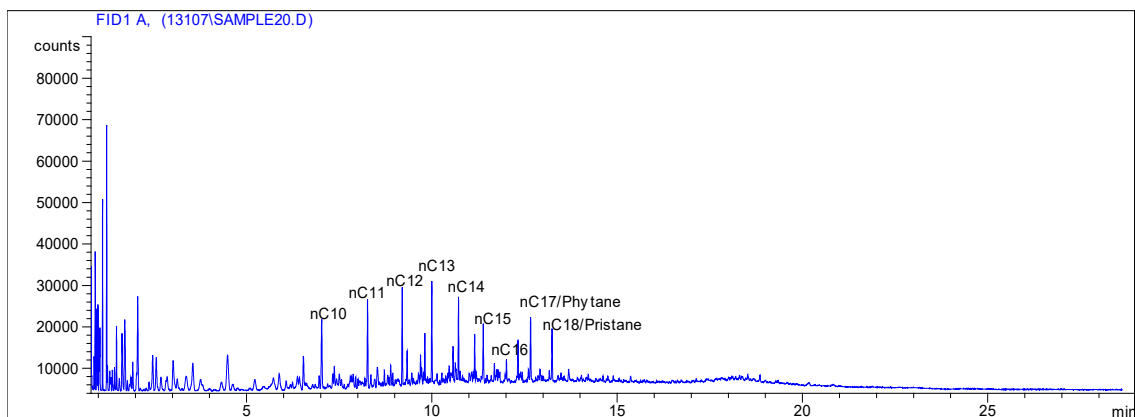


Figure 2. General view of the chromatogram of crude oil taken from Oil Rocks (Station II)

Table 4. Composition of crude oils taken from the 28 May area				
Substances	28 May (I)		28 May (II)	
Alkanes	Area	Ratio %	Area	Ratio %
nC 10	50149	0,92	0,00	0,00
nC 11	48948	0,90	0,00	0,00
nC 12	51185	0,94	9939	0,22
nC 13	49362	0,91	10915	0,25
nC 14	40799	0,75	13746	0,31
nC 15	32639	0,60	19227	0,44
nC 16	10899	0,20	18128	0,41
nC 17	5133	0,09	669	0,02
Pristan	33157	0,61	31041	0,70
nC 18	3848	0,07	678	0,02

Phytane	31326	0,58	22586	0,51
Total amount of hydrocarbons	5430940	100	4417970	100
17/pristan(Pr)	0,259	0,155		0,022
18/phytane(F)	0,173	0,123		0,030
Pr/F	1,253	1,058		1,374

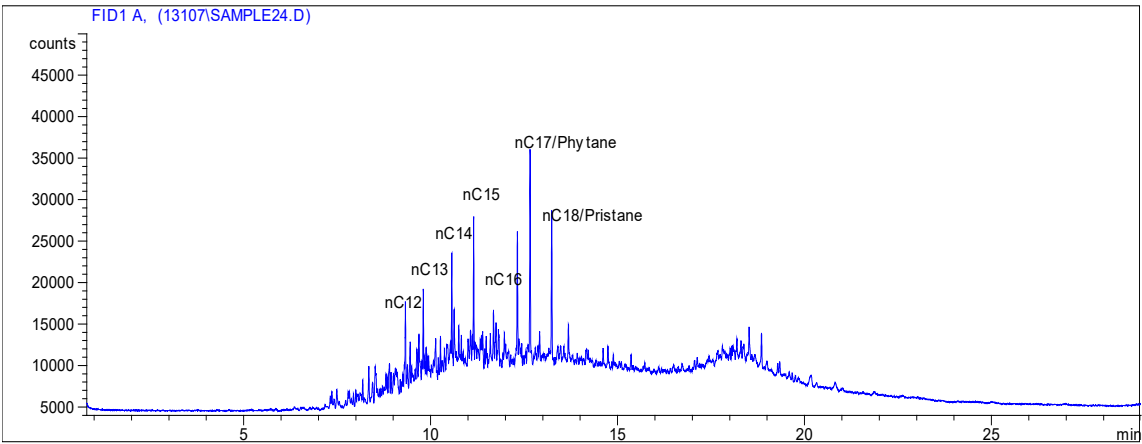


Figure 3. General view of the chromatogram of crude oil taken from the 28 May area (Station I)

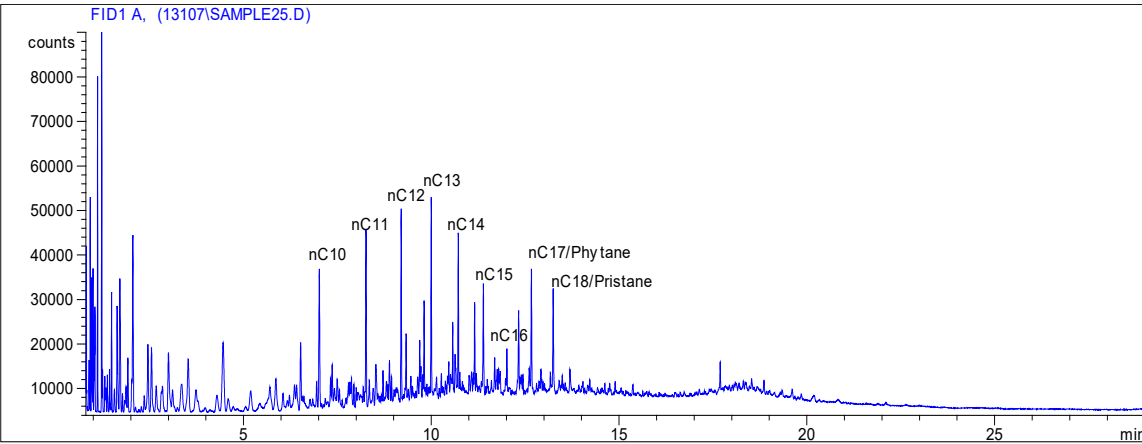


Figure 4. General view of the chromatogram of crude oil taken from the 28 May area (Station II)

CONCLUSIONS

Currently, in connection with the development of industry and technical progress, the problem of pollution of the atmosphere and hydrosphere is one of the global environmental problems. In this regard, based on the conducted research, new perspective directions in solving the problem of environmental pollution have been analyzed. The processes taking place in various areas of the Oil Refinery, production processes taking place in the catalytic cracking area cause pollution of the environment, especially with organic toxic substances - polycyclic aromatic hydrocarbons. Crude oil was taken from certain areas of the Caspian Sea, in our case from Neft Dashlari and 28 May, determined, and its impact on the environment was ecologically assessed.

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CONFLICT OF INTEREST

None.

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Chapter 06

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Evaluation of Artificial Stimulation Methods in the West Absheron Field Based on Hydrodynamic Model

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ABSTRACT

The application of modern approaches to the selection of stimulation methods in fields in the initial stage of development is one of the serious factors affecting the efficiency of the process. Stimulation methods to maintain the development rate and enhanced oil recovery were simulated based on the three-dimensional geological and hydrodynamic models of the productive horizons of the Western Absheron field, and the issues of efficiency evaluation of these methods were considered. On the basis of geological-geophysical-mining data, geological and hydrodynamic models of the field were established, initial geological resources were evaluated, and the development history was restored in the hydrodynamic model. Selection of more efficient stimulation method was investigated on the basis of the hydrodynamic model, the processes of water, polymer solution, hot water and steam injection into the formations were simulated, the optimal placement of new production and injection wells was defined, the field performance were predicted and compared according to various options. Based on a comprehensive analysis of geological, geophysical, and field data, we have developed detailed geological and hydrodynamic models of the West Absheron field. This has enabled us to estimate the initial geological reserves and to restore the development history in the hydrodynamic model. Based on the results of similar studies conducted at similar fields, the dependencies of phase permeabilities of gas-oil and water-oil ratios were developed for the productive horizons of West Absheron field and corrected in the process of restoring the development history. Using the hydrodynamic model, we studied the issue of choosing the optimal formation stimulation method. We predicted development parameters in six different options and compared the results.

Keywords: Field; Layer; Well; Development; Model; Stimulation Technique; Prediction.

INTRODUCTION

Currently, in accordance with international standards, the field reserves estimation, substantiating and determination of the drilling trajectories of new production and injection wells, development plans and projects of hydrocarbon reservoirs, the implementation of various geological and process works, the feasibility studies of the given processes are performed based on the hydrodynamic model. Since exploration works in new fields, well drilling in producing fields, various stimulation methods, drawing up development projects, etc. require a large amount of financial resources, the model is an important tool in predicting the results at any stage of the process.^(1,2,3,4,5,6,7,8,9)

The main objective of reservoir modeling with a comprehensive and accurate study is to determine its condition in advance and explore ways to increase the final oil recovery factor. It

is not excluded that the selection of efficient stimulation methods and the study of the factors affecting the process efficiency are performed through the model. ^(10,11,12,13,14,15,16,17,18)

Research Object

The article is devoted to the simulation of the development process of the Western Absheron field; selection of stimulation method for the full utilization of the residual resources of the field and efficiency evaluation issues are considered, the results are compared, and the field performance is predicted by applying different stimulation methods.

Development of the Western Absheron field started in 1989. The field is dissolved gas drive. The main productive horizons are the Girmaky (QD) and Girmaky Alti (QA) suites. The analysis of actual process parameters, the current oil recovery factor and the prediction of the final oil recovery factor prove the necessity of selection and application of stimulation methods to maintain the field development rate and increase the oil recovery factor. The mentioned task is carried out on the basis of field geological and hydrodynamic simulation.

Geological Model

Field database was created for the development process simulation at first. It included coordinates, altitude, inclinometry, digital log diagrams, oil, gas and water production data for each well, information on measured initial and current reservoir pressures, reservoir temperature, physical and chemical, thermodynamical properties of reservoir fluids and other research results. Generally, the results of various laboratory studies conducted on the basis of formation fluids and core samples of the Western Absheron field were systematized, digitized and adapted to appropriate formats and uploaded to the Open Works database.

Determination of reservoir parameters is one of the most important factors in field modeling. For geomodelling, determination of such parameters as the depths of the top and bottom of the horizon, the depth of the water-oil contact, the effective thickness and oil-gas capacity, the porosity coefficient, permeability, sand content, clay content, oil-gas saturation is necessary. The main information source is the results of core sample analysis and interpretation of logging diagrams.

Core samples were taken from 10 wells in the course of exploration and drilling operations in the Western Absheron field, and dependencies were established based on the statistics of their physical properties. Based on the results of this analysis and dependencies, the formation parameters were determined through the entire depth for all wells.

Correlation of the results of the core samples analyzes with the results of the geophysical research conducted in the wells and their interpretation made possible estimation porosity, clay, carbonation, and permeability limits in the field and separation reservoir and non- reservoir rocks.

Specific resistance (SR), well potential (WP), neutron log and gamma ray log (GR) data were used as main objects in the petrophysical interpretation. Clay content (V_{Shale}) on the logs was identified first in defining the formation parameters.

The porosity coefficient values were continuously determined throughout the depth by means of the dependences derived from the ration of the porosity value (at the depth corresponding to the core sample values) and the values derived from the clay log.

The value of permeability was determined after definition the values of the porosity coefficient. The permeability-porosity curve established as a result of laboratory studies of core samples taken from wells was used fort his purpose (figure 1). By processing this dependence, an equation reflecting the dependence of permeability on porosity was built for productive horizons, and permeability values were calculated by this equation.

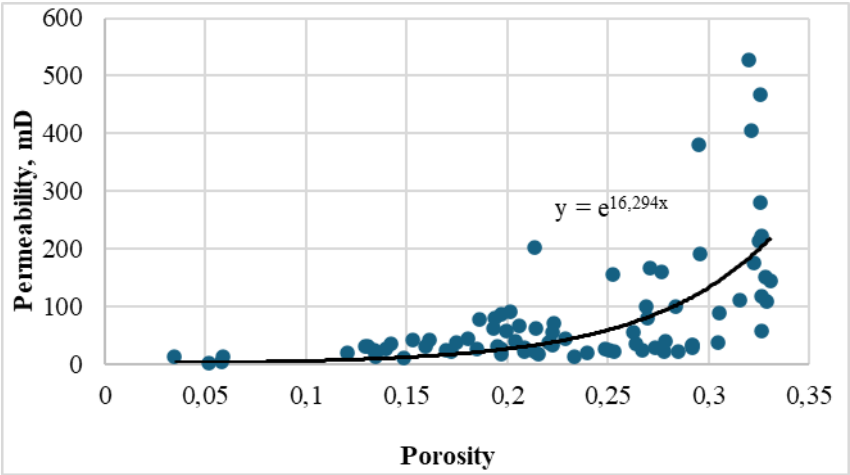


Figure 1. Permeability - porosity curve in the West Absheron field

Change in saturation in the wells was determined with the definition of the values of porosity coefficient. Water saturation value was determined by Archie’s method, based on the value of the porosity coefficient, the specific electrical resistance of the formation and formation fluid.

The average values of formation parameters for the horizons of the Western Absheron field are given in table 1.

Table 1. Average values of formation parameters obtained from log interpretation				
Horizon	Sandiness, v.h.	Porosity factor, v.h.	Permeability, mD	Water saturation, v.h.
QD1	0,30	0,21	61,0	0,35
QD2	0,33	0,21	66,0	0,35
QD3	0,38	0,21	74,0	0,35
QA	0,35	0,20	79,0	0,34
Note: in calculating the formation parameters, their limit (boundary) values were taken as 11 % for the porosity coefficient (Poro), 50 % for the clay content (Vshale), and 50 % for the water saturation (Sw)				

Since permeability (Perm) is related to porosity (Poro), i.e. defined from the Poro curve, the boundary (limit) value of permeability is defined by the boundary value of porosity.

For geological model, compile of two-dimensional maps, and three-dimensional geological models of the reservoir based on these maps provides more accurate results and assists accuracy control of the results. For this, the logging diagrams of all the wells drilled in the formation were

correlated, and depth of the top and the bottom of the horizons were specified. Correlation scheme of longitudinal-section as an example is described in figure 2.

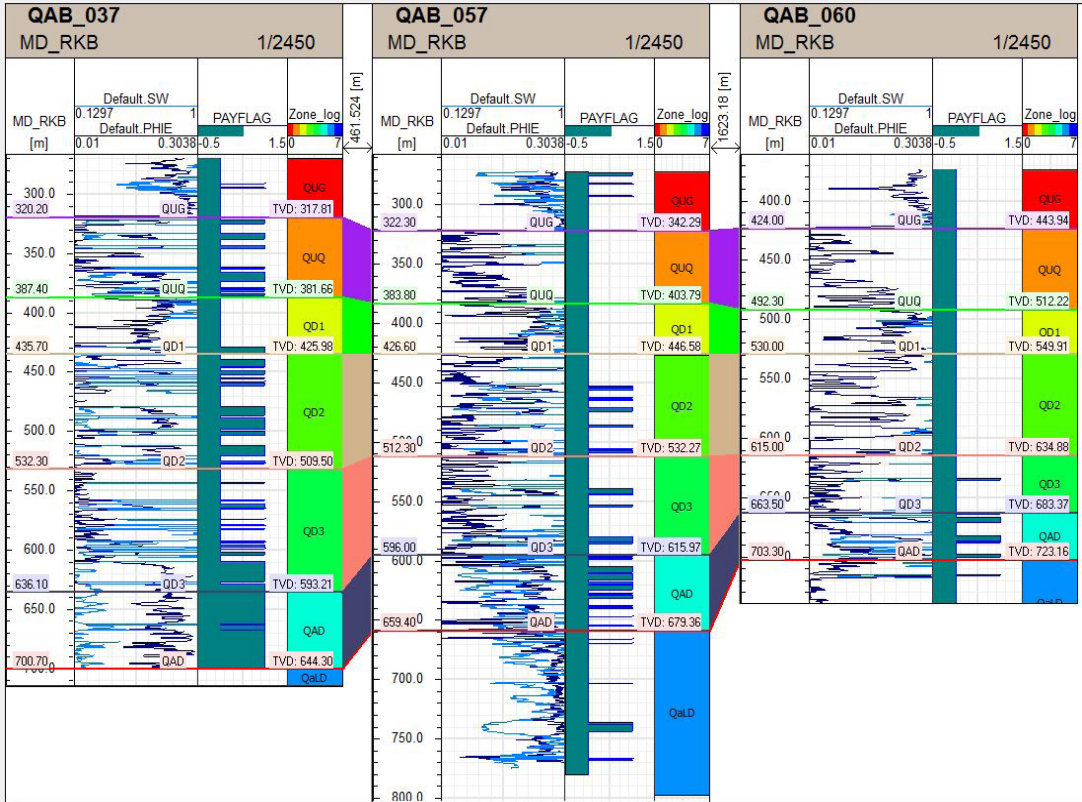


Figure 2. Well correlation schemes

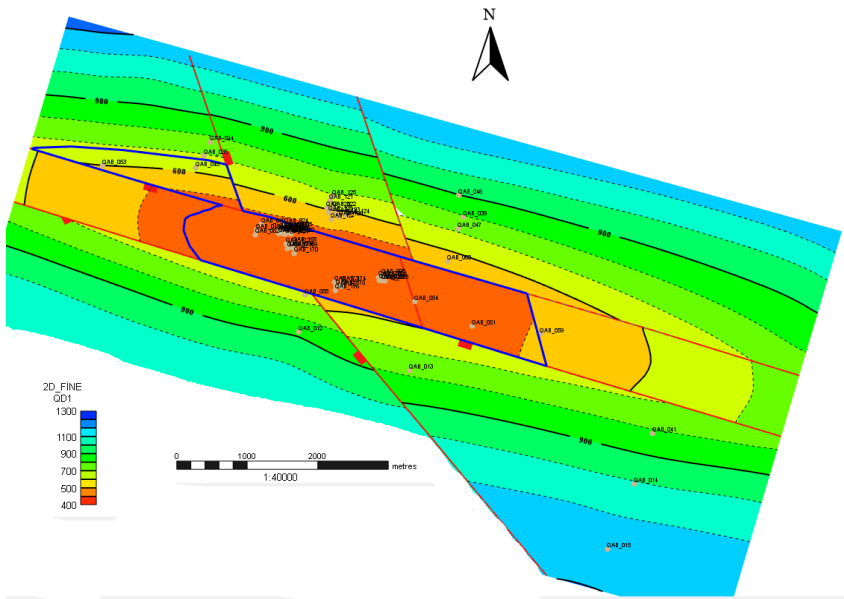


Figure 3. Structural map according to top of the horizon QD1

Despite the fact that the West Absheron field has been in operation since 1985, fundamental seismic exploration work has not been carried out here. For this reason, occurrence mode, depths and faults of the formations have been studied on the basis of logging diagrams. Two-dimensional structural maps of horizons and formations were built on the basis of well correction schemes, top-bottom depths of horizons and absolute values of these depths. Since the main resources in the Western Absheron field are concentrated in QD and QA suite, the QD suite was divided into 3 parts (horizons) (QD1, QD2 və QD3) to make it easier to study the field more accurately and develop the compiled 3D model by programs. As an example, Figure 3 shows a structural map according to the top of the QD1 horizon.

The construction of a three-dimensional geological model is started with structural modeling. Firstly, the frame of the structure was built. During the construction of the structural frame, the tectonic deformations identified according to the well data were three-dimensionally simulated (figure 4). The profile view of horizons in lateral section and their cutting by fractures are also shown in the picture.

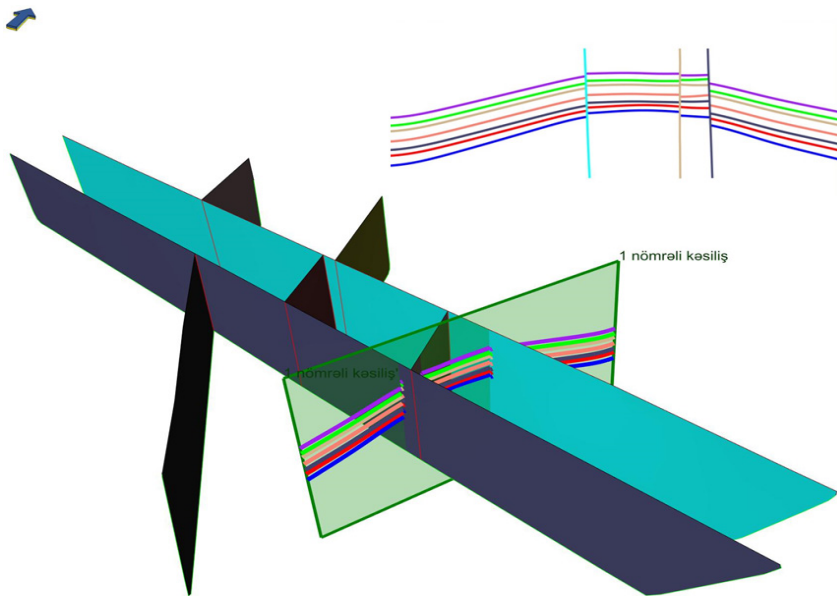


Figure 4. Three-dimensional fracture model

According to the data obtained as a result of interpretations carried out in the drilled exploratory wells, 2 parallel fractures were discovered along the arch in the longitudinal direction of the field. The amplitudes of these fractures change between 50-300 m.

In addition to the longitudinal fractures in the North-West-South-East direction, 5 more fractures have been identified that cross section the field. The amplitudes of these fractures change between 25-100 m. It is highly likely that the transverse fractures are a continuation of each other.

After the fractures, the surfaces were three-dimensionally simulated according to the top of the QUG, QUQ, QD and QAD Suite of the Western Absheron field (figure 5).

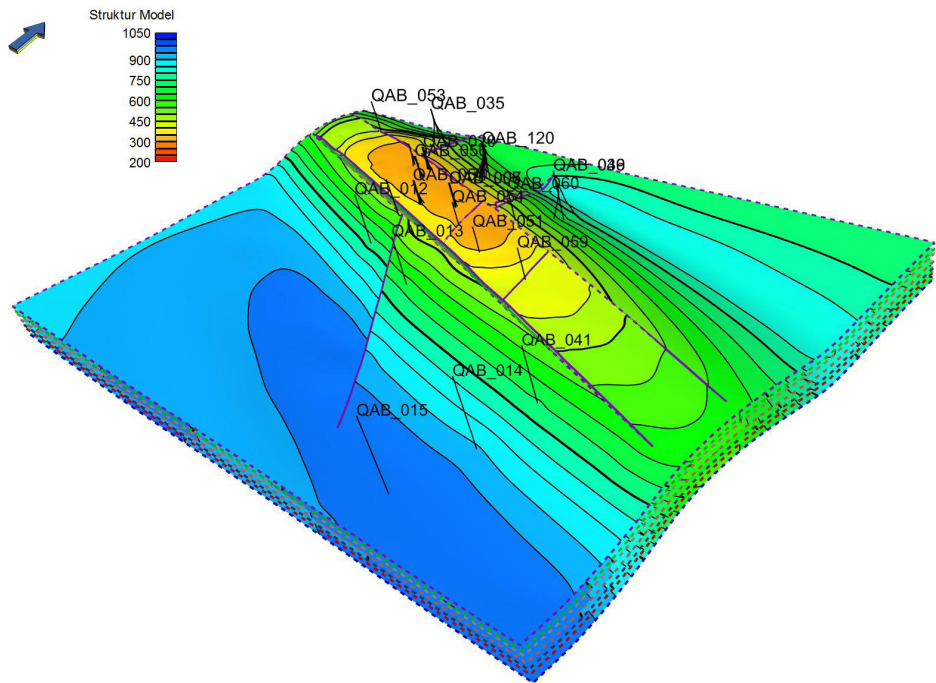


Figure 5. Structural model of the Western Absheron field

After the three-dimensional frame of the horizons is ready, in order to increase the accuracy of the geomodelling, layer parameter distribution, and reserve calculation processes, the horizons are divided into total 1804275 small cells, longitudinal -99 along the X axis, transverse - 45 along the Y axis, and depth-405 along the Z axis , a geological grid was established.

It should be noted that the dimensions of the geological grid are taken as 50x50m along the XY axes. Information about the established geological grid is shown in table 2.

Table 2. Information about the dimensions of the geological grid				
Horizon	geological grid (50m×50m)			Number of grid
	X	Y	Z	
QÜG	99	45	60	267 300
QÜQ	99	45	1	4 455
QD1	99	45	90	400 950
QD2	99	45	60	267 300
QD3	99	45	100	445 500
QAD	99	45	94	418 770
Cami	99	45	405	1 804 275

After the geological grid of the field was established, a facies model was built. The distribution of two facies (sand, clay) was carried out on the basis of the conceptual model adopted in the litho-facies modeling of the zones. Then, the distribution of petrophysical parameters (porosity, permeability, water saturation) on selected litho-facies was carried out.

A stochastic distribution algorithm was selected for facies distribution by analyzing the depositional conditions and interpreted well logs in the formation of production horizons of the Western Absheron field. For this purpose “Kriking” method was used in “Indicators” module of “Irap RMS” modeling program. One of the main advantages of using this module is the reconciliation of distribution results with well data and user-specified parameters.

To make the stochastic distribution more deterministic, the results of variogram analysis, 2D sand thickness distribution trend maps prepared on the basis of the accepted concept on horizons, and 1D vertical proportion curves trends obtained from the vertical distribution of facies on the horizon obtained from the interpreted well data analysis were used. In general, variogram analyzes were used to determine vertical and horizontal uncertainty at each stage of constructing parameter models. Averaging the results of experimental variograms with theoretical dependences is used as an input parameter during modeling.

Variogram analyzes were used to each parametric modeling. With the help of variogram analysis, the interval of changes in the heterogeneity of formations on vertical and horizontal sections was determined

Various variogram analyzes were performed for the distribution of facies, and finally, an exponential curve was chosen, and in the facies model, the azimuth was 350, 1000 m in the direction parallel to the azimuth, 1000 m in the normal direction, and 2 m in the vertical direction.

Various variogram analyzes were carried out for the distribution of facies, and finally, 350° azimuth, 1000 m in parallel to the azimuth, 1000 m in the normal direction, and 2 m in the vertical direction was taken by selecting an exponential curve in the fascial model.

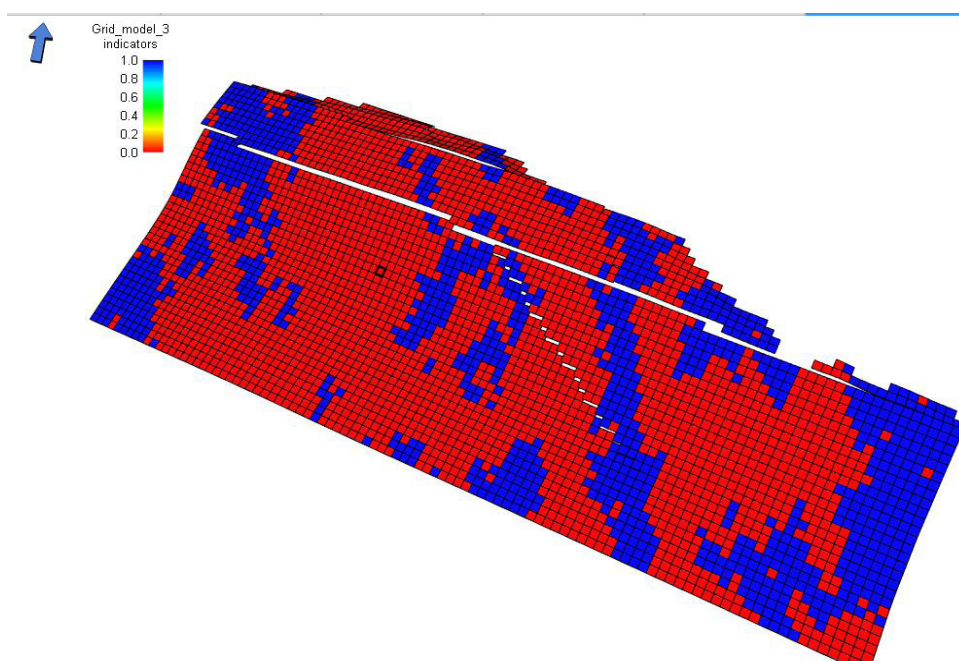


Figure 6. 3D fasial model

The lithologic-facies model of the Western Absheron field was built based on all the well data, the results of the core sample studies, the interpretation of the geophysical research methods of the wells and the general analysis of the results obtained from these studies

A lithologic and facies model of the Western Absheron field was built on the basis of all the well data, test report of drill sample, the interpretation of the geophysical exploration techniques of wells and the general analysis of the results obtained from these studies. In other words, the regularity of distribution of sand-clay facies on the deposit by depth and area has been determined.

The facies model of the Western Absheron field is shown in figure 6.

In the following steps, a petrophysical model (Cube) was built. Porosity, permeability and water saturation parameters were simulated in petrophysical modeling.

A 3D porosity (Phie) model was built with a stochastic distribution by cricking simulation of the effective porosity value after performing multiple analyzes on well data. Different variogram models were tested, and finally, azimuth 350°, parallel 1000 m, normal 1000 m, vertical 1 m distribution variogram with an exponential curve was used (figure 7).

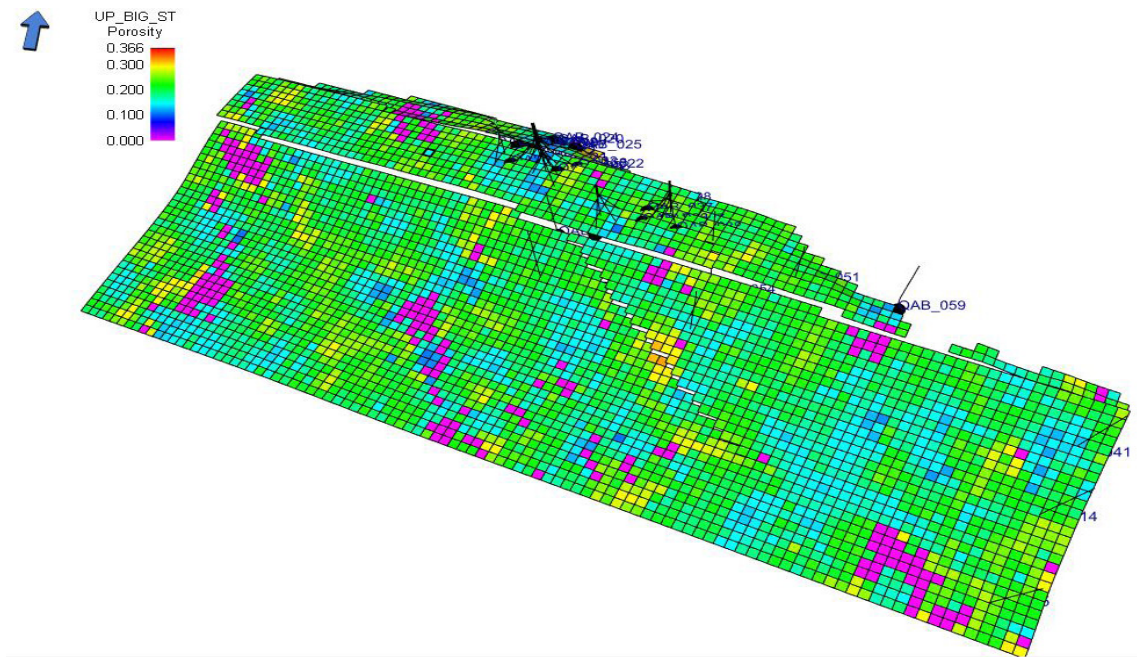


Figure 7. 3D Porosity model

The permeability parameter (Perm) is constructed by a function obtained from both the petrophysical distribution and the porosity dependence. Since the obtained results are similar, finally, it was considered appropriate to establish by the function $K=3,5227 * e^{11,121 \cdot m}$ obtained from the porosity (figure 8).

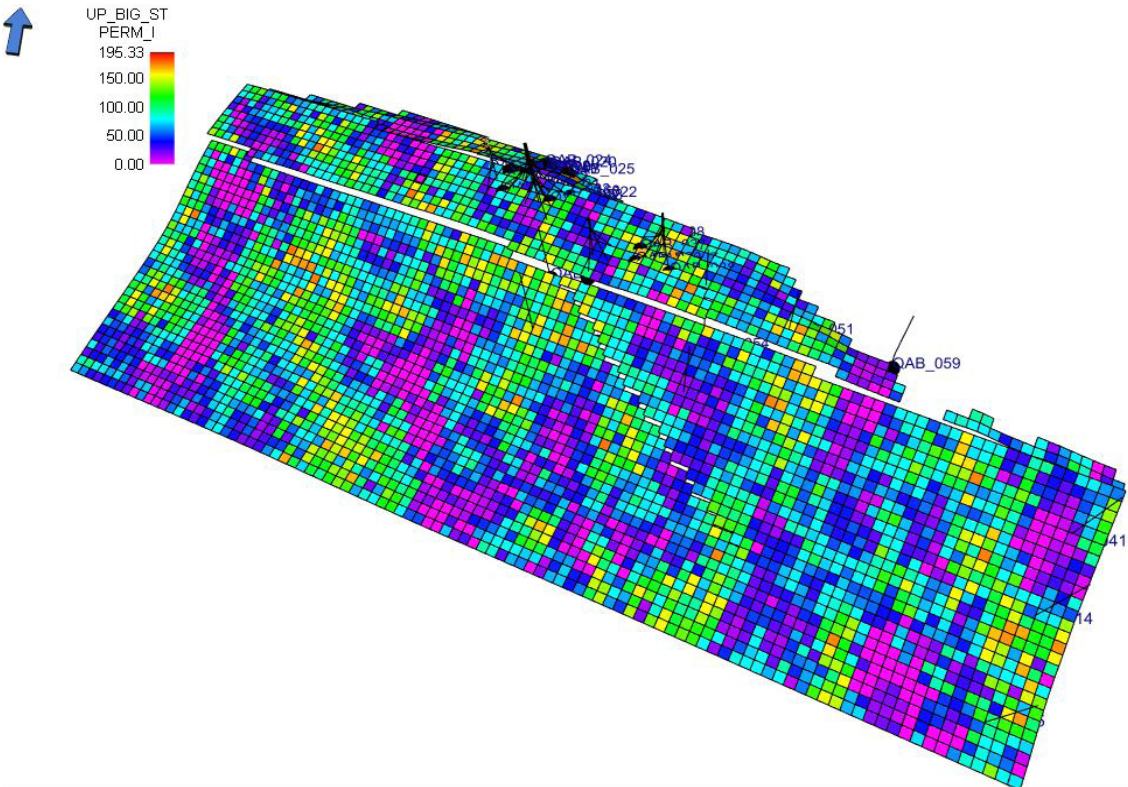


Figure 8. 3D Permeability model

A simplified J-function method using porosity (Poro), permeability (Perm), height (H) above the free water level and petrophysical constants (a, b) was established to build a model of water saturation (SW) (figure 9). The distribution of water (oil) saturation by horizons in the Western Absheron field is shown in figure 10.

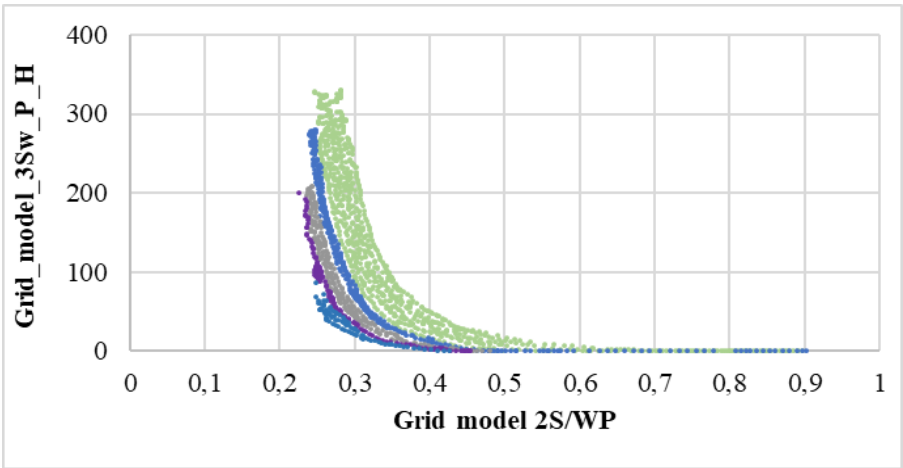


Figure 9. Scatterplot set between SW on horizons and height (H) above free water level

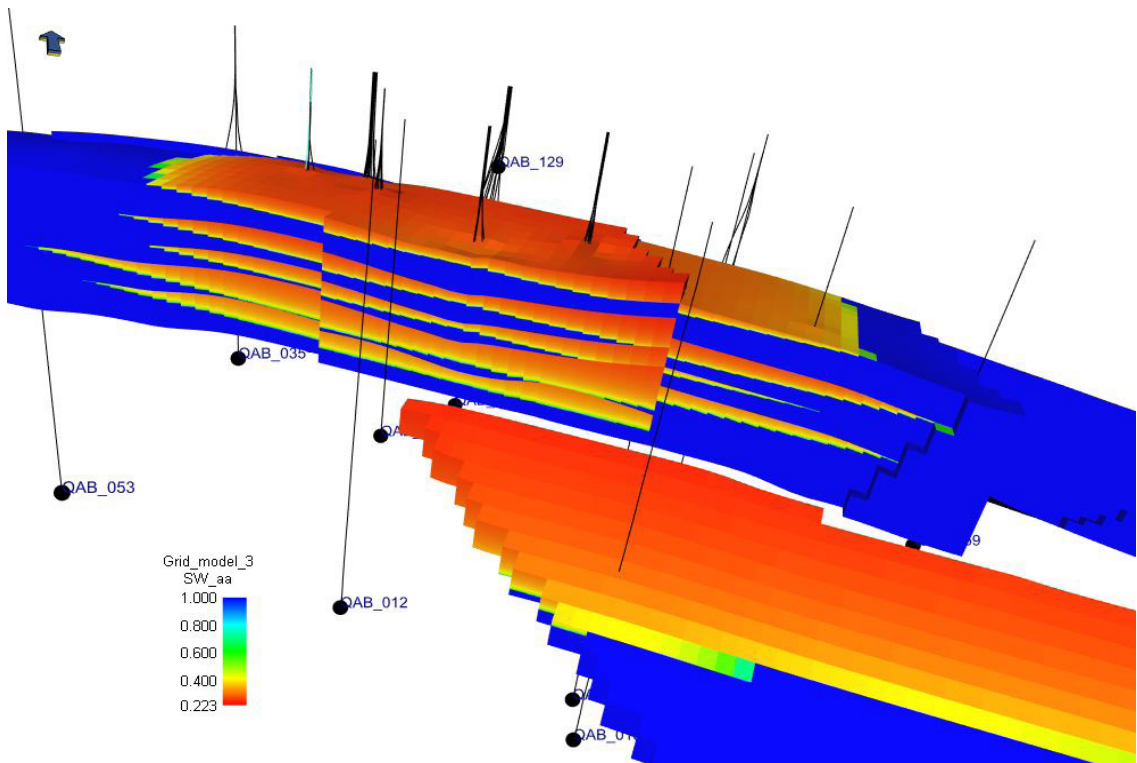


Figure 10. 3D saturation model

After the petrophysical cube is ready, the necessary parameters for the calculation of the oil reserves of the Western Absheron field along the horizons have been determined. Oil and gas effective thickness, porosity and water saturation coefficients were taken based on the results of well data interpretation, as well as the results of the petrophysical model built based on these results. The values of the mentioned parameters are given in table 3.

Table 3. Values of reserve calculation parameters					
Horizon	Porosity factor			Water saturation	
	Min	Max	Medium	Min	Medium
QÜG	0,11	0,28	0,20	0,24	0,34
QD1	0,11	0,28	0,21	0,22	0,35
QD2	0,11	0,27	0,21	0,23	0,35
QD3	0,11	0,28	0,21	0,23	0,35
QAD	0,11	0,28	0,21	0,23	0,35

The determination of the initial oil volume coefficient (Bo) was based mainly on the results of the analysis of samples taken from the first exploration wells drilled in the field^(19,20,21,22) and was accepted as stable for all horizons.

In the map and model constructed according to the calculation plan, oil-water contours are shown in cross-sections both horizontally and vertically (figure 11).

Given that some fractures in the area have non-conductive properties, it is normal for fluid contacts to be located at different depths in the modeled horizons and blocks. The depths of the oil-water contacts (OWC) have been determined separately for each block and the horizons they are divided into (table 4). In determining the contacts, mining-geophysical indicators and production data from wells have been used.⁽²³⁾

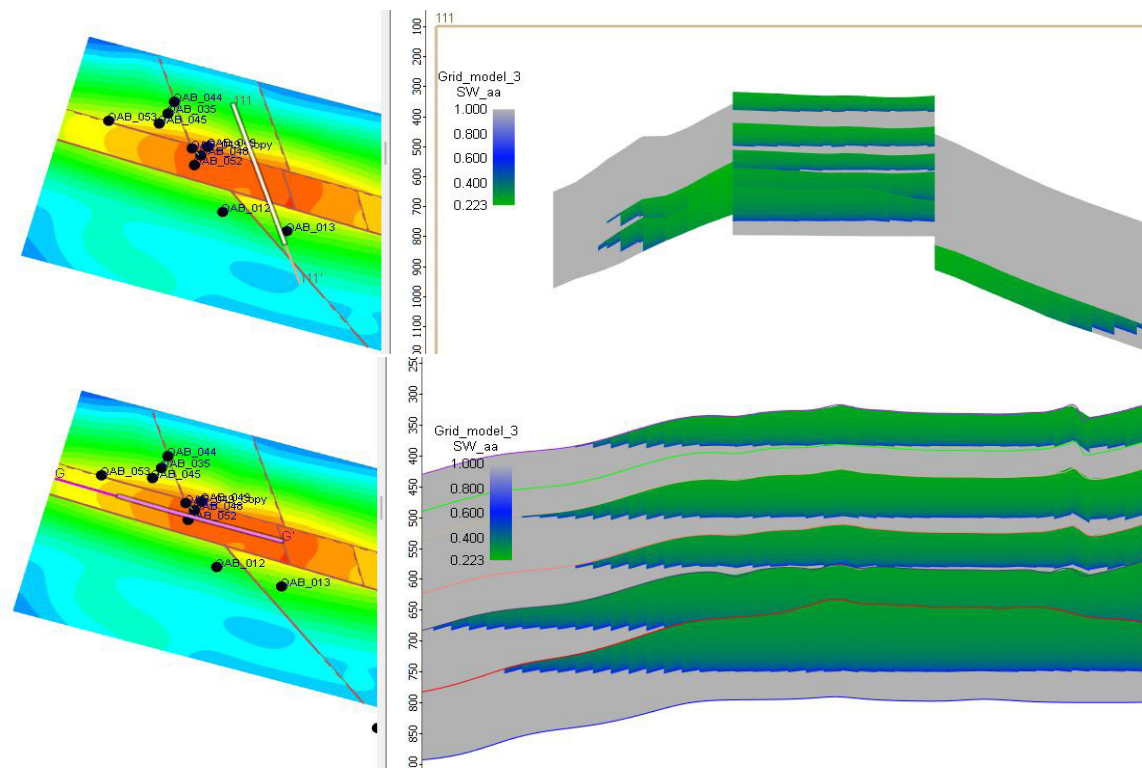


Figure 11. The general appearance of fluid contacts in the longitudinal and transverse cross-sections noted in the saturation map of the horizons

Table 4. Information about the depths of the oil-water contacts (OWC) for the horizons							
Horizon	Oil-water contact (OWC) depth for tectonic blocks, in meters						
	1	2	3	4	5	6	7
QUG	0	0	375	384	0	0	0
QD1	0	0	510	500	670	0	0
QD2	0	0	560	580	770	750	0
QD3	0	0	652	680	900	835	720
QAD	1116	1205	0	750	900	0	0

Using the parameters listed above - such as porosity, thicknesses, saturation, depths of oil-water contacts, and the physical-chemical properties of oil and gas - the initial balance reserves of hydrocarbons in the productive horizons of the Western Absheron field and the tectonic blocks created by fractures in these horizons have been estimated.

Hydrodynamic Model Construction

To construct a hydrodynamic model, the three-dimensional geological model must first be loaded into the hydrodynamic simulator. To achieve this, the geological model must be prepared for loading into the hydrodynamic simulator. Very small-sized geological cells (grids) with millions of units are not suitable for conducting hydrodynamic calculations. This is because, in a hydrodynamic model, filtration equations are solved for each grid, incorporating dependencies of the physical-chemical and thermodynamic properties of formation fluids on pressure, phase permeability variation functions, and other factors. This leads to an increase in the number of calculations to an excessive extent, resulting in a very long computation time. To increase and optimize computation speeds in a hydrodynamic simulator, the number of grids in the model should be reduced. For this reason, when the geological model is loaded into the hydrodynamic model, the more detailed geological ‘grid’ should be replaced with a relatively coarse hydrodynamic ‘grid’ that has a smaller number of elements, in other words, it is necessary to transition from the geological model to a hydrodynamic framework with larger grid sizes. Note that the framework of a hydrodynamic grid is constructed based on the same structural model, and this process is called “upscaling”.

When upscaling the geological model of the Western Absheron field, the number of cells was reduced along the horizons with isotropic distribution in the vertical direction, while the cell sizes were doubled in the X and Y directions. When constructing the hydrodynamic grid, 8-point cells were used instead of the geological grid, and the cells were confined by vertical boundaries. Each fault has been accounted for in the grid by applying a 50 % column adjustment. This method allows for the replacement of a precisely constructed geological grid with a relatively coarse hydrodynamic grid, i.e., one with fewer cells, which enables the equations of fluid flow to be solved more quickly in each cell.

During the transition from the geological grid to the hydrodynamic grid, several options were examined to determine the optimal cell sizes in the X and Y directions, with the goal of preserving vertical and horizontal heterogeneities for all parameters. When the cell sizes are taken to be equal to 100 meters, the production wells do not pass through the same cell (grid), and this size is considered optimal for the X-Y directions. Considering that several wells in the Western Absheron field are producing from multiple horizons, in order to perform hydrodynamic calculations simultaneously across all horizons, cell sizes in the Z direction were also optimized, reducing the total number of cells from 1,8 million to 262 845.

Table 5. Comparison of the hydrodynamic grid with the geological grid						
Horizon	Geological grid (50×50)			Hydrodynamic grid (100×100)		
	X	Y	Z	X	Y	Z
QUG	99	45	60	99	45	10
QÜQ	99	45	1	99	45	1
QD1	99	45	90	99	45	14
QD2	99	45	60	99	45	8
QD3	99	45	100	99	45	10
QAD	99	45	94	99	45	16
Sum	99	45	405	99	45	59
Total	1 804 275			262 845		

Proportional divisions of the main productive horizons in the Z direction and the quality check during the averaging of geological parameters in the hydrodynamic grid have shown that there is no significant difference between the geological and hydrodynamic grids. The absence or minimal difference provides a strong basis for conducting hydrodynamic calculations efficiently. The dimensions of the constructed hydrodynamic grid and its comparison with the geological grid are provided in table 5.

The discrete parameter NTG (net-to-gross ratio) is converted into a continuous parameter. NTG, PHIE (effective porosity), and S_w (water saturation) parameters have been averaged using an arithmetic method. The PERM (permeability) parameter has been averaged using the full tensor method. Since the permeability values vary in the lateral and vertical directions, the full tensor method was used to obtain the Perm parameter for each of the I, J, and K directions.

The quality check of the ‘upscaling’ between the geological and hydrodynamic grids was conducted by comparing petrophysical parameters (porosity, water saturation) using histogram diagrams, and for the facies parameter, based on the vertical distribution curve.

After the upscaling process of geological model parameters to the hydrodynamic grid was completed, the initial geological balance reserves of hydrocarbons were calculated in the hydrodynamic grid. Comparing the reserves calculated in the geological and hydrodynamic grids is a way to verify the quality of the ‘upscaling’ process. According to international standards for modeling the development process of fields, it is considered inappropriate to continue the modeling process if this difference exceeds 10 %. In such cases, either the construction process of the geological model or the upscaling process of the geological model parameters to the hydrodynamic grid must be re-evaluated.

The initial geological reserves of the Western Absheron field were calculated in the hydrodynamic grid and compared with the values computed in the geological model, and it was determined that the differences were within acceptable error limits.

During the loading of the geological model into the hydrodynamic simulator, the coordinates of the wells, their altitudes, inclinometrics, the depths of the water-oil contacts, the depths of the formation tops and bottoms, and the cubes of the formation permeability parameters are also incorporated into the hydrodynamic model.

It is known that the reservoir pressure decreases progressively during the production process. Since the physical-chemical and thermodynamic (PVT) properties of the reservoir product depend on pressure, changes in pressure during the production process lead to changes in the thermodynamic properties of the reservoir product. On the other hand, calculations within the hydrodynamic model are performed not only for the conditions based on the initial reservoir pressure and the initial thermodynamic properties of the fluid but also for the current pressure values at each step and the corresponding thermodynamic properties of the reservoir fluid for those pressures. Therefore, knowing in advance the regular changes of the thermodynamic properties of the formation product depending on the pressure is an important for the accuracy of the hydrodynamic model. These data are determined only on the basis of thermodynamic experiments of the formation product in laboratory conditions. Based on the experiments, the pressure dependent points of these parameters are established, and these points in subsequent calculations using the appropriate equations with special programs are adapted to the pressure-temperature change and loaded into the model as a function.

Change of PVT properties of Western Absheron oil depending on pressure was obtained from the correlation and interpolation of the laboratory experiments results based on samples taken from wells No. 22, 24 and 28.

As an example of the adaptation of the physico-chemical and thermodynamic properties of the formation product in the model, the curves showing the adaptation of the experimental values of the oil volume coefficient and viscosity depending on the pressure in the model are given in figures 12 and 13.

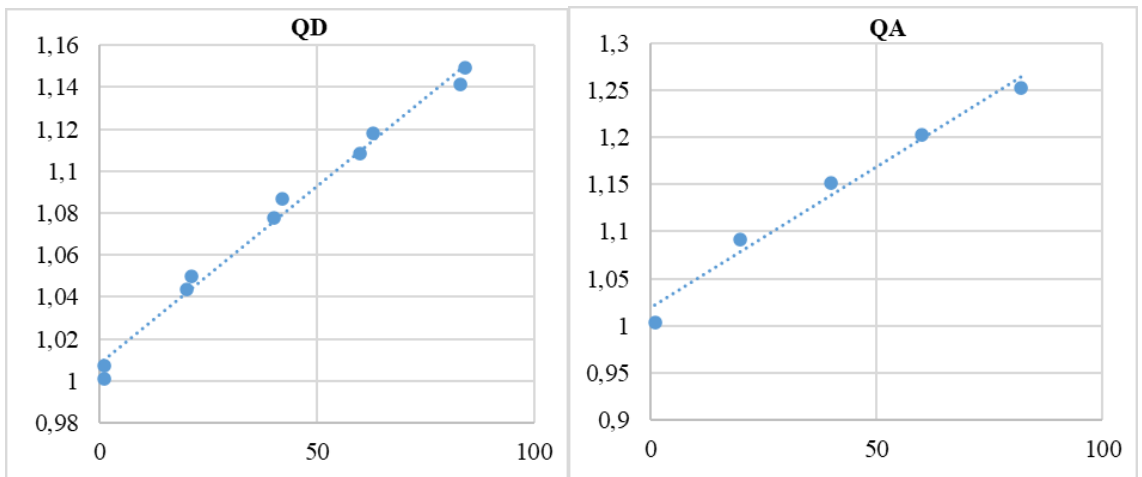


Figure 12. Adjustment of the calculated values of the oil volume coefficient to the experimental values

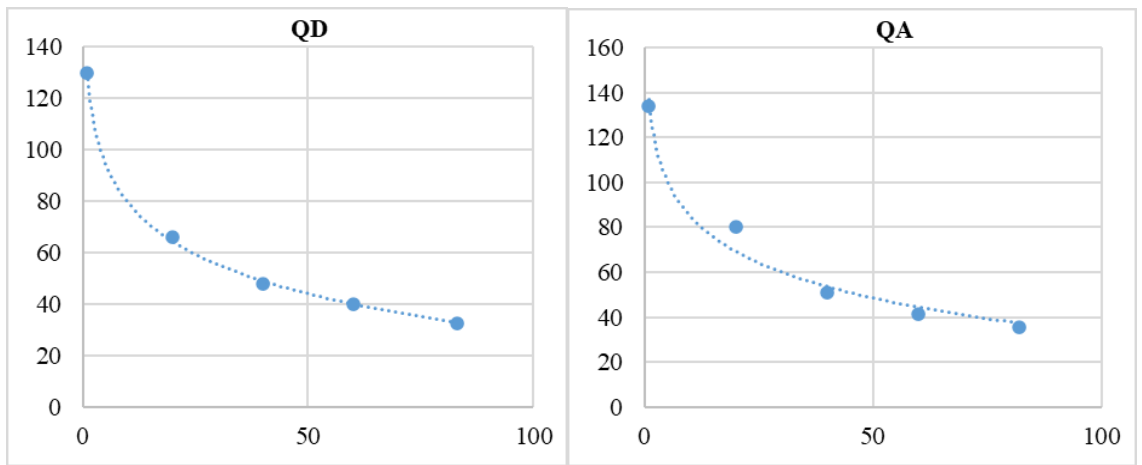


Figure 13. Adjustment of calculated values of oil viscosity to experimental values

As seen from the figures, the regular change of the physico-chemical and thermodynamic parameters of the formation product depending on the pressure is very well adapted to the values obtained as a result of the relevant tests. This creates a great basis for the proper functioning of the hydrodynamic model and accurate results in the future.

The most important parameter for the accurate operation of the hydrodynamic model and the adequacy of the predictions is the values of the relative phase permeability. The correct

values of this parameter mean that the percolation equations and hydropermeabilities of the formations describe the ongoing processes more accurately and the process of predicting the performance indicators is accurate. Note that the values of these parameters are determined as a result of laboratory analyzes of core samples taken during drilling.

Since no such studies were conducted for the Western Absheron field, relevant data from similar fields were used in the model, and corrected in the restoring process of the development history. Dependencies of gas-oil and water-oil relative phase permeability used in the model are shown in figures 14 and 15.

It should be noted that “Tempest Enable” software was used to build the hydrodynamic model, and “Black oil” model was selected for calculations.

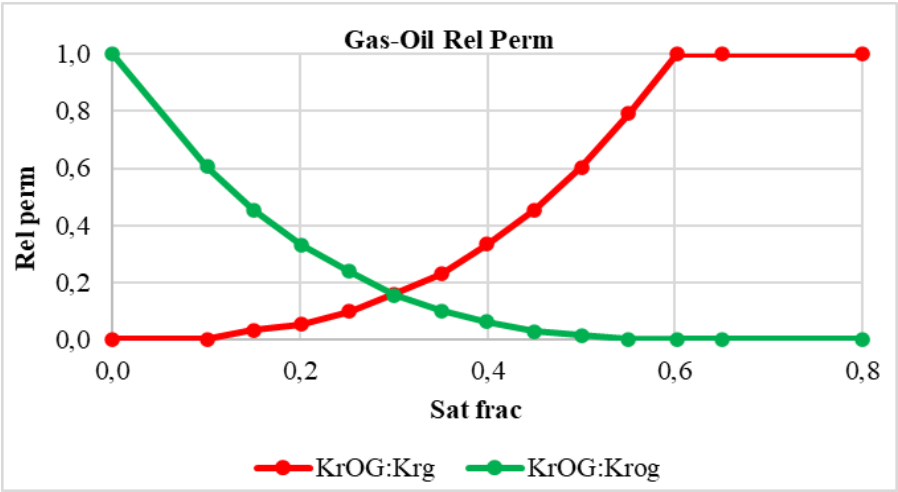


Figure 14. Gas-oil relative phase permeability used in the model

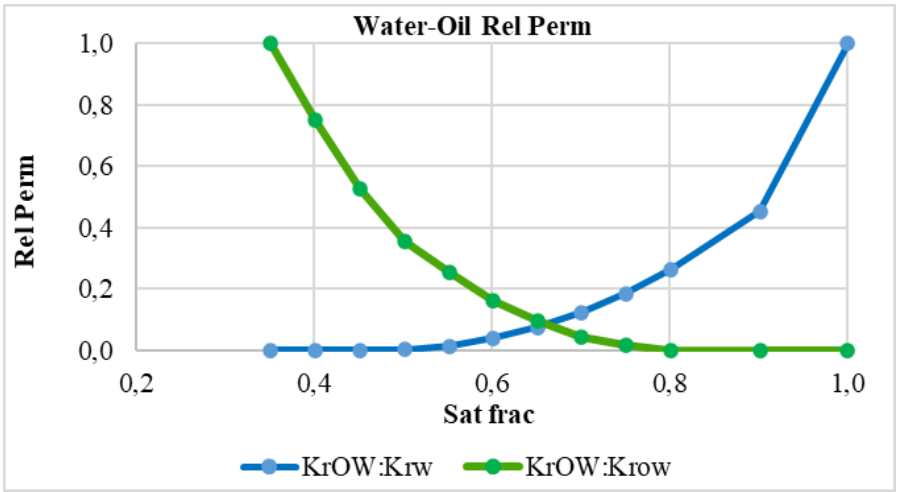


Figure 15. Water-oil relative phase permeability used in the model

After the hydrodynamic model corresponding to the initial condition of the field was ready, the development history restoring, i.e., the process of adapting the parameters included in the model to the fact, was carried out.

Since the production of oil, dissolved gas and water is considered more accurate and informative, adaptation of these parameters was taken as a basis. Production (history) recovery curves for the general Western Absheron field are shown in figure 16, 17 and 18.

Completion of the adaptation process means receiving the report of the current status of all performance parameters of the horizon. That is, the condition of the contours, the volume of the produced product, the volume of residual resources, location, etc. parameters correspond to the current state of the horizons development process.

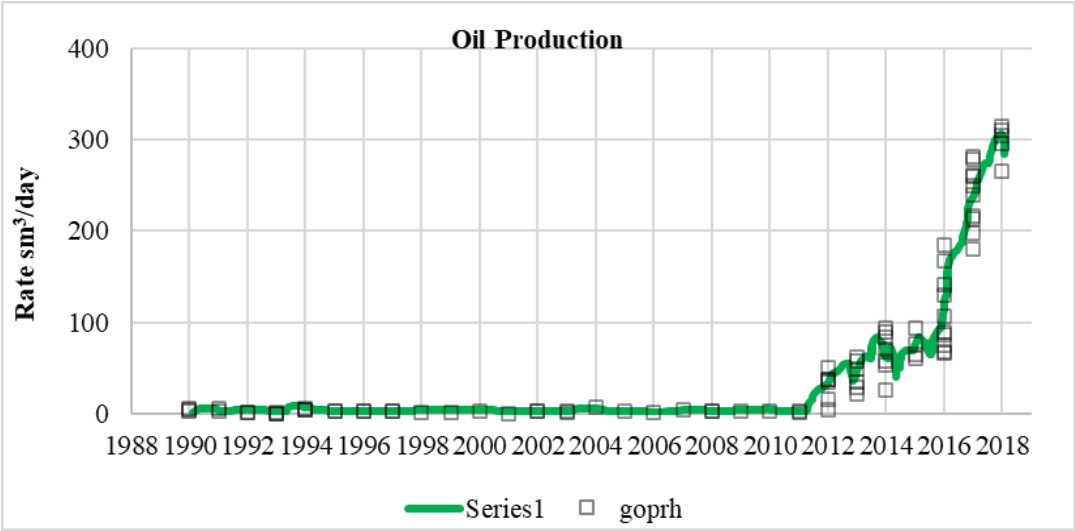


Figure 16. Oil production recovery curve

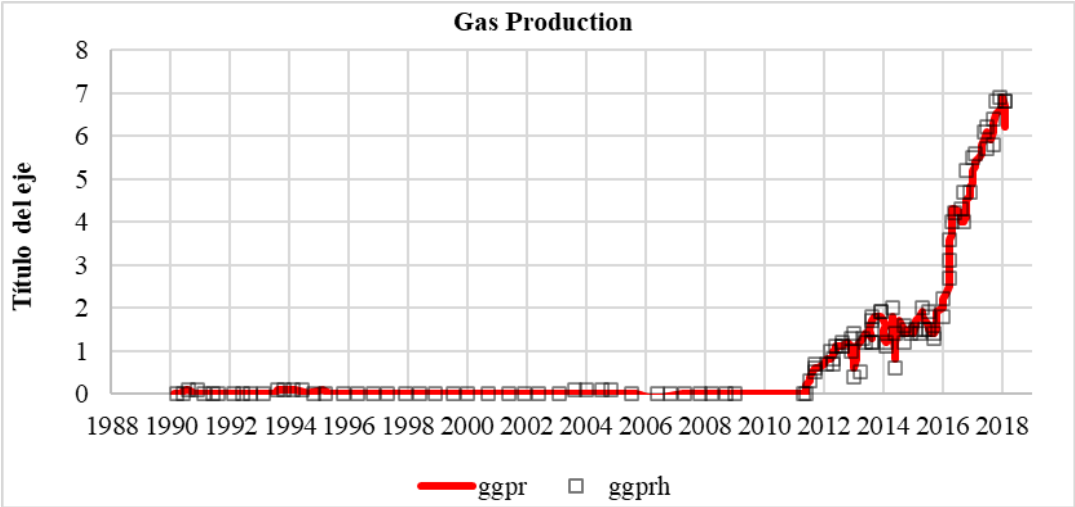


Figure 17. Gas production recovery curve

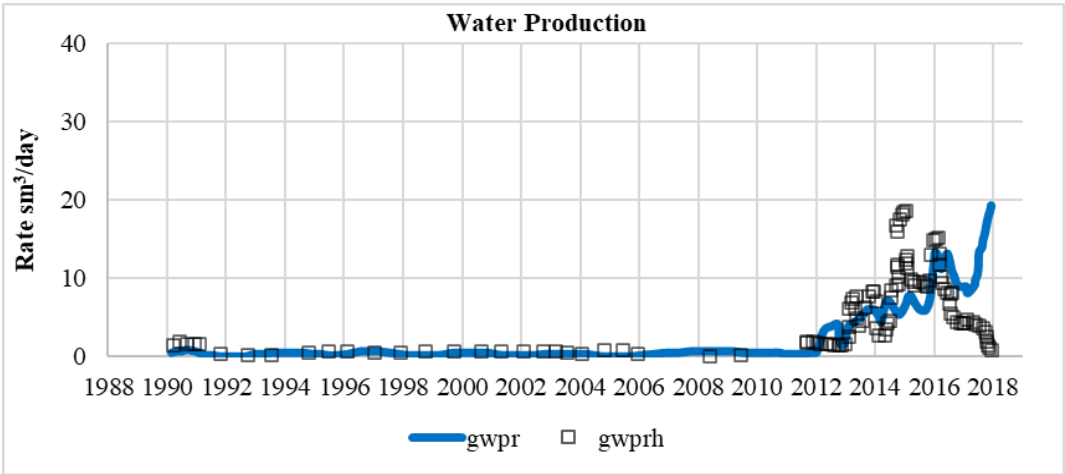


Figure 18. Water production recovery curve

The process of restoring the development history based on the hydrodynamic model, as well as the actual production data, show that currently 455 thousand m³ of oil and approximately 10 mln. m³ of gas were produced from QD3 and QA formation.

In the West Absheron field, production parameters up to 2050 with operating wells are predicted by the model (figures 19 and 20).

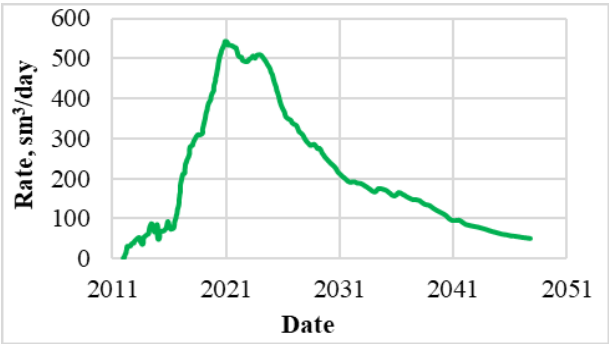


Figure 19. Prediction of the average daily oil production of the field with the existing well stock

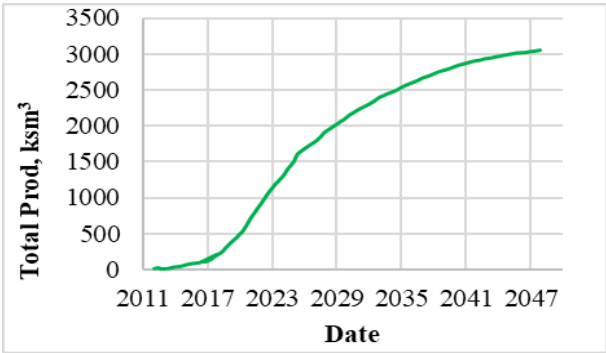


Figure 20. Prediction of total oil production of the field with the existing well stock

According to the calculations carried out in the hydrodynamic model, as seen from the figures, with current well stock a total of 1,7 mln. m³ (QD3-1,1 mln. m³; QAD-0,6 mln. m³) of oil is predicted from QD3 and QA formations. This figure is a very low indicator in terms of full exploitation of horizons' resources. Therefore, in order to fully exploit the residual resources of the Western Absheron field, the issue of planning new production wells in the hydrodynamic model was considered.

For this purpose, a total of 61 new production wells were placed, 23 in the QD horizon and 38 in the QA horizon, based on the comparative analysis of different options, in the areas with the best indicators on the joint distribution map of the porosity, sandiness, thickness and residual oil saturation parameters according to the current state of the field development stage. the numbers of wells to be drilled, horizon project, commissioning dates and initial productions were determined and included in the model (figure 21).

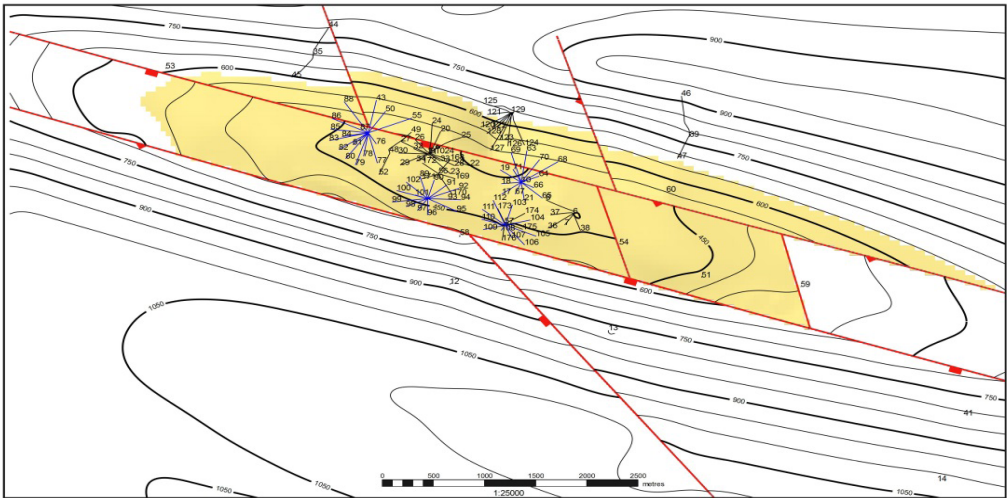


Figure 21. Location scheme of the proposed new wells on the structural map

Taking into account the new production wells, the operating parameters of the QD3 and QA formations have been predicted until 2050. The forecast of parameters is shown in figure 22 and 23. As seen from the figures, despite the new production wells being put into operation, by 2050, 3,06 mln. m³ of oil and 496,34 mln. m³ of dissolved gas production is predicted.

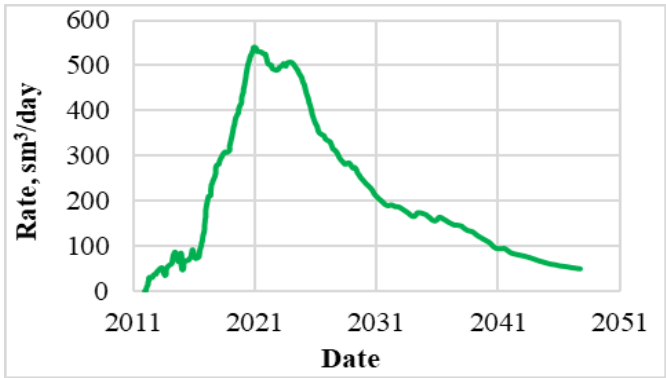


Figure 22. Prediction of average daily oil production of the field with new planned wells

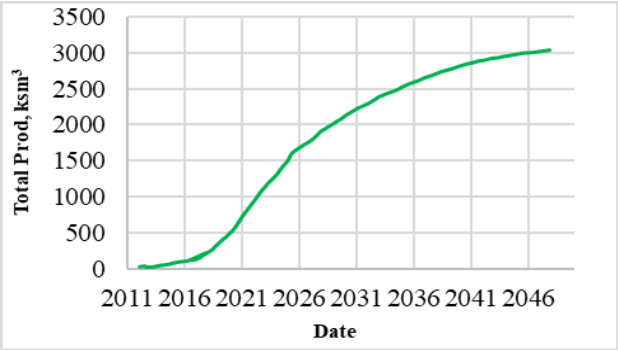


Figure 23. Prediction of total oil production of the field with new planned wells

Modeling of Stimulation Techniques

In order to increase the final recovery coefficient of the Western Absheron field, several stimulation techniques have been studied. For this purpose, the processes of injecting water, polymer solution, hot water and steam into the formation were modeled and the obtained results were compared. In order to neutralize the influence of other extraneous factors on the process, when modeling each stimulation technique, the number of new production and injection wells, start-up dates, sequences and other parameters were taken as the same for each horizon.

Water displacement: firstly, periphery injection process into QD and QA formations is modeled. For this purpose, in addition, 8 water injection wells are planned for the QD formation and 6 for the QA formation. 100 m³/day of water was pumped from each well. It should be noted that the production parameters of the planned new production wells were also taken into account during the modeling of all formation stimulation techniques and production forecasting.

The forecast results are shown in figures 24 and 25. As seen from the figure, 3,91 mln. m³ of oil, 71,7 mln. m³ gas purchase is predicted.

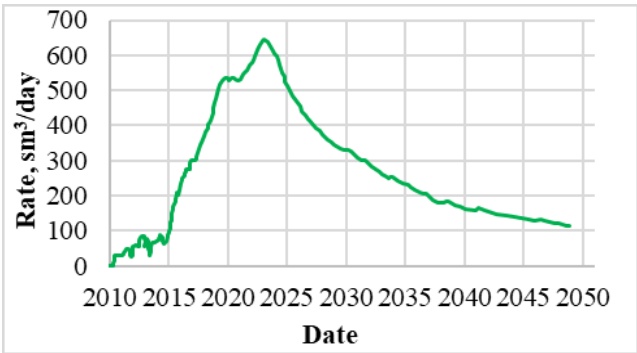


Figure 24. Prediction of average daily oil production of the field during watering by year

Oil displacement by polymer solution: to prevent the risk of water tonguing that may occur during formation stimulation and to ensure piston-like oil displacement, to ensure a decrease in the ratio between the viscosities of the displacing and displaced fluids and to bring the viscosity ratio to one, the process of displacement of high-viscosity oil from West Absheron by an aqueous polymer solution was modeled.

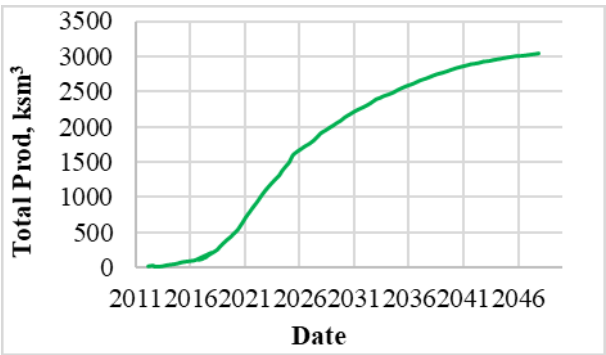


Figure 25. Prediction of total oil production of the field during watering

For this purpose, injection of polymer solution behind the contour from operating wells used for modeling the water injection process was considered. Water injection was modeled with a polymer concentration of 0,016 kg/m³ into the layer, then the polymer solution was displaced with normal water. The law of viscosity fluctuation depending on the polymer concentration was studied in laboratory conditions, the obtained result was included in the model in the form of current factor of viscosity (figure 26). The results of predicted oil production are shown in figures 27 and 28. As you can see, it is predicted that by 2050, a total of 4,12 million m³ of oil and 441,16 million m³ of gas will be purchased. Current factor for oil viscosity and polymer concentration.

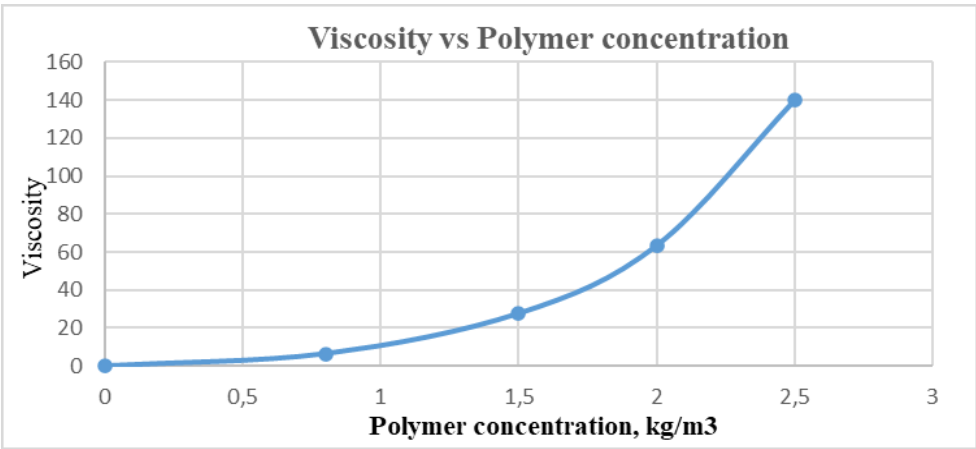


Figure 26. Graphical chart of viscosity on polymer concentration

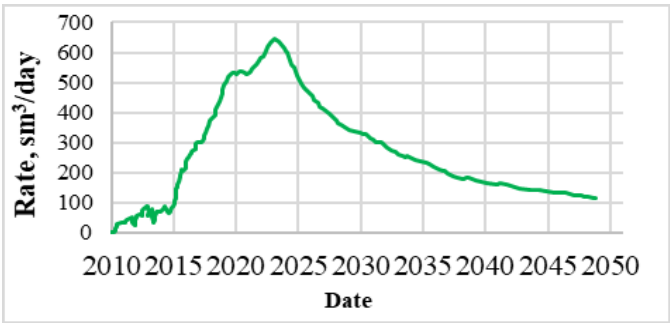


Figure 27. Prediction of average daily oil production of the field during polymer solution stimulation by year

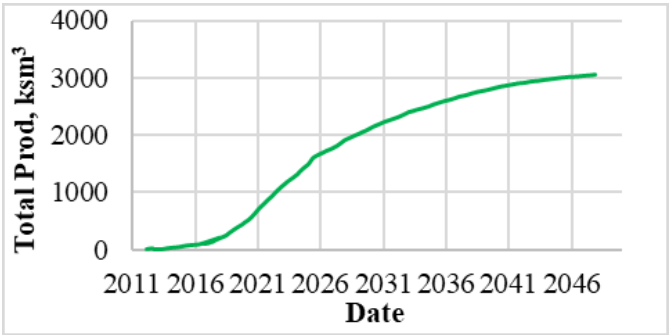


Figure 28. Prediction of field total oil production during polymer solution stimulation

Hot water injection into layers: In this option, concomitantly with the drilling of 61 new producing wells, the drilling of 14 new injection wells is planned. Of the 14 wells drilled, hot water was injected into the Kirmaki suite (QD) of eight wells and into the under-Kirmaki suite (QAD) of six wells. The regularity of viscosity change depending on temperature was studied in laboratory conditions, the obtained result was included in the model in the form of current factor of viscosity (figure 29). The production forecast results for this option are shown in figures 30 and 31. As can be seen from figure, it is predicted that 5,27 mln.m³ of oil and 388,8 mln.m³ of dissolved gas will be obtained from the field by 2050 during hot water stimulation into layers.

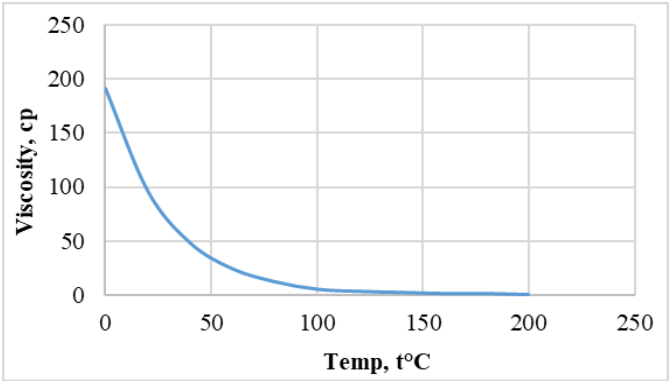


Figure 29. Temperature-viscosity curve

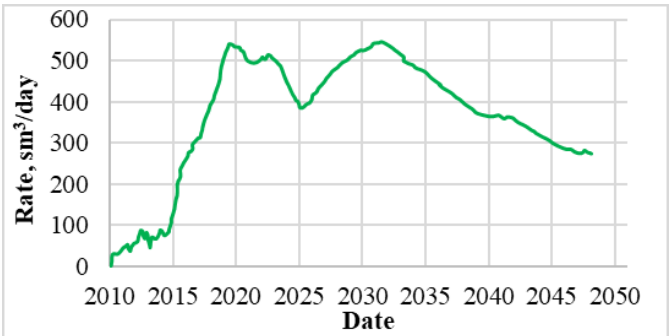


Figure 30. Prediction of average daily oil production of the field during hot water stimulation by year

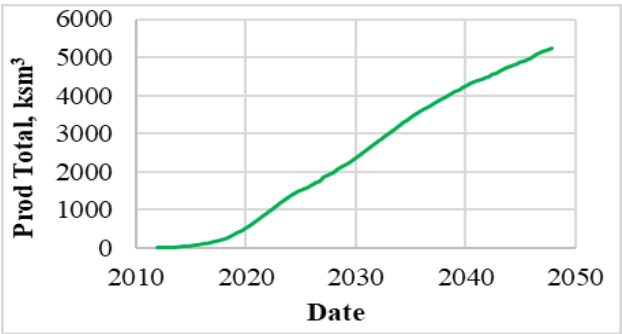


Figure 31. Prediction of field total oil production during hot water stimulation

Steam injection into layers: the mode of steam stimulation on the West Absheron field is also modeled. For this option, it is planned to drill 61 new producing wells and 14 new steam injection wells in the productive horizons of the field.

The prediction results of the steam injection option are shown in figures 32 and 33. As can be seen from figure, it is predicted that 4,05 mln.m³ of oil and 412,0 mln.m³ of dissolved gas will be obtained from both layers by 2047 during the steam stimulation into layers.

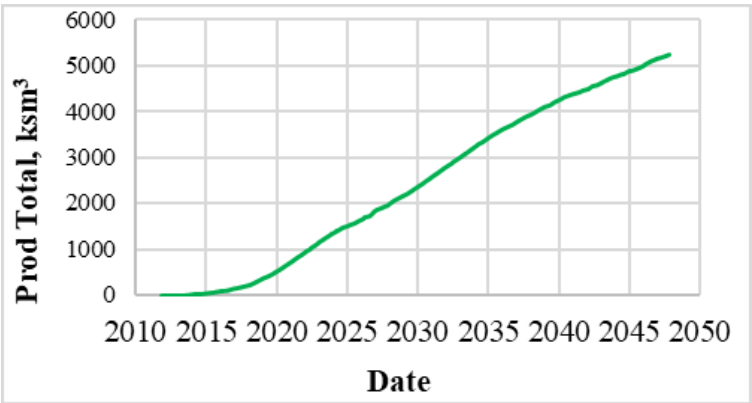


Figure 32. Prediction of average daily oil production of the field during steam stimulation by year

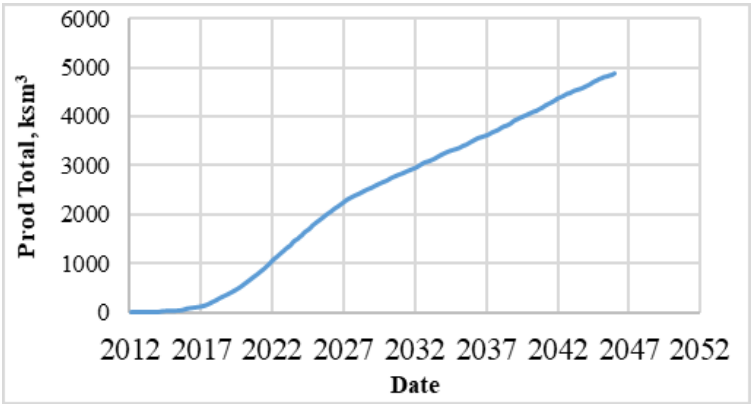


Figure 33. Prediction of field total oil production during steam stimulation

Thus, based on a complete modeling of the development process of West Absheron field, 6 different development options were proposed with 4 methods of formation stimulation (water, polymer solution, hot water and steam) - only with active wells stock (basic option); with active wells stock and planned new producing wells; active wells stock, planned new producing wells with various methods of formation stimulation are predicted and the predicted parameters obtained for a certain period of development are compared (table 6).

A more accurate decision can be made on which of the modeled methods of formation stimulation is more efficient and to be applied in West Absheron field after conducting feasibility report.

n	Calculation options	Total oil production, mln.m ³	Total gas production, mln.m ³	Additional oil production, mln.m ³	Additional gas production, mln.m ³
1	Base Option	2,36	191,05	-	-
2	Planning Wells	3,06	496,30	0,70	305,25
3	Water injection	3,91	442,50	1,55	251,45
4	Polymer	4,12	441,20	1,76	250,15
5	Hot water	5,27	388,80	2,91	197,75
6	Steam	4,05	412,00	1,69	220,95

CONCLUSIONS

Based on geological, geophysical and field data, geological and hydrodynamic models of West Absheron field were developed, initial geological reserves were estimated, and the development history was restored in the hydrodynamic model.

Based on the results of similar studies conducted at similar fields, the dependencies of phase permeabilities of gas-oil and water-oil ratios were developed for the productive horizons of West Absheron field and corrected in the process of restoring the development history.

Using the hydrodynamic model, the issue of choosing the optimal formation stimulation method was studied, development parameters were predicted in 6 different options, and the obtained results were compared.

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None.

AUTHORSHIP CONTRIBUTION

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Drafting - original draft: Vugar J. Abdullayev, Mehti A. Huseynov.

Writing - proofreading and editing: Vugar J. Abdullayev, Mehti A. Huseynov.



Chapter 07

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Technological Integration in Oil and Gas Industry Supply Chain Management

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ABSTRACT

The oil and gas industry exists at 3 main sectors (upstream, midstream, downstream), each of which includes a set of different processes. The management of these processes is related to different areas. One of these areas is supply chain management, namely transportation. Supply chain management assumes the responsibility of managing many complex processes, from the acquisition of oil and gas products as raw materials to their delivery to consumers. However, the management of these processes gives rise to some issues, the solutions of which require the integration of modern technologies. Some of these technologies are IoT, Blockchain, Big Data Analytics, Artificial Intelligence, which are also mentioned in the article. The article examines Supply Chain Management issues in the Oil and Gas industry, the integration of the listed technologies for improving this sector, and their benefits.

Keyword: Oil and Gas; Supply Chain; Management; Logistics.

INTRODUCTION

Oil and gas, as a raw material, unites many industries around itself. One of them is the supply chain and, accordingly, logistics. These two industries are responsible for many processes, from the acquisition of oil and gas as a raw material to its delivery to the end user. Supply chain and logistics are concepts that are often used together, but they are not the same. However, it is possible to consider logistics as part of the supply chain.

Yildiz⁽¹⁾ gave the following definitions regarding supply chain and logistics in his article: “The definition of logistics is the planning, implementation and control of the efficient flow of goods, services and related information from the point of origin to the point of consumption in order to meet the needs of customers. Supply Chain covers the entire supply chain from raw materials to finished products. Its management is a control process and involves the integration of activities between different organizations to maximize the flow of goods, information and services from suppliers to customers. It includes tasks such as supply ordering, production planning, inventory tracking, distribution channel management, etc.”

Supply chain models are divided into different purposes. In general, the most well-known supply chain models are as follows:

- Continuous flow model: a traditional model that has the property of stability.

- Agile model: the adaptation of the supply chain to changing market demands in the shortest possible time. Which is further accelerated by adaptive artificial intelligence models in the modern era.
- Fast supply chain model: one of the modern models applied by enterprises with products with short life cycles.
- Efficient Supply Chain Model: a model that has the property of maximizing efficiency.
- Custom-configured model: a model designed for a personalized approach.

Professionals should base their choices on the nature of the industry, customer requirements, and overall business goals.⁽²⁾

PAL⁽³⁾ outlined the main parts of this model as follows: the most basic model of supply chain management is the ITO model, which includes input-transformation-output components. The simple structure of the ITO model⁽⁴⁾ is as follows:

INPUTS (things, people) TRANSFORMATION (manufacturing, service) OUTPUTS (goods, services)

Additionally, it also includes resources, which include employees, equipment, facilities, systems, suppliers, etc. Another supply chain management model is the SCOR model.

The Supply Chain Operations Reference (SCOR) model is a powerful tool for assessing and comparing supply chain operations and performance. SCOR provides a unique framework that integrates business processes, metrics, best practices, and technology into a single structure to support communication among supply chain partners and improve the effectiveness of supply chain management and related supply chain improvement activities.⁽⁵⁾

The main processes of the SCOR model are: Planning, Source, Make, Deliver and Return. These were the 5 main processes of the previous versions, and in the new versions a new process has been added. The Enable process.

This process is a supporting tool, reflecting the increasing importance of activities that ensure the effective functioning of the main processes such as quality management, sales operations planning and supply chain risk management.⁽⁶⁾

The GSCF (Global Supply Chain Forum) model, like SCOR, focuses on the processes that connect the supply chain and the description of the physical flow of goods between supply chain members.⁽⁷⁾ It is implemented through three main elements, the supply chain network structure, supply chain business processes, and management components.⁽⁸⁾ There are eight relevant processes in the GSCF model: Customer Service Management, Demand Management, Order Fulfillment, Production Flow Management, Supplier Relationship Management, Product Development Management, and Returns Management. Logistics also plays an important role in the supply chain processes in the GSCF model.⁽⁹⁾

The concept of incorporating environmental sustainability procedures into a conventional production network is called “green supply chain management (GSCM).”⁽¹⁰⁾ The process of Green Supply Chain Management ensures the integration of environmentally sustainable procedures into all stages, from the acquisition of raw materials to their delivery to the end user.

One of the key elements of GSCM is a circular supply chain that minimizes waste by creating closed systems where products and materials are reused, recycled, or remanufactured.^(11,12)

Modern supply chain management is forcing businesses to change their models and strategies in this direction by integrating factors such as reducing costs and increasing customer satisfaction.

Logistics involves the coordination and transportation of goods from the production area to the delivery point, including the warehouse area. Its main goal is to optimize costs, space, and time to ensure the efficient distribution of goods and services.⁽¹³⁾

Supply chain management also includes logistics and is applied in various fields. One of these is the oil and gas industry.

Logistics and Supply Chain Management in the Oil and Gas Industry

The oil and gas industry is of great importance in the global context. It plays an important role in the world market, being used in small and large industries such as transportation, heat and electricity generation. The oil and gas industry is usually divided into three main sectors: upstream, midstream and downstream.^(14,15)

- Upstream sector: this sector involves the search for potential underground or underwater crude oil and natural gas deposits, the drilling of exploratory wells, and the drilling and operation of wells that subsequently produce and bring the crude oil or crude natural gas to the surface. The upstream industry is sometimes known as the exploration and production (E&P) sector.
- Midstream sector: it processes, stores, markets, and transports commodities such as crude oil, natural gas, natural gas liquids, and sulfur. The midstream provides a vital link between remote oil production areas and population centers where most consumers are located.
- Downstream sector: this includes refineries, petrochemical plants, petroleum product distributors, retail outlets, and natural gas distribution companies.

The supply chain is interconnected with all three sector. Blueoceanacademy⁽¹⁶⁾ on its website states the role of supply chain in the oil and gas industry as follows: “Each stage of the oil and gas chain is interconnected with the next. This means that there are several chain links that need to be analyzed and properly understood. These may include transportation, sales, materials management, technology, processing and other processes. In addition, there are supply chain management systems and tools that are used. Supply chain management in the oil and gas sector must be strictly adhered to from the planning stage to the execution stage. Companies should have a dedicated staff to act as consultants for the entire supply chain management in the oil and gas sector. These consultants should liaise with refinery managers and supervisors and operating engineers. These consultants aim to understand the entire operation of oil refineries and pipelines, propose and implement new technology to improve efficiency, and develop new strategies to increase production capacity.”

Thus, as mentioned, the sequence of processes consisting of several chain blocks maintains the competitiveness of the oil and gas industry even in the era of increasing renewable energy. Although the transition to renewable energy is currently being more widely accepted by various countries, the demand for the oil industry continues and will continue in the near future. In fact, the Global Oil and Gas Industry Market is predicted to reach 8,79 Trillion US Dollars in 2034.⁽¹⁷⁾

The potential scope of supply chain management in this industry includes the following:⁽¹⁸⁾

- Strategic supplier relationships.

- Customer relationships.
- Green purchasing and production management.
- Information sharing.
- Internal environmental management.
- Distribution and logistics.

Lisitsa et al.⁽¹⁹⁾ in their article “Supply-chain management in the oil industry” identified the following as the main factors for reducing costs and increasing company profits in supply chain management:

- Demand management.
- Efficient distribution of petroleum products among customers.
- Better transportation scheduling.
- Warehouse management.
- Quality and timeliness of data.

And it accepted all of these as parts of a unified process.

Technological Approaches in Supply Chain Management

A number of innovative approaches have been adopted to improve supply chain management in the oil and gas industry. Recent developments in the oil and gas industry include the increasing demand for better and faster customer service, the globalization of the oil and gas business, and the availability of information technology to facilitate information exchange.⁽²⁰⁾

Overall, supply chain management in this industry is being improved by the integration of a number of technologies and is driven by digitalization. Technological advancements such as the Internet of Things (IoT), blockchain, big data analytics (predictive analytics), and artificial intelligence (AI) have revolutionized SCM in the oil and gas industry.^(21,22)

Internet of Things in Supply Chain Management

IoT is being applied in the oil and gas industry for various purposes: Asset Management, Supply Chain Management, Monitoring and Control, Predictive Maintenance

Supply Chain Management and Logistics Optimization: IoT can optimize supply chain management and logistics by tracking shipments in real time and automating commercial documents and payments. The oil and gas industry can benefit greatly from using IoT in supply and inventory management, including higher efficiency, reduced costs, improved security, and increased sustainability.⁽²³⁾

The increasing complexity of logistics and supply chains in the oil and gas industry highlights the need for improved operational visibility and efficiency, which is fueling growth in this sector. Monitoring and control, with a market value of this sector expected to grow to US\$12,5 billion by 2032, also plays a crucial role by enabling real-time monitoring of operations, quickly eliminating inefficiencies, and ensuring compliance with industry safety regulations.⁽²⁴⁾

Blockchain in supply chain management

Blockchain is a chain of interconnected blocks that continuously grow by storing transactions in blocks.⁽²⁵⁾ Blockchain technology generally has the key features of decentralization, consistency, anonymity, and auditability. With these features, blockchain can significantly save costs and increase efficiency.⁽²⁶⁾ There are two types: permissioned and permissionless blockchains.

A good example of the permissionless classification is public blockchains. In a public blockchain, any user can enter or exit the chain at any time. Permissioned blockchains themselves are divided into two main groups: private blockchains and consortium blockchains.⁽²⁷⁾

Some of the applications of blockchain in oil and gas are:⁽²⁸⁾

- Optimizing Control of Physical Assets.
- Improving Transactions with Smart Contracts.
- Improved Land Registry Management.
- Improved Data Storage.
- Seamless Supply Chain Management.
- Transparency and Accountability in Transactions.

Most of the systems designed to control and manage trade in the oil industry are centralized, unreliable, and highly opaque.⁽²⁹⁾ Blockchain acts as a key tool in solving these problems. One of the main problems of blockchain is the financial issue. Because blockchain technology is a new technology for supply chain management and requires high investment.⁽³⁰⁾

The supply chain segment is expected to grow at a CAGR of 40,8 % from 2025 to 2034 due to greater transparency and improved operational efficiency in oil and gas transportation. Blockchain technology enables end-to-end tracking and anti-fraud records, eliminating fraud and errors in the supply chain.⁽³¹⁾

Blockchain and smart contracts, combined with IoT devices, can transform the traditional supply chain for oil and gas with the advantages of transparency and immutability. Blockchain takes the supply chain of oil and gas companies to the next level by providing a secure system for recording data and implementing and executing smart contracts. With the power of smart contracts and IoT devices, the oil supply chain can have the ability to source and secure.⁽³²⁾

Big Data Analytics in Supply Chain Management

Large data sets that are unmanaged, unmaintainable, and unusable for analysis using typical database systems are often described as “big data.”⁽³³⁾ This type of data can be found in various sectors and, if properly managed, can be highly beneficial. Many processes such as statistical analysis, forecasting, and strategy development rely on well-managed large data sets. Big data analytics is the process of analyzing large data sets to uncover unknown relationships and associations, market trends, and valuable insights.⁽³⁴⁾ It has types such as Prescriptive Analytics, Predictive Analytics, Diagnostic Analytics, Descriptive Analytics.⁽³⁵⁾

One of the areas where big data analytics is used is the oil and gas industry. Big data analytics helps to regulate key oil and gas operations such as exploration, drilling, production, and supply across three sectors - upstream, midstream, and downstream.⁽³⁶⁾

The emergence of big data allows for the consideration of complex factors in supply chain design, thus enabling the development of a robust supply chain network.^(37,38)

The successful use of big data analytics in the oil and gas supply chain requires a strategic approach to address these challenges, enabling organizations to develop the dynamic capabilities needed to thrive in a volatile and complex industry. Big data analytics has the potential to transform supply chain management in the oil and gas industry by delivering real-time insights, improving demand forecasting, and improving decision-making.^(39,40)

Artificial Intelligence in Supply Chain Management

Since the 1970s, artificial intelligence has been theoretically studied in the oil and gas industry. This includes widespread artificial intelligence methods such as fuzzy logic, artificial neural networks and evolutionary algorithms, etc. It is applied to solve many problems in each sector of the oil and gas industry - upstream (exploration and production), midstream (transportation and storage) and downstream (oil refining and sales). Artificial intelligence already today allows you to increase the efficiency of field exploitation: parameters such as well flow, waterlogging, and bottomhole pressure are analyzed, and optimal operating methods are selected to increase production and reduce costs.⁽⁴¹⁾

Currently, the application of Artificial Intelligence in the oil and gas industry is developing rapidly, as the concept of artificial intelligence is gradually integrated into various stages of the industry, such as smart drilling, smart production, smart pipeline, intelligent processing, etc. Areas such as digitalization, automation, forecasting, security, intelligence, supply chain management can be examples of the application of Artificial Intelligence in the oil and gas industry.⁽⁴²⁾

From the point of view of Artificial Intelligence, the exploration of oil and gas resources is a set of operations that result in the creation of a 3D geological model of an oil/gas field or reservoir.^(15,43)

AI in supply chain management is being applied to solve many issues such as improved efficiency, cost reduction, and improved customer satisfaction. In the oil and gas sector, AI optimizes supply chain processes by forecasting demand, managing inventory, and improving logistics operations. AI-based solutions analyze historical data, weather conditions, and market trends to predict supply chain disruptions and adjust logistics accordingly. This improves resource allocation, reduces delivery delays, and ensures more efficient supply chain flow.

In general, the impact of artificial intelligence in the oil and gas industry can manifest itself in several ways. These are:

- Improve Safety.
- Optimize Supply Chain.
- Increase Operational Efficiency.
- Minimize Environmental Impact.
- Reduce Carbon Footprint.

Along the supply chain, it can support sustainability by improving the efficiency of resource extraction, refining, transportation, and energy use. Artificial intelligence (AI) can uncover overlooked energy-saving opportunities by examining operational variables and historical data. Furthermore, by simplifying transportation routes and schedules, AI can reduce fuel consumption in logistics and greenhouse gas emissions associated with the transportation of goods, gas, and oil.^(44,45,46,47,48)

CONCLUSIONS

The process of supply chain management in the oil and gas industry is further improved by integrating modern technologies and approaches. These technologies and approaches include the Internet of Things, Big Data Analytics, Blockchain, Artificial Intelligence. Integration in the oil and gas industry allows the supply chain to improve in the following areas:

- Within the framework of the Internet of Things, higher efficiency, reduced costs, improved security, and high sustainability are achieved.

- End-to-end traceability and anti-fraud records are achieved within the blockchain framework, eliminating fraud and errors in the supply chain.
- Big data analytics enables real-time insights, demand forecasting, and improved decision-making.
- Within the framework of Artificial Intelligence, it is possible to support sustainability by increasing the efficiency of resource extraction, purification, transportation and energy use, enable energy savings, simplify transport routes and schedules, and reduce fuel consumption in logistics and greenhouse gas emissions associated with the transportation of goods, gas and oil.

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Chapter 08

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Waste Oil Monitoring and Water Informatics Using AI and IoT

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ABSTRACT

The paper addresses one of the major issues of modern technogenic society, that is the pollution of water areas by oil and petroleum products. It is noted that timely and accurate detection of oil spills along with trajectory prediction allows for their prompt localization, subsequent collection, and minimization of environmental damage. The aim of the present review is to assess the efficiency of modern technologies for detecting oil pollution in various conditions, particularly focusing on the application of sensor networks and the Internet of Things (IoT) technologies, as well as artificial intelligence methods. The paper provides a description and comparative analysis of various technologies, ranging from visual identification, technology of scattered light, fluorescence, and microscopy, to remote, optical, and wireless sensing techniques. The characteristics of devices for detecting oil spills have been presented. The potential of applying Visible Sensors, Infrared Sensors (TIR), Ultraviolet Sensors (UV sensors), Synthetic Aperture Radars (SAR), Side-Looking Airborne Radars (SLARs), Microwave Scatterometers, and Microwave Radiometers is described. Advanced systems capable of accurately measuring the thickness of an oil slick have been described, such as Laser Ultrasonic Remote Sensing of Oil Thickness (LURSOT), Effective Oil Thickness (EOT), and others. A review of multiphase sensors for crude oil facilities and transportation pipelines has been presented. It has been established that this type of sensors is unsuitable for operation under natural aquatic conditions. A potential solution to this problem is the deployment of systems comprising multispectral sensors, radiometers, sorbent materials, dip plates, imaging devices, tube samplers, acoustic detectors, and photometric sensors - so-called hybrid and remotely operated systems. The study describes the following modern systems: Multi-modality Systems, Remotely Operated Systems, and Microwave Sensors. A substantial paragraph is devoted to oil spill detection and monitoring using artificial intelligence, particularly Traditional Machine Learning Techniques. The possibility of using the following algorithms for classifying oil spills and their analogues has been considered: artificial neural network (ANN), support vector machine (SVM), decision tree (DT), K-nearest neighbor (KNN), genetic algorithm, random forest (RF), maximum likelihood, and linear discriminant analysis. The potentialities of monitoring oil spills using Artificial Neural Networks, Support Vector Machines, and Deep Learning Techniques have been outlined.

Keywords: Synthetic Aperture Radar (SAR); Optical Sensors; Internet of Things (IoT); Deep Learning; Remotely Operated Systems.

INTRODUCTION

Water and oil: the former is a source of life on the planet, without which the development of modern post-industrial society is impossible. The latter represents one of the key pillars

of energy sector (accounting for 36 % of global demand for primary energy); it is also used as raw material in the oil refining and chemical industries for the production of fuels, plastics, synthetic rubber and synthetic fibers, ethyl alcohol, detergents, and a wide range of other products. However, the processes of extraction, transportation, and processing of oil, given oil's toxic impact on the environment, are associated with certain risks. Particularly dangerous are leaks from offshore drilling platforms, discharge of ballast water from ships, pipeline ruptures, and sudden emergency discharges from wastewater treatment systems at oil refineries.

The difference between marine and terrestrial oil spills lies in the rate at which oil moves or disperses and in the corresponding size of the affected area. Oil spills in water are carried by wind and currents and often over long distances. However, oil movement on land is typically slower, it follows a downslope path, and tends to accumulate in natural lowlands, making it generally easier to predict.

Annually, 2,4 million tons of oil enter marine waters, forming a surface film with an area of about 48 000 000 km². Under the influence of several factors, such as temperature, ultraviolet rays, wind and wave currents, as well as the processes of diffusion, sedimentation, emulsification, evaporation, and biological decomposition, physical and chemical parameters of oil slicks gradually change. Toxic light oils evaporate quickly. Heavy oils are less toxic but persist in the environment for much longer periods. Heavy oils can bind with pebbles and sandy shorelines, where they can remain for years. Over time, oil slicks thin out, forming what is visually recognized as “oil sheen” caused by the difference in the refractive indices of oil and water, as well as the thickness of the film. According to the Bonn Agreement⁽¹⁾, the codes for the visual appearance of oil are presented in table 1.

Table 1. Appearance of oil on a calm water surface ⁽¹⁾			
Code	Description Appearance	Layer Thickness Interval (µm)	Litres per km ²
1	Silvery sheen	0,04 to 0,30	40 - 300
2	Rainbow sheen	0,30 to 5,0	300 - 5000
3	Metallic	5,0 to 50	5000 to 50 000
4	Discontinuous true oil color	50 to 200	50 000 - 200 000
5	Continuous true oil color	200 to more then 200	200 000 to more then 200 000

The data from the above-mentioned table are used both to determine the degree of sheen formed by the oil slick layer on the surface and to estimate its thickness and volume.

All fractions of oil cause irreparable harm to the environment by altering the parameters of the water surface, reducing oxygen levels, and worsening living conditions for plants and animals. Therefore, monitoring and detection of oil slicks are essential components of emergency response planning in the event of oil spills. Accurate detection of oil spills with trajectory prediction is necessary for their timely containment, they are beneficial for fisheries, wildlife protection, resolution of liability disputes, and resource management for monitoring and preservation of the marine ecosystem. However, visual detection of oil spills (table 1) is unreliable, since during daylight hours it can be mistaken for marine algae, and in the evening or at night, as well as in foggy conditions, visual detection is simply impossible.

The aim of this paper is to assess the efficiency of modern technologies for detecting oil pollution in water under various conditions, particularly focusing on application of sensor networks and the Internet of Things (IoT) technologies, as well as artificial intelligence methods.

METHOD

Methods and Technologies for Monitoring Oil Pollution in Aquatic Areas

Traditionally, oil monitoring in water has been carried out manually. For example, to detect bilge water discharges, technologies such as that of scattered light, fluorescence, and microscopy have been applied.

Scattered light technology is a popular choice onboard ships due to its relatively low cost and insensitivity to water color. On the other hand, an excessive amount of suspended particles may affect instrument readings. It is also necessary to take into account the influence of external factors that alter the properties of oil and thereby lead to errors in classifying oil types. This technology allows determining oil concentration based on the results of measuring the intensity of light passing through the water column. Oil particles present in the sample “refract” light depending on the level of oil concentration in the water. The higher is the oil content in the water, the greater is observed light diffusion. It should be noted that solid particles are also capable of scattering light. However, unlike the spherical molecules of oil, the irregular shape of solid particles affects the refraction of a light beam in a different way. The use of multiple sensors installed at different angles highlights the shape of the molecules and allows solid particles to be disregarded.

The quantitative assessment technology involves determining oil content by infrared absorption of the sample extract. At the first stage, after sampling, the samples are acidified to a low pH level and then extracted using chemical reagents. At the second stage, an infrared quantitative assessment is conducted, determining the oil content based on the infrared absorption of the extract and the total methylene (CH_2) content.

Fluorescence is a phenomenon in which a substance absorbs light energy and then emits it as light of a different wavelength. Oil particles are known to possess the ability to fluoresce under ultraviolet (UV) radiation. Since each type of oil responds to a specific light wavelength, the use of waves of known ranges makes it possible to determine the corresponding type of oil. However, the simultaneous presence of several types, especially in the presence of accompanying pollutants, may lead to measurement inaccuracies.

Microscopy is the determination of oil concentration by measuring the size of its droplets in bilge water using image processing and recognition software. A high-speed camera takes pictures of a sample at the speed of several shots per second. These images are analyzed using an existing database of components that can identify visible differences between oil, gas, and solid particles.

All the methods mentioned above relate to direct—stationary determination of oil products under laboratory conditions. It should be noted that this type of sampling has a number of limitations. Firstly, point samples, unlike continuous ones, are taken only at a specific moment in a specific location, which does not allow researchers to obtain a complete real-time picture of environmental pollution. Secondly, when using some methods, there may be potential confusion regarding the concentrations of “dissolved” and “dispersed” oil, since both are extracted using solvent extraction. As a result, fractions of dissolved oil may be included in the dispersed state, making it difficult for operators to accurately determine the ratio of fractions in accordance

with environmental requirements.

Based on the above, it can be concluded that current conditions urgently demand the application of innovative methods and technologies, including those based on artificial intelligence (AI), for tracking oil discharges, resource management, and environmental risk assessment.

Such methods include remote, optical, and wireless sensing techniques (table 2). Information required to model the spread of an oil spill can be obtained from multi-temporal imaging captured by remote sensing sensors. Devices of remote sensing include infrared video and photography, thermal infrared imaging, airborne laser fluorescent sensors, airborne and satellite optical sensors, as well as airborne and satellite SAR. Although satellite remote sensing provides a synoptic view, it suffers from low spatial and temporal resolution. The following information can be provided by sensors for an oil spill: location, area, and movement of oil slicks on the water surface; thickness of the film and the volume of spilled oil; and the classification of oil type for assessing environmental damage.

The information can be collected through remote sensing by both active and passive methods. Active sensors emit radiation directed toward the target, collecting reflected radiation from it. Passive sensors, on the other hand, collect and measure naturally available energy, such as solar radiation.⁽²⁾ The characteristics of major remote sensing technologies for detecting oil spills over marine waters are presented in table 3.

Table 2. The main methods for oil slicks detection ⁽³⁾		
Categories	Methods/Techniques	Description of the Methods
Remote sensing	Camera in visible and infrared spectrum ⁽⁴⁾	Include passive observation, optical techniques, visible spectrum, infrared sensors, radar, satellite radar systems, laser fluorosensors, and slick thickness measurements using ultrasonics and chemical analysis
	Underwater acoustic method ⁽⁵⁾	Detection feasibility of Hazardous and Noxious Substances (HNS) using two methods. Firstly, a tank experiment with 200-kHz active sonar utilized castor oil as a chloroform alternative to examine underwater acoustic detection, and secondly, a computer simulation evaluated the potential of side scan sonar for detecting chloroform and tetrachloride randomly distributed on different seabed types.
	Multi-temporal approach ⁽⁶⁾	Change Vector Analysis (CVA) was employed to examine the present image of the region and compare it to a reference image dataset that had undergone statistical analysis to lessen sea spectral variability across time to develop an automatic detection algorithm.
Optical sensing	Light Emitting Diode (LED) and Light Dependent Resistor (LDR) ⁽⁷⁾	The study proposes an optical sensor system using LEDs to monitor oil concentration in irrigation ditches. The sensor differentiates between the presences of diesel engine oil, identifies the gasoline engine oil source, and estimates the concentration of oil from 0 to 0,20 mL/cm ² range. The algorithm combines signals from white, blue, and red LEDs for comprehensive oil monitoring in the irrigation system.

Wireless sensor	Light Detection and Ranging (LIDAR) sensor ⁽⁸⁾	A 905 nm laser LiDAR system, with 3 channels and 3 Hz scanning, distinguishes seawater from oil. It detects various oil thickness, presenting thick oil as brighter pink on the seawater surface. Key parameters include sensed area, spill thickness, detection Field-of-View (FoV), and time.
	L a s e r - i n d u c e d fluorescence (LIF) sensor	Discuss LIF spectral features for different states of oil products in seawater and thin slicks. It introduces a calibrated LIF method for identifying and measuring ocean pollution from bilge water disposal, along with a small-sized LIF sensor for unmanned aerial vehicles (UAVs) to monitor oil pollution at sea.
	Optical reflectance ⁽⁹⁾	The proposed method effectively estimated the thickness of oil samples in laboratory conditions and accurately determined the volume of thicker oil samples in outdoor settings using RGB images.
	Wireless Sensor Networks (WSNs) ⁽¹⁰⁾	The method involves incorporating intelligence at multiple aggregation levels, transforming sensor nodes into active, intelligent observers, thus enhancing the efficiency of the network and contributing to the improvement of oil spill detection in oceanographic research.
	Internet-of-Things (IoT) ⁽¹¹⁾	The study describes the creation of an autonomous oil–water separator that is Internet of Things (IoT)-based and supports water ecosystems’ oil pollution monitoring system. The water-oil separation was carried out by applying semi-permeable membrane nanotechnology.
	Satellite Aperture Radar (SAR) An MPRI Technical Report	This study introduces a novel method for detecting oil spills using satellite synthetic aperture radar (SAR) systems. The technique employs convolutional neural networks (CNNs) trained with an adversarial loss function for image-to-image translation, demonstrating promising results in discriminating between real oil spills and lookalikes in SAR data from Radarsat-2 and Sentinel-1 over the Mediterranean Sea, Atlantic Ocean, and the North Sea.

Table 3. RS technologies for detecting oil spill over marine water ⁽¹²⁾			
RS Technique	Sensor	Principle of detections	Results
Optical Remote Sensing	Visible	Color, absorption of sun-glint on water surface, optical properties differences.	Easy distinguishing the oil spill due to color contrast ^(13,14)
	Infrared	Absorption of light at specific wavelengths	Identification of oil slicks ⁽¹⁵⁾
	Thermal Infrared	Detection of oil spill on the bases of Thermal characteristics difference between oil and marine water	Thickness of oil spill over water surface ⁽¹⁶⁾
RADAR (SAR)	Microwave	The dampening action of the spilled oil causes a change in surface roughness.	Oil spills can be easily distinguished from other ocean features ^(17,18)

The studies by Goodman⁽¹⁹⁾ contain the characteristics of remote sensing bands and related instruments used for oil spill detection (table 4).

Table 4. Remote sensing bands and related instruments used for oil spill detection⁽¹⁹⁾

Band	Wavelength	Type of Instruments
Radar	1-30 cm	SLAR/SAR
Passive microwave	2-8 mm	Radiometers
Thermal infrared (TIR)	8-14 μm	Video cameras and line scanners
Mid-band infrared (MIR)	3-5 μm	
Near infrared	1-3 μm	Film and video cameras
Visual	350-750 nm	Film, video cameras and spectrometers
Ultraviolet	250-350 nm	Film, Video cameras and line scanners

Visible Sensors: despite a number of disadvantages that hinder the accurate identification of the exact location of spills (such as sun glint and surface ripples creating the illusion of oil sheen; presence of marine algae and darker shorelines mistakenly interpreted as oil spills), Visible Sensors continue to be widely used in remote sensing. The advantages of Visible Sensors include their wide availability and ease of installation on aircraft. A number of recent innovations in the development of this technology should be noted. Drones are equipped with both visible and infrared cameras. Recent advancements in sensor technology have enabled the creation of hyperspectral sensors like the Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) and the Airborne Imaging Spectrometer for Applications (AISA). Hyperspectral imagery captures data across dozens or even hundreds of spectral bands, allowing for the identification of an object's unique spectral signature.⁽²⁰⁾

Infrared sensors: in the studies^(21,22) the authors discuss the use of infrared sensors for determining the properties of oil spills. Oil absorbs solar radiation and re-emits a portion of it as thermal energy, primarily in the thermal infrared spectrum (8-14 μm). In the study by Salisbury et al.⁽²³⁾ the authors noted that since oil has lower emissivity, its spectral signature in the thermal infrared range (TIR) is clearly visible against the water background. Thicker layers of oil absorb more radiation and therefore appear warmer in thermal infrared (TIR) imagery. Oil with medium thickness tends to appear cooler in this region, while thin sheens are generally undetectable in TIR. The minimum detectable oil thickness ranges from 20 to 70 μm , and the transition from a warm to a cool appearance occurs within the 50 to 150 μm thickness range.⁽²⁴⁾ At night, the reverse pattern is observed: heat loss in oil is faster than in water and therefore, thick oil appears cooler than water. The drawback of infrared sensors is their inability to detect oil emulsions, since emulsions contain up to 70 % water and their thermal properties are similar to those of background water.⁽²⁴⁾

Ultraviolet Sensors make use of reflected sunlight in the ultraviolet region (0,32-0,38 micron) for oil spills detection. A UV sensor can detect thin sheens (less than 0,1 micron thick), whereas oil spills of thickness more than 10 micron are not generally detected by this type of sensors. UV images are only capable of providing information concerning the relative thickness of oil slicks.⁽²⁵⁾ Additionally, there are a number of interferences that hinder accurate detection, such as wind-driven ripples, sun glint, and algae accumulation. As these interferences differ from those that affect infrared measurements, the combination of IR and UV sensing can provide a more accurate indication of the presence of oil than using either method alone.

Radar: the radar functions as an active sensor, operating within the radio wave region, and is used for detecting oil in a large area. Ocean water is imaged brightly as a result of radar waves

being reflected by capillary waves.⁽²⁶⁾ The presence of oil in the ocean reduces reflectance by diminishing capillary waves. Therefore, oil can be detected as a dark area in a bright image of the ocean.⁽²⁷⁾

There are two main types of radars used for remote sensing of oil spills: Synthetic Aperture Radars (SAR) and Side-Looking Airborne Radars (SLARs). The latter is an older and less expensive technology that achieves spatial resolution using a long antenna. The synthetic aperture radar uses the aircraft's forward motion to create a very long antenna, achieving excellent spatial resolution (independent of range) but requiring sophisticated electronic processing.⁽²⁴⁾ Compared to SLAR, SAR radars, although more expensive, offer a wider range and better resolution.⁽²⁸⁾

The radars are characterized by a number of serious flaws because of numerous deception targets. Fresh water slicks, wind slicks (calms), shadows cast by waves, land or structures, weed beds, which calm the water just above them; glacial flour, biogenic oils and the sea state are all factors to be considered.⁽²⁴⁾ A number of studies highlight the impact of wind speed on radar readings.^(29,30) Indications are that wind speeds of at least 1,5 m/s (3 knots) are required for detection, and speeds of 6 m/s will remove the effect again. Shipborne radars suffer from similar limitations and have the additional drawback of low installation height, which limits their range to 8-30 km depending on the antenna height.⁽³¹⁾

Microwave Scatterometers: a microwave scatterometer is a device that measures how a target scatters microwave or radar energy. Just as it does for radar sensors, the presence of oil reduces the scattering of microwave signals. However, this is subject to a large number of interfering factors, as mentioned above.⁽²⁴⁾ Microwave scatterometers are characterised by two main disadvantages: the inability to discriminate between oil and the lack of imaging capability.

Microwave Radiometers: both seawater and oil are sources of microwave radiation. However, oil is a stronger emitter, as evidenced by a comparison of their emissivity coefficients: for seawater the emissivity coefficient is 0,4, while for oil it is 0,8.^(32,33) Microwave Radiometers detect this difference and thereby enable detection of pollution by oil. Additionally, there is a signal change in thickness, which, in theory, means the device could measure it. Having analyzed the studies,^(24,34,35) it can be concluded that passive microwave radiometers can be used as all-weather oil detection sensors. However, their potential as a reliable device for measuring the thickness of an oil slick is questionable.

Slick Thickness Sensors: accurate measurement of the thickness of an oil slick would enable more effective response actions, including dispersant application and in-situ burning. As early as the late 1980s and early 1990s, a number of laboratories conducted research on thermal remote sensing methods. The first results were described in the study,⁽³⁶⁾ and the method was later named accordingly - «thermal mapping». In this technique, an infrared camera is used to examine the temperature profiles created over a small region near the heated oil. These profiles are the result of a laser being used to heat the oil. The thickness of the oil determines the temperature profiles that are created.

Another, more advanced method—Laser Ultrasonic Remote Sensing of Oil Thickness (LURSOT)—was first described in the works.^(37,38) This system consists of three lasers, one of which is connected to a Fabry-Pérot interferometer for precise measurement of oil layer thickness.⁽³⁸⁾ The sensing process is initiated by a thermal pulse generated in the oil layer by the absorption of a powerful CO₂ laser pulse. Rapid thermal expansion of the oil layer occurs near the surface, where the laser beam was absorbed.

This results in a step-like increase in the surface of the sample, as well as a high-frequency, large-bandwidth acoustic pulse (~15 MHz for oil). The acoustic pulse moves through the oil until it hits the oil-water interface. At this point, it is partly transmitted and partly reflected back towards the oil-air interface. This causes a small movement of the oil surface. The time taken for an acoustic pulse to travel through the oil and back to the surface again depends on the oil's thickness and acoustic velocity. A second laser probe beam is used to measure the displacement of the surface. This beam is aimed at the surface.^(24,27) Surface motion causes a phase or frequency shift (Doppler shift) in the reflected probing beam. This phase or frequency modulation of the probing radiation can then be demodulated using a confocal Fabry-Pérot interferometer).⁽³⁹⁾ The thickness can be determined by measuring the propagation time of the acoustic wave between the upper and lower surfaces of the oil slick. This method is considered to be well-established and reliable for assessing the thickness of oil layers.

Thermal remote sensing methods have been capable of estimating the Effective Oil Thickness (EOT) from image pixels with a significant oil presence, regardless of the type of oil emulsion.⁽⁴⁰⁾ Daniel Leifer et al.⁽⁴¹⁾ applied thermal infrared (TIR) remote sensing to estimate the thickness of oil slicks using a numerical three-layer heat transfer model based on thermal contrast. It was found out that the thermal profile decreased linearly through optically thin oil both with and without illumination, and through thick oil without illumination. Thus, this method is dependent on the type of oil, varying environmental conditions, and surface illumination. More recent developments include multiphase sensors and measurement systems for separation tanks in crude oil facilities and transportation pipelines.^(42,43) The systems in question include floaters (displacers) based on density, differential pressure transmitters, ultrasonic transducers, gamma-ray sensors and multi-electrode capacitive sensors.^(4,5)

In the studies^(6,8) sensors specialized in detecting emulsion layers in oil tanks are described. Furthermore, the work of S. Chakraborty et al.⁽¹¹⁾, presents sensor characteristics capable of detecting contamination levels in air-oil-water systems in industrial facilities, oil tanks, and transportation pipelines. However, all the aforementioned multiphase sensors were developed for operation under controlled industrial conditions and are not suitable for measuring oil slicks on open water. This is due to the continuous variation of the physical properties of oil mixtures in open water conditions, influenced by weather and sea dynamics. Moreover, oil spills create complex and sometimes unpredictable properties of oil-water mixture, which in certain cases cannot be identified using traditional autonomous calibration methods. These complications make the measurement of oil slick thickness one of the most challenging tasks during oil spill events.

A potential solution to this problem is the deployment of systems comprising multispectral sensors, radiometers, sorbent materials, dip plates, imaging devices, tube samplers, acoustic detectors, and photometric sensors (table 5).⁽⁴⁴⁾

Multi-modality Systems: these systems integrate several techniques, such as capacitive, inductive, conductive, ultrasonic, and optical methods to measure the oil thickness collaboratively.

Inductive monitoring systems are widely used for multi-interface contamination level measurements at industrial processing plants. They typically consist of several inductive coils distributed vertically along a guiding rod. Their operating principle is based on detecting changes in induced current in each coil, which correlates with the conductivity of the surrounding

medium. Therefore, they are limited to differentiating between conducting and non-conducting materials—such as oil and water—but cannot distinguish between non-conducting substances like air and oil. One advantage of these systems lies in their reduced susceptibility to contamination issues due to the magnetic nature of their measurements. This principle was employed in the inductive-capacitive dual-mode sensor, which has combined arrays of flat electrodes and coils to achieve multiphase level measurement.

Table 5. Hybrid & remotely operated systems properties ⁽⁴⁴⁾					
Modality	Structure	Target Application	Resolution (mm)	Range (mm)	
Capacitive and inductive ⁽⁴⁵⁾	Capacitive array for non-conductive - inductive array for conductive materials	Multiphase gravity separators	Not reported	< 200	
Capacitance and resistance ⁽⁴⁶⁾	Combining tomograms from commercial ECT (M3C) and ERT (V5R) systems	Visualizes gas-oil-water multiphase flow in horizontal pipelines	Pixel dimension of 1x1	T o m o g r a m (60x60 pixels)	
Capacitive and ultrasonic ⁽⁴⁷⁾	Capacitive sensor array to detect the oil-water interface - ultrasonic sensor to detect the air-oil interface	Measures the oil slick thickness	2 (handheld), 12 (skimmer)	< 92 (handheld), < 552 (skimmer)	
Acoustic ⁽⁴⁸⁾	Acoustic sensors mounted on ROVs and AUVs	Measures the oil slick thickness	Not reported	< 6	
Multispectral ⁽⁴⁹⁾	Multispectral sensors mounted on UASs	Classification of oil slick thickness from thin sheens to actionable oil	0,01	0,0005 to 20	
Ultrasonic ⁽⁵⁰⁾	Ultrasonic sensors (2,25 MHz and 5 MHz central frequencies) mounted on an ROV	Measures oil slick thickness	0,5	1 and 4,5	
Ultrasonic and Vision ⁽⁵¹⁾	ROV with ultrasonic sensors combined - an airborne drone with an optical camera	Measure thick oil slick thickness and estimate the oil volume	Not reported	> 0,5 (< 7,5 tested)	

Remotely-operated Systems: the method for measuring the thickness of an oil slick involves the use of acoustic sensors positioned beneath the slick. This technique is used for real-time quantification of the rate and efficiency of in-situ burning. Experimental results demonstrated its capability to measure oil slick thickness within the range of 1 mm to 10 mm. Unmanned aerial vehicles (UAVs) have been employed to measure oil slick thickness using multispectral sensors. ⁽⁴⁹⁾ Experimental evaluation has shown that this method could classify oil thickness ranging from thin rainbow-colored sheens (a few micrometers thick) to dark oil patches (several millimeters to centimeters thick).

The study ⁽⁵¹⁾ presents research on measuring oil slick thickness using two ultrasonic sensors (2,25 MHz and 5 MHz) mounted on an ROV. Ultrasonic reflections were collected from beneath the oil slicks while the ROV was either stationary or in motion. Oil layer thickness was estimated

based on the analysis of ultrasonic transit time within the oil slick. As a result of the conducted experiments, the minimum measurable layer thickness was determined to be 0,8 mm and 0,45 mm for the 2,25 MHz and 5 MHz transducers, respectively. The two transducers were able to measure oil slick thickness in the range of 1 mm to 4,5 mm with a maximum absolute error of approximately 0,3 mm when the ROV was stationary.

Microwave (MWR): the microwave (MWR) is a passive sensor. It is used for oil spill detection. It can also be used for oil thickness measurements. Microwave radiation is stronger from oil than from water, and it looks brighter too. The measurement of oil thickness using MWR is affected by the presence of radiation from the upper and lower boundaries of the oil film. However, microwave sensors are favored over optical ones because they are capable of acquiring data at any time, regardless of lighting conditions. Microwaves are emitted by satellites, which then use reflected waves to identify the presence of oil spills on the water surface. The dissipation of waves is accelerated and their growth is slowed down by oil due to its viscoelastic properties. There are a number of ways to detect oil spills using satellite images. These include image segmentation, dark spot detection and feature extraction. The methods are based on the idea that isolated image sections are easier to investigate.^(52,53) Additional Requirements - MWR (Microwave Radiometry) requires a specialized antenna to receive the emitted microwave radiation, as well as extensive information on numerous environmental characteristics and oil properties. All of these factors indicate both the complexity of system operation and its high cost.

Oil Spill Detection and Monitoring Using Artificial Intelligence. Studies on remote sensing of oil spills^(54,55,56,57) have primarily focused on the advantages of utilizing different sources of remotely sensed data and various techniques for oil spill detection and delineation. However, they have not considered applying modern machine learning (ML) techniques for identifying oil spills/slicks. A wide range of studies have examined and adopted the use of RS technologies and ML algorithms for detecting and monitoring oil spill slicks, with these technologies being used in a synergistic way.^(58,59,60,61) The analysis of remote sensing data has demonstrated the efficiency of using ML techniques for detecting oil spills in an automated mode.

Figure 1 illustrates the process of developing and adopting machine learning (ML) models for oil spill detection.⁽⁶²⁾

Traditional Machine Learning Techniques: the main stages of oil spill detection using this technology include: preprocessing of remote sensing data; image segmentation to identify dark spots; determination of distinguishing features and classification of objects in the image for distinguishing oil spills and their look-alikes. The method is based on the results of recursive and iterative analysis of possible solutions from a predefined database of sample inputs and features, without explicit programming.⁽⁶³⁾ The following algorithms may be used for classifying oil spills and their look-alikes: artificial neural network (ANN),^(64,65,66) SVM,⁽⁶⁷⁾ decision tree (DT),⁽⁶⁸⁾ K-nearest neighbor,^(69,70) genetic algorithm⁽⁷¹⁾ random forest (RF),⁽⁷²⁾ fuzzy logic,⁽⁷³⁾ maximum likelihood, linear discriminant analysis,⁽⁷⁴⁾ k-means,⁽⁷⁵⁾ ensemble learning.⁽⁷⁶⁾

Artificial Neural Network: the basic topological structure of Artificial Neural Networks (ANNs) consists of three layers: input, hidden, and output. The training process of artificial neural networks (ANNs) consists of three key stages: feeding the input data forward through the network, computing the error between the predicted output and the actual output, and updating the connection weights accordingly.⁽⁷⁷⁾ After completing training and validation, the neural network model can accurately identify oil spills in new data with similar features. A key

issue in using ANNs for oil spill classification is determining the optimal combination of ANNs hyperparameters, such as the number of hidden units, the size of batches, training iterations, learning rate, and momentum, since poor choices may negatively impact its accuracy and computing performance. The accuracy of the ANN method in oil spill studies ranges from 72 % to 99 %.

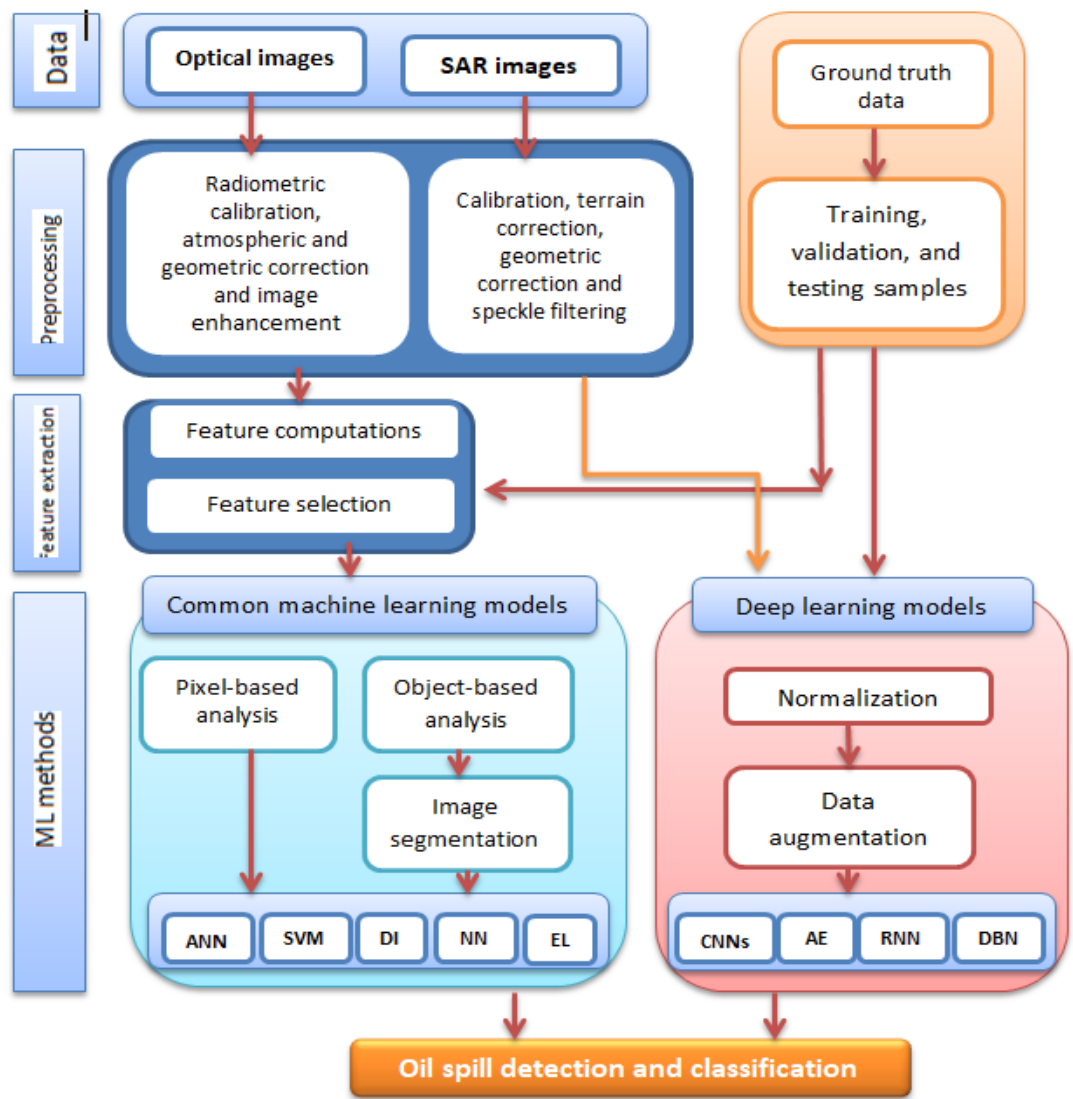


Figure 1. Framework of oil spill detection⁽⁶²⁾

Support Vector Machine: SVM,⁽⁷⁸⁾ a non-parametric controlled machine learning technique, based on the principle of minimization of statistical learning theory, has been successful in a large number of remote sensing applications. The SVM method allows processing of a multidimensional feature space and provides achieving satisfactory classification results with a limited number of training samples. SVM focuses on samples that lie close to the class boundaries in the feature space, referred to as support vectors. The SVM method aims to determine the location of a separating hyperplane (decision boundary) that provides optimal class separation to minimize

classification errors and achieve satisfactory generalization capability. The accuracy of SVM in oil spill studies ranges from 71 % to 97 %.

Decision Tree: DT is a simple non-parametric machine learning classifier that recursively divides the input dataset into branches of data subsets; each subset is described by a set of features, threshold values, and class labels.⁽⁷⁹⁾ DT is widely used to assist in developing rule sets for classifying remote sensing data using an object-based image analysis (OBIA) approach, due to its ability to handle non-linear relationships between features and feature values from different scales or value ranges and classes. Tree-based classifiers are highly sensitive to even minor variations in the training data. Therefore, it is essential to carefully develop a training dataset that can successfully distinguish between oil spills and lookalikes.⁽⁶⁸⁾ The accuracy of DT in oil spill research ranges from 80 % to 96 %.

Deep Learning Techniques: Deep Learning (DL) algorithms represent a series of distinct deep neural networks (DNNs) that automatically learn complex discriminative features from significantly larger volumes of data in a hierarchical manner, extracting information through multiple high-level abstraction layers.⁽⁸⁰⁾ Unlike traditional machine learning methods, deep learning is entirely data-driven, where the inherent relationships between inputs and outputs are automatically established, and the feature representations are learned directly from the data without manual intervention.⁽⁸¹⁾ The step involving the extraction of features is no longer dependent on the construction of hand-crafted features by experts before the classification phase of the oil spill.

Various DL models have demonstrated excellent results in oil spill detection using SAR and optical images, due to their ability to automatically extract discriminative learned features for recognizing oil spills and their look-alikes. Moreover, the generalization capabilities of these models can account for the case-specific nature of traditional methods. These models have been used to perform various tasks such as oil spill detection and recognition,⁽⁸²⁾ Classification on the basis of fragments, definition and semantic segmentation.^(83,84) Among the widely adopted architectures in deep learning are convolutional neural networks (CNNs), autoencoders (AEs), recurrent neural networks (RNNs), deep belief networks (DBNs), and generative adversarial networks (GANs).^(85,86)

CONCLUSIONS

1. The paper addresses one of the major issues of modern technogenic society, that is the pollution of water areas by oil and petroleum products, which can be partially resolved through the use of modern technologies for early oil spill detection.
2. The technologies used for solving this issue include the following: the technology of scattered light, fluorescence, microscopy, as well as remote, optical, and wireless sensing methods, each with specific conditions of application and detection ranges.
3. A review of multiphase sensors for crude oil facilities and transport pipelines has led to the conclusion that these sensors are not suitable for operation in natural aquatic areas. A potential solution is the implementation of hybrid and remotely operated systems.
4. Of particular interest are modern developments in the field of remote determination of oil slick thickness: remotely operated systems, microwave sensors, and the use of multispectral and ultrasonic sensors (with frequencies of 2,25 MHz and 5 MHz) installed in unmanned aerial vehicles (UAVs).
5. The most advanced technologies for oil spill monitoring are based on Artificial Intelligence, particularly Artificial Neural Networks and Deep Learning Techniques. DL

algorithms represent a set of individual deep neural networks (DNNs) that automatically study complex discriminant features from large volumes of data in a hierarchical manner to extract information through multiple high-level layers of abstraction. Additionally, for classification of oil spills and their analogues, other algorithms can be applied: artificial neural networks (ANN), SVM, decision tree (DT), K-nearest neighbor, genetic algorithm, random forest (RF), maximum likelihood, and linear discriminant analysis.

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Part III

Advanced Materials,
Metal Complexes,
and Nanoscience



Chapter 09

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Ecological Basis for the Use of Iron and Manganese-Based Metal Complexes

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ABSTRACT

A series of reactions were carried out in the interfacial H_2SO_4 /DEAN catalytic environment based on ferrocene and cymantrene, and new derivatives were synthesized. The obtained derivatives exhibited antidetonation properties. DEAN-diethylammoniumnaphthenate- $(\text{C}_2\text{H}_5)_2\text{NHCOOR}$ (R-naphthene residue), which plays the role of a carrier in the process, is obtained from the interaction of diethylamine $(\text{C}_2\text{H}_5)_2\text{NH}$ with naphthenic acid. The main feature of this compound is that it reacts with strong acids, in our case concentrated sulfuric acid, to form an intermediate complex, and then enters into ion exchange reactions. Using this property of them, it was possible to use them in interphase catalysis reactions. In this regard, by using DEAN, it was possible to overcome the immiscible interphase barriers by transferring one of the reactants from the aqueous medium to the organic phase. In this case, by using a carrier, it was possible to ensure the solubility of organometallic compounds in organic solvents, taking into account the hydrophobicity of the compounds, and to increase the yield of the reaction product. As a result, the yield of the reaction product was relatively high.

Keywords: Cyclic Ketone; DEAN; Sulfuric Acid; Interfacial Catalysis; Ferrocene; Cymantrene.

INTRODUCTION

The use of additives in fuels is very important. What is more important is how the additives added to fuels affect the environment from an ecological perspective. Until 1980, tetraethyllead (TEL), which was widely used as an additive in fuels, polluting the environment and causing very serious diseases in the human body, completely limited the possibilities of using this substance. Tetraethyllead was very profitable as an additive, it was added in an amount of 0,5-0,8 g per 1 kg of gasoline. Since it has an ecologically toxic and carcinogenic effect, many countries banned its use in accordance with Euro-2 standards at that time, and only then did research begin on many substances for use as anti-knock additives.

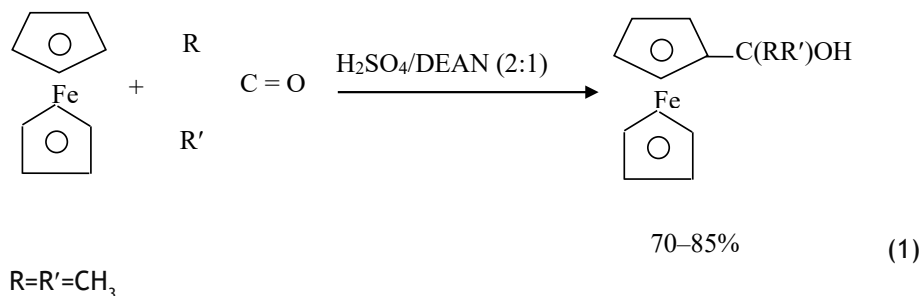
In our modern era, the requirements of Euro-5 standards are completely different. Better yet, the use of electric vehicles with zero pollution for the environment is one of the main requirements of the modern era. However, since a complete transition to electric vehicles is economically difficult, new standards must be developed to make fuel-powered engines safe or at least slightly dangerous for the environment. In this case, the main issue facing us is the development of environmentally friendly additives that are as harmless as possible to the environment. In this direction, the use of organometallic compounds and derivatives based on them has been one of the main directions in finding a solution to environmental problems. As the metal contained in organometallic compounds converts the oxygen that provides combustion into more effective atomic oxygen, it is also added to the fuel in a very small amount (37 mg/

ml). This makes the use of these substances efficient and prevents the formation of metal oxides, even in small quantities, during combustion in the process. It should be noted that the industrially produced cement-based anti-knock additive composition produced by the German company “hi-tech”, as well as the FK-4 ferrocene-based compositions of the Russian “Khimki” plant, have wide production and application areas in many oil refining production areas.

The possibility of using more effective additives for environmental protection is always on the agenda. As the demand for gasoline and diesel fuel has increased in recent years, it is very important to have environmentally friendly additives. For this purpose, we have investigated the possibilities of using organometallic compounds in motor transport. The most widely used representatives of organometallic compounds: ferrocene and cymantrene have been the main objects of our research.

Many substances based on ferrocene and cymantrene have anti-knock properties. On the other hand, these compounds, like octane number enhancers, also have a smoke-reducing effect by ensuring normal engine operation. In order to increase the compression resistance of low-octane motor fuels, a large amount of additives is required. In this case, certain problems arise: as a result of the deposition of metal oxides in the combustion chamber and on the surface of the burning spark plugs, the engine fails and eventually becomes unusable from an ecological point of view. In order to ensure normal engine operation, the amount of metal in various brands of gasoline is determined according to international standards. According to these standards, the amount of iron is 17-37 mg/l, and the amount of manganese is 28-55 mg/l. This amount is also considered useful from an ecological point of view. In order to reduce the amount of metals (Fe, Mn) in ferrocene and simantrene molecules, alkyl and oxyalkyl groups that do not have an antiknock effect are introduced into the molecules. For this purpose, alkylation reactions of ferrocene and simantrene were carried out based on Friedel-Crafts reactions. For the first time, we used pyrocondensate, which is a pyrolysis product of naphtha gasoline, for the alkylation of ferrocene. Pyrocondensate contains 32-35 % unsaturated hydrocarbons of various structures.

Below is the synthesis reaction of ferrocene-based derivatives in an interfacial catalytic environment. Here, depending on whether the ketone used is aliphatic or cyclic, the yield of the reaction product varies. Thus, when $\text{H}_2\text{SO}_4/\text{DEAN}$ was used in a 2:1 ratio, the corresponding ferrocenylcarbinols were obtained in high yields with aliphatic and cyclic ketones.^(1,2)



It should be noted that the reactions considered were first carried out in the presence of concentrated H_2SO_4 acid. The course of the process is described below.

METHOD

A three-necked flask with a volume of 0,5 liters is blown with nitrogen. After adding 15 ml of pungent-smelling cyclohexanone (cyclopentanone) to the flask, it is cooled to -10°C under cold

conditions with an ice-cold NaCl (salt) solution, and 20 ml of 92 % H_2SO_4 acid, previously cooled to -10°C , is added to it. Then the mixture is stirred in a mixer for 30 minutes. It should be noted that the process is exothermic, so it proceeds with the release of heat. This has a negative effect on the course of the reaction and the yield of the reaction product.

Therefore, the process is carried out with constant cooling with ice water (-10°C). The color of the mixture is light yellow, but gradually the color becomes brown and dark. Then, with stirring in a medium-speed mixer every 10 minutes, ferrocene in the form of an orange powder with a total mass of 9,8 grams is added in portions to the reaction mixture. Stirring is carried out until the dark brown color obtained in the process (a greenish color is visible on the walls of the beaker) remains unchanged, stirring continues for about two and a half hours. The reaction mixture obtained in this way is neutralized in parts with a solution of NaHCO_3 (baking soda). At this time, foam forms on the solution. Through the baking soda, the carbinol derivative of ferrocene rises to the solution through the foam. The foam is collected by filtration, washed several times with distilled water, and dried in a drying cabinet. In the process, a solid substance, ferrocenylcyclohexanol, is obtained, which changes color from orange to yellowish. The obtained substance has a specific odor. The soda solution used as a neutralizer is prepared as follows:

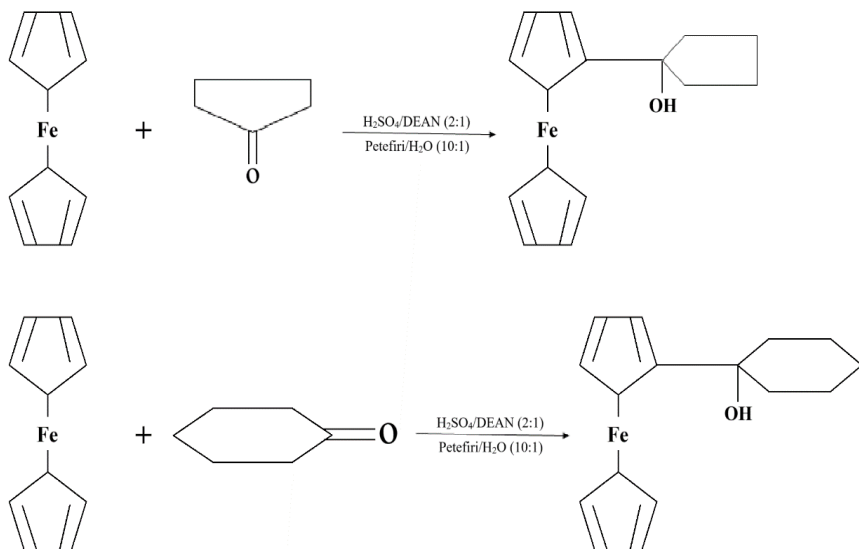
NaHCO_3 (baking soda) was added in portions to one liter of distilled water previously placed in the refrigerator and mixed. Then, this solution was added in portions (10 ml) to the reaction mixture. At this time, the foam that formed on the surface of the solution brought the newly formed yellow substance to the solution. It was collected through a skimmer into a filter covered with a sieve, washed once or twice with cold distilled water, and dried in a drying cabinet. A total of 22-23 grams of NaHCO_3 baking soda were used in the process. After drying, the powder was weighed on an analytical balance and the amount of reaction product was calculated based on the molar amount of ferrocene. Since the yield was not high, the same reaction was also carried out in an interfacial catalysis environment.

Thus, concentrated sulfuric acid and diethylammonium naphthenate were used to create the interphase medium. These substances were taken in different ratios and the best result was obtained in the ratio $\text{H}_2\text{SO}_4/\text{DEAN}$ 2:1. The process flow is given below.

The same reaction was carried out in the presence of diethylammonium naphthenate (DEAN), a viscous and dark brown substance. The synthesis process was carried out as above, but the difference was that two phases were used in the course of the reaction. For this, 30 ml of petroleum ether with a specific odor, boiling at $30^\circ\text{--}70^\circ\text{C}$, was taken. 15 ml of cyclic ketone (cyclopentanone or cyclohexanone), 9,8 g of orange-colored powder-ferrocene were added to it and mixed. At this time, no reaction occurred. 20 ml of 92 % H_2SO_4 solution was added to this mixture, then 10 ml of brown viscous diethylammonium naphthenate (DEAN). In the process, 92 % sulfuric acid served two functions: sulfuric acid was used both as a catalyst and to neutralize the acidic environment. The inorganic phase was transparent, and the organic phase was colored chestnut after the addition of ferrocene. At the boundary (separating boundary) of these two phases, brown DEAN was located. After heating the flask to 10°C , the onset of the reaction was observed. Since, as we mentioned above, the process is exothermic, it was sufficient to initially heat the flask to a temperature of 10°C for the reaction to proceed. The onset of the reaction was determined by the gradual browning of the transparent color in the inorganic phase. First, 92 % sulfuric acid was added to the inorganic phase, that is, water, and then petroleum ether. At this time, the organic and inorganic phases separated. When left

to stand, the organic phase formed in the upper part of the flask, and the inorganic phase in the lower part. After the phase separation was complete, a cyclic ketone (cyclopentanone or cyclohexanone) was added to the organic phase, i.e. the upper phase, and then a metal organic compound (ferrocene or cymanthrene) in a 1:1 molar ratio. Only then was the carrier DEAN-diethylammonium naphthenate ($(C_2H_5)_2NHOCONaf$) added to the system to initiate the reaction. The process was carried out by heating at positive temperatures: in the temperature range of 20-40°C. Thus, the preparation of the corresponding derivatives of organometallic compounds with cyclic ketones using a phase-shifting catalytic medium ensured, on the one hand, its one-step process, and, on the other hand, its loss-free and high-yield preparation. At the same time, the purity of the obtained substance was also high. The yield of the reaction product obtained by this method was up to 85 %.

The main purpose of DEAN in the process was to transport H_2SO_4 acid to the organic phase. It should be noted that, although $H_2SO_4/DEAN$ was taken in different ratios, the most optimal state was observed at a ratio of 2:1. When the ratio was 2:1, DEAN was able to transport H_2SO_4 acid to the organic phase in catalytic amounts. After the solid H_2SO_4 acid, which was involved as a catalyst in the process, passed into the organic phase, the interaction of ferrocene with cyclic ketones (cyclopentanone and cyclohexanone) occurred in the organic phase. In this regard, sulfuric acid was used as a catalyst in the process and to create an acidic environment. In order to separate ferrocenylcyclocarbinol from the upper part of the flask, i.e. from the organic phase, 4-5 ml of a 1 liter pre-prepared cold 5 % $NaHCO_3$ solution was added to that phase in portions and mixed. Due to the CO_2 gas released from the reaction mixture during each mixing, the reaction product appeared on the surface of the solution in the form of a yellow foam. The yellow foam was collected on a sieve with a perforated skimmer and washed 1-2 times with cold distilled water. The observed reaction was completed in exactly 1 hour and 30 minutes. The obtained substance was dried in a drying cabinet for 24 hours. Then, the purity of the obtained substances was checked using the thin layer chromatography method. Thus, the reactions of ferrocene with cyclic ketones under interfacial catalysis conditions of $H_2SO_4/DEAN$ (2:1 ratio) were carried out and the corresponding derivatives were synthesized.⁽¹⁾ The optimal temperature during the reaction was taken between 20-40°C, at which time the yield of the reaction product was obtained between 70-85 %.⁽³⁾ The temperature used during the reaction directly affected the yield of the reaction product.



(2)

If the temperature is too low during the reaction, the reaction does not occur, and the flask must be slightly heated to start the process. At high temperatures (above 40°C), the yield of the reaction product is very small, 20-22 %, due to the decomposition of the metal-organic complex.⁽⁴⁾ Compounds obtained based on cyclic ketones have occurred in the same interfacial catalysis environment as aliphatic ketones.^(5,6,7)

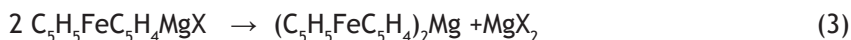
The general formula for organometallic compound (I) was $C_{15}H_{18}FeO$, and for compound (II) it was $C_{16}H_{20}FeO$. The results of elemental analysis of the organometallic compounds under consideration are given below:

$C_{15}H_{18}FeO$ C% 66,66 H% 6,61 O% 5,92 $C_{16}H_{20}FeO$ C% 67,60 H% 7,04 O% 5,63

Interpretation and discussion of the results

It is known that the reactions of ferrocene and cymanthrene occur more easily with aliphatic ketones than with cyclic ketones, and the yield is higher than with them. This can be explained by the spatial structure of the substance. The yield of the product in the reactions under consideration was therefore low. It was possible to increase the yield of the reaction product by using lithium or magnesium derivatives of ferrocene and cymanthrene.⁽⁸⁾ On the other hand, it was found that when both ferrocene and simantrene react with cyclic ketones, the temperature factor greatly affects the process, so it is possible to keep it under constant control and obtain a product with a high yield. For this purpose, reactions were carried out by selecting different conditions. It should be noted that by choosing the right temperature, it was possible to increase the yield of the reaction product up to 85 %. Thus, by choosing the right temperature, it is possible to increase the yield of the reaction product by 3-4 times. The reaction mixtures were taken in certain proportions and placed in certain phases in sequence.

Toluene and a lithium-substituted derivative of ferrocene were used as phase-forming media. It should be noted that the yield of the reaction product was not high in this case, 23-28 %. However, when studying the factors affecting the course of the reaction, it was determined that the most important thing for the process to proceed in one direction is the correct selection of the reaction medium and the temperature factor. Otherwise, the reaction becomes reversible and the yield of the product decreases. On the other hand, the reason for the low yield of the reaction product is that the active Grignard reagent $C_5H_5FeC_5H_4MgX$ dimerizes to form the symmetrical compound $(C_5H_5FeC_5H_4)_2Mg$. At this time, its reactivity decreases.



The removal of derivatives obtained from the reactions of organometallic compounds with cyclopentanone and cyclohexanone from the reaction mixture poses certain difficulties. Thus, choosing the right environment is also very important for the lossless removal of the organometallic compound cyclopentanol and cyclohexanol mixture from the reaction mixture. Thus, after the reaction is complete, the hydrolysis of the product obtained from the reaction mixture was carried out by creating a weakly acidic environment. At this time, the alkaline solution $Mg(OH)_2$ or $XMgOH$ (X-organic radical) formed acted on the ferrocene nucleus and caused the iron in the molecule to oxidize to the Fe^{+2} cation, resulting in the complete decomposition of the ferrocene molecule. This means that the iron and cyclopentadienyl rings are separated from each other. Therefore, the method of decomposition of part of the product as a result of hydrolysis of the reaction product was not considered suitable. Also, the formation of intermediate products in the reaction reduces the yield of the reaction product. Regarding the yield of the reaction

product, when investigating the reason for the low reaction product, it was determined that the metallizing effect of the magnesium compound is low at low concentrations. Also, the reaction product is subject to decomposition when stored for a long time. In this regard, based on these shortcomings, the method was not considered suitable. For this, it was necessary to develop a more suitable method, and for this purpose, an interphase environment was created. In this case, the process was carried out using organic and inorganic phase-forming substances. Thus, an immiscible two-phase system was created and the direct reaction of organometallic compounds with cyclic ketones was carried out. In other words, the synthesis of organometallic compounds with cyclopentanone and cyclohexanone was carried out in an interfacial catalytic environment. When creating an interfacial environment, the resulting two-phase system should not mix with each other. For this purpose, petroleum ether, a light fraction of gasoline, was used as the organic phase, and water was used as the inorganic phase. The ratio of petroleum ether to water was taken as 10:1 by volume (figure 1)

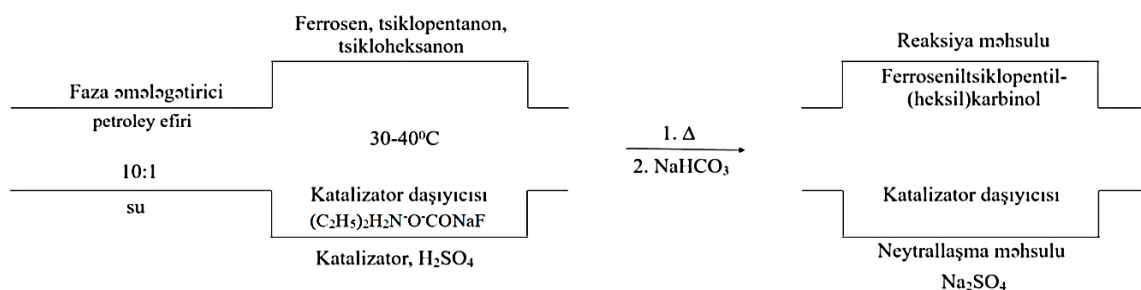
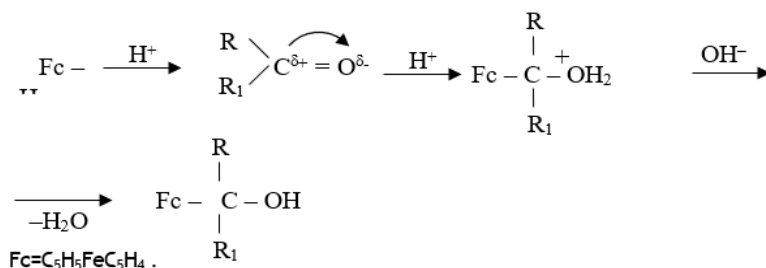


Figure 1. Description of the interfacial catalytic environment

Both ferrocene and cymanthrene react with ketones via an electrophilic substitution mechanism. Since the cymanthrene molecule is easily decomposed, reactions with ferrocene have been studied more extensively. It has been shown that the hydrolysis ability of the intermediate carbocation obtained in the process, as well as the steric factors created by this carbocation, directly affect the yield of the reaction product. These reactions with cymanthrene occurred in a much lower yield than with ferrocene. This was explained by the decomposition of the cymanthrene molecule in the presence of concentrated sulfuric acid during the reaction and the failure of the reaction. Corresponding reactions with simantrene were also carried out in the presence of hydrochloric and phosphoric acids, but no positive results were obtained.

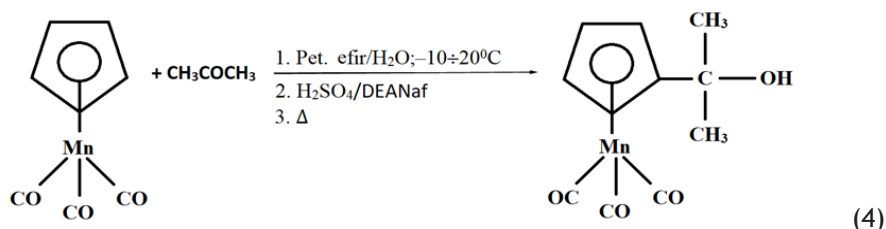
The mechanism of these reactions in an acidic environment can be generally described as follows:⁽⁹⁾



During the reaction, ketones and sulfuric acid were taken in different ratios. The correct selection of these ratios directly affects the yield of the reaction product obtained. In an acidic environment, it was more expedient to take the ratio of ketones to sulfuric acid (92 %) as 45

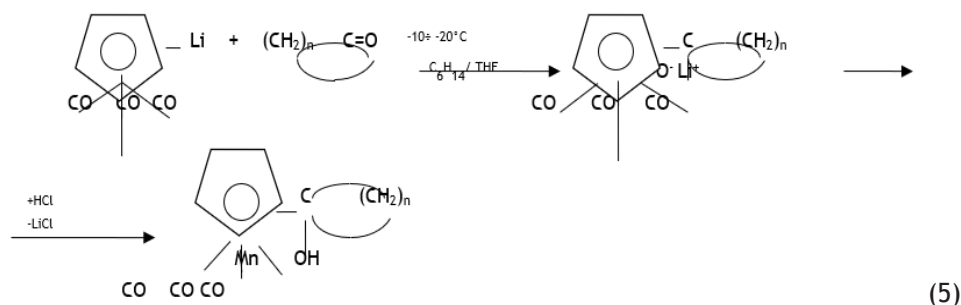
ml:15 ml. The main purpose of taking sulfuric acid at a high concentration was to prevent the hydrolysis of the intermediate complex obtained from the interaction of the ketone with the acid. At lower concentrations, the intermediate complex obtained usually decomposes. The kinetics of the process was studied based on the formation of the corresponding ferrocenylcarbinol between ferrocene and acetone. In order to study the kinetic regularities of the process, the reaction between the aliphatic ketone acetone and ferrocene was studied in detail. In the presence of diethylammonium naphthenate and sulfuric acid (1:2) in the interfacial catalysis medium, the reaction of acetone to ferrocene proceeded at an increasing rate for two hours, and then a gradual weakening of the rate was observed. The process was carried out for about two hours in total. In the process, 85-87 % of ferrocene entered the combination reaction, and the rest was decomposed for certain reasons. When studying the kinetics of the process, the change in the substances entering the reaction with time was found to be nonlinear. At first, ferrocene entered the reaction quickly, at this time its consumption was high, but as it progressed, its consumption in the reaction decreased. The high rate of obtaining the main products in the initial stage of the reaction occurred due to the rapid increase in the combination products. As the product of the compound increased, the amount of ferrocene entering the reaction decreased sharply in parallel. Very little of the ferrocene decomposed in the process for certain reasons.

The derivative of simanthrene, simanthrene dimethylcarbinol, was obtained by reacting simanthrene with corresponding aliphatic ketones (acetone).



All the reactions considered were carried out in an interfacial catalytic environment. Analogously to ferrocene, the kinetic regularities of the reaction of symanthrene with acetone $(\text{CH}_3)_2\text{CO}$ were also studied.⁽¹⁰⁾

The reactions of ferrocene and symanthrene with cyclic ketones were also carried out. The reactions of symanthrene with cyclic ketones were carried out at lower temperatures than the reactions with ferrocene.



The yield of products obtained from the reactions of both ferrocene and cymanthrene with

cyclic ketones was very small compared to aliphatic ketones. This depends on many factors; reaction temperature, number of active collisions of molecules, steric factors, etc. The obtained metal organic complexes have antiknock properties and have been widely used in various brands of gasoline.^(11,12)

The structure of cyclocarbinols obtained from the reactions of ferrocene and cymanthrene with cyclic ketones (cyclopentane and cyclohexane) was studied. IR spectra were recorded on a Specord M80 device based on ferrocene and cymanthrene.

As can be seen from figure 1, the valence absorption frequency of the C=O group of cyclopentanone, which was taken for the preparation of new derivatives of ferrocene with cyclic ketones, was $\nu_{\text{C=O}}$ 1680 cm^{-1} according to IR spectroscopy (Specord M80), and that of cyclohexanone was $\nu_{\text{C=O}}$ 1690 cm^{-1} . After the reaction, no signals corresponding to these groups were observed in the spectrum. This is explained by the transition of the ketone group (C=O) to the hydroxyl (OH) group. Based on the IR spectroscopy of ferrocene organometallic derivatives obtained with cyclopentanone and cyclohexanone, signals corresponding to OH groups were obtained in the region of 3420-3480 cm^{-1} for ferrocenylcyclopentanol, and in the region of 3450-3510 cm^{-1} for ferrocenylcyclohexanol.⁽¹³⁾ Thus, for ferrocenylcyclopentanol (a) and ferrocenylcyclohexanol (b), the valence absorption frequencies ν_{OH} 3448 cm^{-1} and ν_{OH} 3468 cm^{-1} were obtained, respectively. These groups did not interact with the central atom either intramolecularly or intermolecularly.

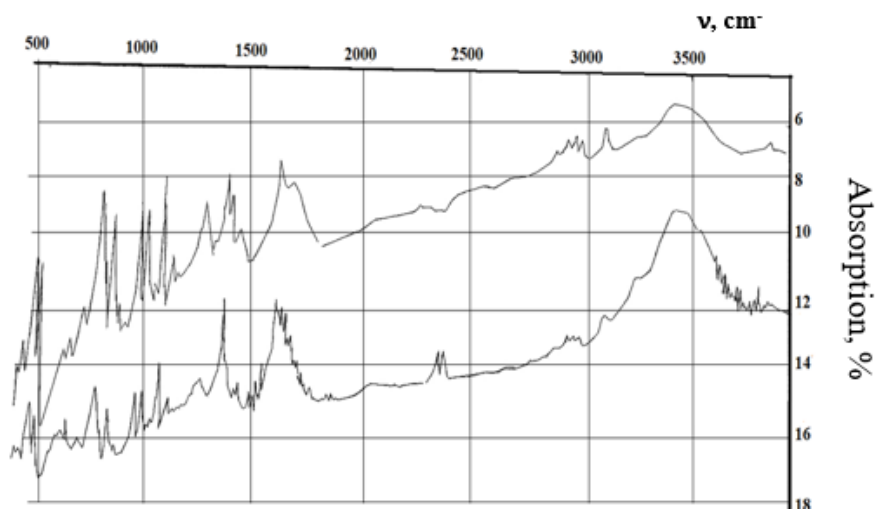


Figure 1. IR spectrum of ferrocenylcyclopentanol and ferrocenylcyclohexanol

Then, simantrenylcyclopentanol obtained by the same method was also analyzed by IR spectroscopy. The spectra were recorded in vaseline oil. No vibrational frequencies belonging to the ketone (CO) group were observed in the compound obtained as a result of the reaction. This suggests that the cyclic ketone taken as the initial reagent was used to obtain the corresponding carbinol. When analogous reactions were carried out with aliphatic ketones, no vibrational frequencies belonging to the CO-ketone group were observed in the end.⁽¹⁴⁾

As can be seen from figure 2, a valence absorption frequency of $\nu_{\text{C=O}}$ 3415 cm^{-1} was observed for the hydroxyl group. The valence absorption frequency of the CO group, located in the region

of $\nu_{\text{C=O}}$ 1938-2048 cm^{-1} , indicates the absence of intramolecular interaction between the C=O and OH groups.

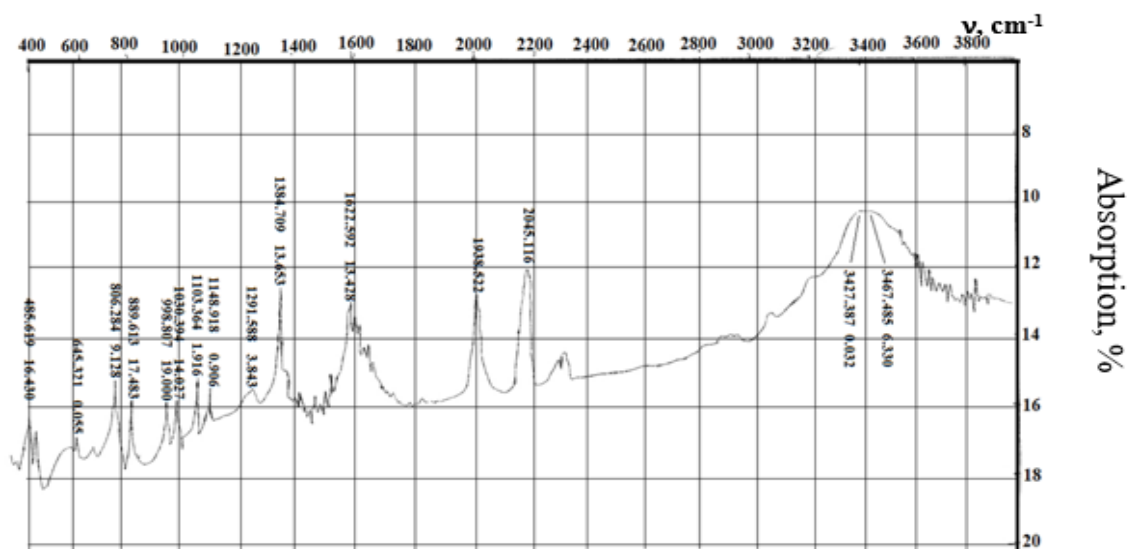
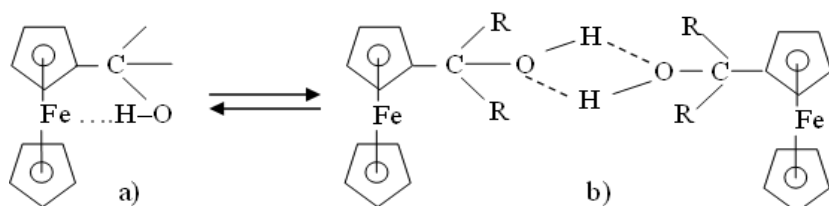


Figure 2. IR spectrum of simantrenylcyclopentanol



^1H NMR analyses were performed on a Bruker instrument. The spectrum was recorded at a temperature of $\text{C}_4\text{D}_8\text{O}$, 22° C. In the ^1H NMR spectrum, a chemical shift of the field for the -OH group in the ferrocene molecule occurred from 2 m.h to 4,30 m.h. In the unsubstituted ferrocene molecule, the chemical shift of the protons in the cyclopentadiene (C_5H_5) ring (ligand) occurred at a field of $\delta\text{C}_5\text{H}_5=4,12$ parts per million. Due to the symmetry breaking after substitution, the cyclopentadiene ligand (C_5H_4) underwent cross-linking in the α and β positions and the protons became more mobile. For protons, chemical shifts occurred at 3,82 and 3,91 m.h. of the field. This is explained by the fact that the substituent group is a strong electron donor. This phenomenon occurred every time a substitution occurred in one of the cyclopentadiene ligands in the ferrocene core. It should be noted that depending on the difference in functional groups in the molecule, chemical shifts may differ slightly, but this difference in chemical shift is not very noticeable.^(15,16,17)

The reactions considered with ferrocene proceeded mainly in an acidic medium. As a rule, these reactions do not proceed in an alkaline medium. It was found that the C-H acidity number of 10-11 in the ferrocene molecule does not affect the proton in its molecule, in this case the proton does not become mobile and, as a result, reactions with ketones do not occur. When the C-H acidity number is above 25, protonation of carbinol groups is ensured and the

reaction proceeds precisely at this time. In this regard, reactions with ferrocene must occur in an environment with a high pH. For the reaction to proceed, it was possible to increase the pH of the environment to 28-30. For this purpose, a strong acid - sulfuric acid - was used in all the reactions considered. Interestingly, when sulfuric acid was replaced with concentrated hydrochloric and phosphoric acids, the reaction did not occur. In the presence of concentrated hydrochloric and phosphoric acids, the molecule of the organometallic compound disintegrates and the reaction does not occur.

CONCLUSIONS

In the reviewed article, the reactions of ferrocene and cymanthrene with cyclic ketones were studied analogously to aliphatic ketones. Metal complex derivatives were obtained in lower yields from the interaction of the corresponding metallocenes with cyclopentanone and cyclohexanone compared to aliphatic ketones. In order to increase the yield, an interfacial catalysis environment was used. The yield of reaction products was relatively higher in the DEAN environment. 92 % concentrated sulfuric acid was used in the process. Reactions with cymanthrene were more difficult compared to ferrocene. Structural analysis of the obtained ferrocenyl- and cymanthrenylcyclocarbinols was carried out. Their structures were studied by IR spectroscopy and NMR method. IR spectroscopy was studied on a Spekord M80 device, and NMR analysis was studied on Bruker devices.

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AUTHORSHIP CONTRIBUTION

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Chapter 10

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Ecologically important properties of bio-oils

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ABSTRACT

Environmental monitoring was carried out in the Caspian Sea's Oil Rocks and 28 May areas. First, the composition of crude oil taken from these regions was determined based on gas chromatography. Then, 15 polycyclic aromatic hydrocarbons and representatives of 11 phenolic organic compounds were analyzed based on mass spectroscopy in seawater. The physico-chemical properties of sea waters were also studied. As the examined seawater samples were exposed to petrogenic pollution, many PAHs and phenolic organic compounds exceeded the permissible concentration limit. Later, in laboratory conditions, the crude oil taken from these two areas was used for the absorption of bio-oils of natural origin to purify drinking and seawater, and it was determined that, oil sorption occurs effectively when the process is carried out in an organic solvent (hexane or heptane). The sorption process was investigated with different oils of natural origin and oil collection on seawater and drinking water for three hours at room temperature was better with soybean and castor oils.

Keywords: Oil Fields; Bio-Oil; Sorption; Hexane; Heptane.

INTRODUCTION

It is known that recently, as a result of anthropogenic effects on the biosphere, as well as due to the effect of the greenhouse effect, the Earth's atmosphere, hydrosphere and lithosphere are being polluted with various types of toxicants.^(1,2,3) From this point of view, it is important to conduct new research methods and modern analyzes in order to find solutions to the ecological crisis and ecological complications.^(4,5,6,7,8)

According to the researchers, if the ecological imbalance is not prevented, the temperature of the Earth's crust is expected to increase by 40C in the last century, which will lead to ecological disasters.^(9,10,11,12) It is important to maintain the temperature of the ground at a maximum of 1,50C. It is known that the main factors influencing the creation of the greenhouse effect are the increase of industrial enterprises, various anthropogenic effects, as well as the environmental damage caused by automobile transport.^(13,14,15,16) The main components of gases that cause the greenhouse effect are carbon dioxide, methane, freons, nitrous oxide, and ozone and traces of water to a lesser extent [17-19]. In an era of nanotechnology development, the growth of industrial and chemical enterprises, as well as the negative impact of conventional fuel-powered automobiles on the environment, are driving the deepening of the environmental threat that will be considered global.^(20,21,22,23) This eventually leads to global pollution of the

atmosphere, lithosphere and hydrosphere, which interact with each other.⁽²⁴⁾

Currently, the problem of pollution of the world ocean and water shortage is one of the main environmental problems.^(25,26,27,28) Due to global pollution, the problem of droughts, depletion of fresh water resources, mixing of wastewater with other water resources and polluting them is currently relevant. These problems are also relevant in our country.⁽²⁹⁾ So, since the extraction of oil from the Caspian Sea and its transportation to different countries is carried out by land, as well as by waterways, various injuries are caused to the hydrosphere layer.^(30,31,32,33) In this case, the protection of the hydrosphere layer is currently considered as an urgent environmental issue of the day, and it is important to investigate efficient ways to implement water treatment.^(34,35,36,37)

It is known that various natural and synthetic sorbents are used in chemical cleaning. The sorption method is a classic method, and it is widely used in cleaning the oil layer accumulated on the water.⁽³⁸⁾

From this point of view, experiments were carried out in laboratory conditions for the effective collection of oil collected on the water surface with oils of natural origin in hexane or heptane environment.

Experimental part

Chemical analysis of the crude oil taken from the two areas examined by us was carried out. Based on the results of gas chromatography analysis, it was conducted to determine which organic hydrocarbons the composition of crude oil consists of (figure 1 and figure 2).

Table 1. Analysis of crude oil taken from two points of Oil Rocks

<i>Alkanes</i>	Oil Rocks (point I)		Oil Rocks (point II)	
	<i>Area</i>	<i>Ratio %</i>	<i>Area</i>	<i>Ratio %</i>
nC 10	28518	1,02	27851	0,99
nC 11	27630	0,99	27647	0,98
nC 12	28438	1,02	28369	1,00
nC 13	27575	0,99	26380	0,93
nC 14	21991	0,79	21159	0,75
nC 15	17601	0,63	12477	0,44
nC 16	6091	0,22	5972	0,21
nC 17	5078	0,18	5190	0,18
Pristane	19617	0,70	18677	0,66
nC 18	2705	0,10	2673	0,09
Butane	15656	0,56	15243	0,54
Total amount of hydrocarbons	2799090	100	2826610	100
Area ratio of isoprenoid hydrocarbons				
17/pristane	0,259		0,278	
18/butane	0,173		0,175	
Pr/B	1,253		1,225	

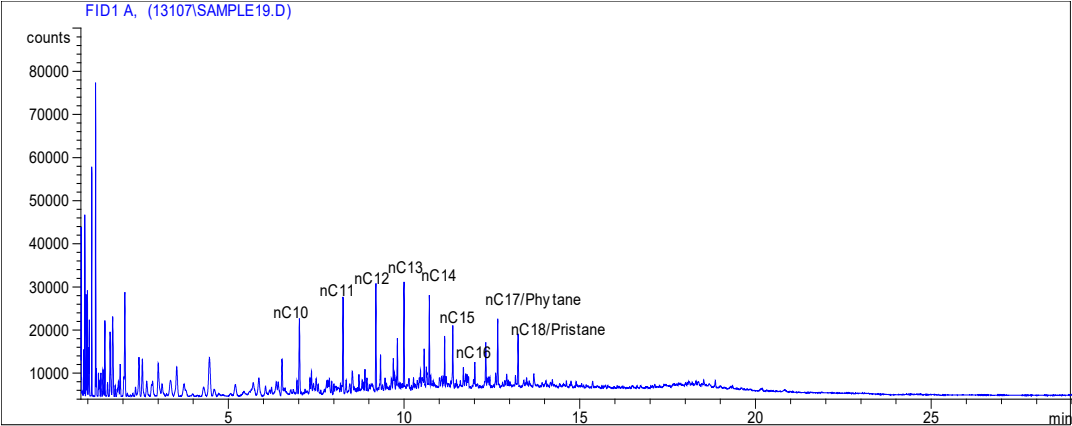


Figure 1. General view of the chromatogram of crude oil taken from Oil Rocks (point I)

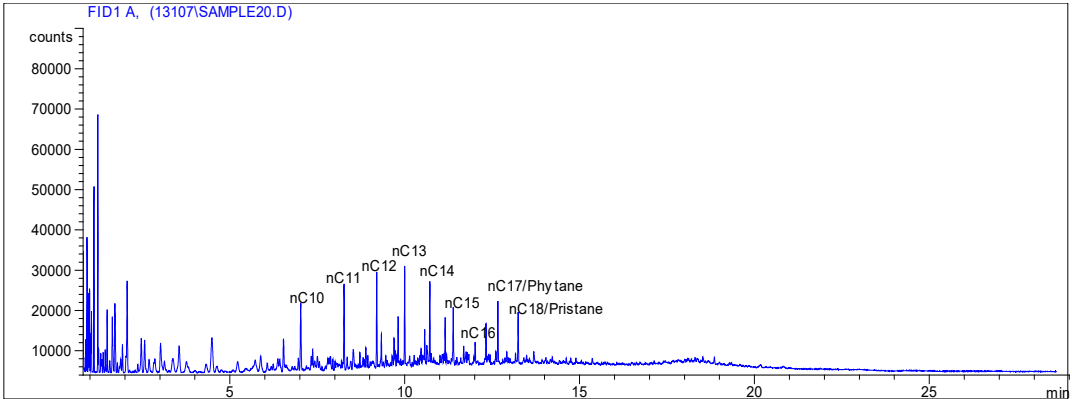


Figure 2. General view of the chromatogram of crude oil taken from Oil Rocks (point II)

Table 2. Composition of crude oils taken from 28 May area		
Substances	28 May oil	
Alkanes	Area	Ratio %
nC 10	50149	0,92
nC 11	48948	0,90
nC 12	51185	0,94
nC 13	49362	0,91
nC 14	40799	0,75
nC 15	32639	0,60
nC 16	10899	0,20
nC 17	5133	0,09
Pristane	33157	0,61
nC 18	3848	0,07
Butane	31326	0,58
Total amount of hydrocarbons	5430940	100
17/pristane(Pr)	0,259	0,155
18/butane(B)	0,173	0,123
Pr/B	1,253	1,058

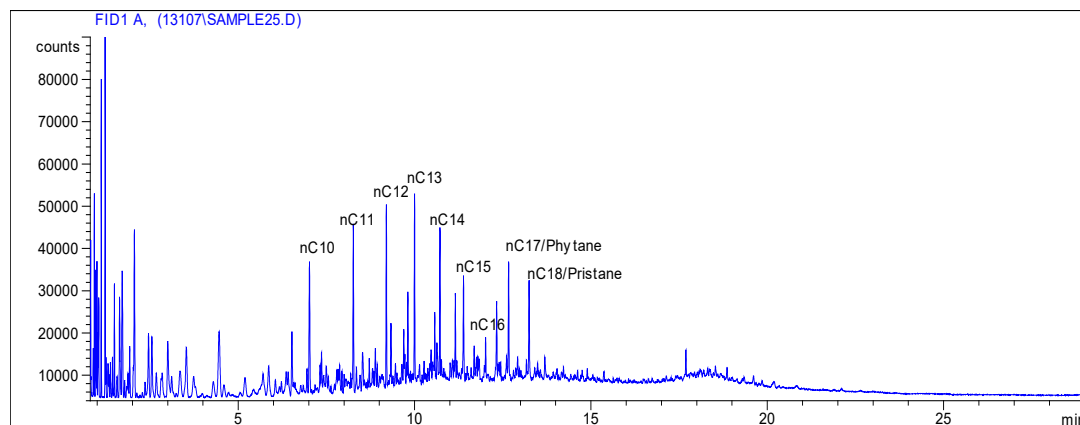


Figure 3. General view of the chromatogram of crude oil taken from 28 May area

Sunflower, olive, castor and soybean oils were used as natural absorbents of biological origin. Based on the comparative analysis of all four containers, it can be said that the property of these substances to collect oil on water occurs only with the presence of hexane (heptane) in that medium. The petri dishes were monitored for several days. Vegetable oils of different origins were taken and compared in the experiments. Better results were obtained with soybean and castor oils in vessels II and IV (table 1). At this time, only 20-30 % of the total area of the vessel remained untreated. Thus, the ability of these natural oils to collect oil was 60-70 %. The diameter of the oil spheres obtained on the water layer and the thickness of the oil layer were measured, and based on this, a graph of dependence between oil collection was constructed depending on time. Then, in laboratory conditions, four petri dishes were separated, 40-50 ml of drinking water was added to two of them (I, II) and sea water was added to the other two (III, IV). Then 0,4-0,6 ml, about 2-3 drops of crude oil taken from two regions of Azerbaijan with oil field (28 May and Oil Rocks) are added to the water in each container, and the solutions remain in a calm state for 1 day. After 1 day, after the oil has completely spread over the water layer, 2,5 ml of hexane (or heptane) was added to the containers with drinking and sea water (I, III), and 2,5 ml to the other containers with drinking water and sea water (II, IV). 5 ml of 50 % solution of oil in hexane is added and kept for some time (2-3 days).

Discussion and interpretation of results

Chemical analysis of crude oils was carried out before experiments. Oil was taken from two regions of Azerbaijan (Oil Rocks and 28 May oil) and its chemical composition was determined. The composition of Azerbaijani oil is mainly rich in paraffins and naphthene, and the amount of sulfur is low. This is one of the unique features of our oil. As the number of higher hydrocarbons in the oil increases, so does its absorption. Table 3 below shows the chemical parameters of crude oils taken from the oil fields of Azerbaijan.

Table 3. Some chemical properties of oils taken from the regions of Azerbaijan			
Type of crude oil	Chlorine salts (mg/l)	Sulphur (%)	Paraffin (%)
Oil Rocks	39,2	0,21	1,65
28 May	31,7	0,27	1,27

After that, sea water samples were taken from the examined areas and polycyclic aromatic hydrocarbons and phenolic organic compounds were determined in them (table 4 and table 5).

Table 4. PAH content in seawater sampled from two regions of the Caspian Sea

PAH (mcg/l)	28 May	Oil Rocks
Naphthalene	0,07	0,12
Accented	0,03	0,05
Acenaphthene	0,04	0,04
Fluorene	0,24	0,03
Phenanthrene	0,29	0,05
Anthracene	0,04	0,05
Fluoranthene	0,03	0,02
Pyrene	0,05	0,02
Benz (a) anthracene	0,01	0,01
Khrezen	0,02	0,02
Benz (b + j + k) fluoranthene	<0,01	0,02
Benz (a) pyrene	<0,01	0,02
Indene (1,2,3-cd)pyrene	<0,01	<0,01
Benz perylene	<0,01	0,01
Diphenanthrene	0,02	0,02

Table 5. Amount of phenolic organic compounds in seawater sampled from two regions of the Caspian Sea

Phenol (mcg/l)	28 May	Oil Rocks
phenol	0,13	0,16
o-cresol	0,04	0,45
2-nitrophenol	0,10	0,13
2,4-dimethylphenol	0,11	0,13
2,4-dichlorophenol	0,03	0,04
2,6-dichlorophenol	0,07	0,08
4-chloro-3-methylphenol	0,14	0,08
2,4,5-TCP	0,07	0,10
2,4,6-TCP	0,07	0,10
2,3,4,6-tetrachlorophenol	0,10	0,12
pentachlorophenol	0,12	0,16

The reviewed chemical analyzes were carried out at the Caspian Ecological Laboratory based on mass spectroscopy equipped with Agilent series gas chromatography.

The physico-chemical properties of seawater taken from the areas considered in table 6 below were also investigated.

Table 6. Some physicochemical characteristics of seawater samples

Areas	Tem. °C	pH	salinity, %	Electrical conductivity, mS/cm
28 May	26,3	8,2	11,0	18,7
Oil Rocks	25,9	7,9	10,5	17,7

After the ecological monitoring of sea waters taken from two regions of the Caspian Sea, oil sorption from these sea waters was examined in laboratory conditions. The concept of rapid accumulation was used to determine the collecting (dispersing) property of oils of biological

origin. The rapid collection constant (K) is based on the faster action of the reagent and its ability to collect oil more quickly. K is equal to the ratio of the total area of the container (S_1) to the area of the oil circle (S) collected after the reaction of the reagent: $K=S_1/S$

The more effective the reagent, the smaller the numerical value of S and the larger the numerical value of K . Here, the total area of the vessel is S_1 , and the area of the oil spheres spread over the water layer is denoted by S . As the thickness (h) of the oil layer in the Petri dish increases, the ability of oil to accumulate (disperse) on the water surface decreases. The thickness of the oil layer was calculated according to the following formula: $h=V/S$

Here, h -thickness of oil layer (cm); V -volume of added oil (ml); S is the area of the oil sphere (cm^2).

However, the best results were obtained with soybean and castor oils. Thus, in the presence of hexane (heptane), almost complete accumulation of oil on sea and drinking water was observed. At this time, the obtained oil balls were completely collected on the water surface (table 7).

Table 7. Main indicators of absorption of oil from sea water and drinking water by bio-oils			
Castor oil	Drink. Water ml	40	50
	h , ml	0,014	0,013
	S , sm^2	34,2	37,4
	K	3	2
Castor oil	Seawater, ml	40	50
	h , ml	0,016	0,013
	S , sm^2	31,25	38,46
	K	2,5	2,1
Soybean oil	Drink water, ml	40	50
	h , ml	0,02	0,02
	S , sm^2	26,3	29,4
	K	2,4	3,7
Soybean oil	seawater	40	50
	h , ml	0,01	0,01
	S , sm^2	27,2	27,7
	K	2,2	2,5

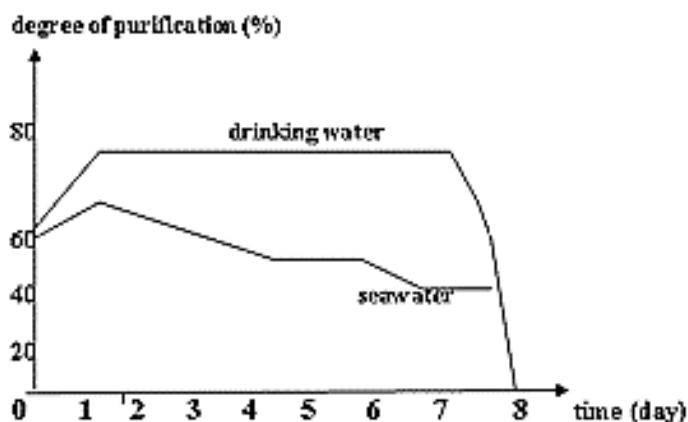


Figure 4. Time dependence of oil absorption

After studying the absorption of both oil samples (Oil Rocks and 28 May) with oils of natural origin in laboratory conditions, it was found that the absorption of both crude oils occurs differently in drinking water and sea water (table 2). Thus, absorption in sea water occurs in different ways at different time intervals, which can be explained by its multi-component composition. As can be seen from Table 2, the value of the aggregation constant (K) is smaller in seawater than in drinking water. This is explained by the fact that the reagent has a more effective effect in drinking water. Thus, as the numerical value of K increases, oil globules have a smaller area, in other words, effective collection occurs (figure 4).

CONCLUSION

Thus, environmental monitoring was conducted in the areas of Oil Rocks and 28 May, and representatives of 15 polycyclic aromatic hydrocarbons and 11 phenolic organic compounds were analyzed based on mass spectroscopy in seawater. The physico-chemical properties of sea waters were also studied. Many of the PAHs and phenolic organic compounds exceeded the permissible concentration limit as the examined seawater samples were exposed to petrogenic pollution. Later, in laboratory conditions, the crude oil taken from these two areas was used for the sorption of bio-oils of natural origin to purify drinking and sea water, and it was determined that the accumulation of oil on sea water and drinking water in hexane or heptane environment, at room temperature for three hours, soybean and castor bean performed better with oils.

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Chapter 11

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Study of the smoke-reducing properties of metal-organic compounds and their industrial applications

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ABSTRACT

Metal-organic compounds possess environmentally significant properties and fields of application. For ferrocene and cymantrene, as well as some of their derivatives, there are reactions of great environmental importance. One of these is the reaction of ferrocene carbinols with Ba(OH)₂ and Ca(OH)₂, resulting in the formation of the corresponding carbinolates – reactions that are of considerable industrial relevance. However, the drawback of this process is that the reaction products are not obtained in high yields. Compared to reactions with aliphatic ketones, those involving cyclic ketones proceed rather weakly. To increase the reaction yield, a phase-transfer catalytic medium has been employed. Reactions with aliphatic ketones yield the corresponding ferrocenylcarbinolates with 60-72 % efficiency.

Keywords: Ferrocene; Cymantrene; Cyclic Carbinols; Cyclic Ketones; Environment.

INTRODUCTION

The issue of air pollution remains topical in our country, as it is globally. Reforms based on the implementation of Euro-5 standards have facilitated the use of fuels that are significantly less detrimental to the environment. According to Euro standards, a primary prerequisite is the virtual absence of sulfur and benzene in the fuels utilized. Furthermore, the octane rating of carburetor fuel must not be less than 95, and the fuel must possess a high smoke-suppressant capability. In this context, the antidetonation and smoke-suppressant properties of novel derivatives synthesized from ferrocene and simanthrene have been investigated. As noted, the corresponding derivatives formed by ferrocene and simanthrene—the principal representatives of organometallic compounds—with ketones are already widely employed for their antidetonation characteristics in fuels.^(1,2,3)

New mono- and di-substituted derivatives of ferrocene and simanthrene were used to create ecologically clean octane-boosting compositions, and their application features were studied. It was determined that the carbinol complexes and ether derivatives of ferrocene and simanthrene exhibit an effect up to three times greater than ferrocene and simanthrene when used in the same concentration in fuel. It has been confirmed that, depending on the origin and composition of the gasoline, these compositions possess the ability to increase the octane number by 12 to 18 units.

As for ferrocene, it is a π -complex with a closed cyclic structure – dicyclopentadienyliron, (C₅H₅)₂Fe. Ferrocene is a widely distributed industrial product and has been extensively studied in coordination chemistry. It differs from other representatives of its class by its unique properties. Specifically, ferrocene is the only compound among transition metal complexes that

decomposes at temperatures above 500 °C, a characteristic that distinguishes it from other metal-organic compounds.

In our study, the alkylation of pyrocondensate was carried out using the Al + CCl₄ system. Experimental results showed that the alkylation of ferrocene with pyrocondensate proceeds through substitution occurring only on one of the cyclopentadienyl rings of the ferrocene molecule, resulting in mixtures of alkylferrocenes with different compositions. The melting and boiling points of the variously structured alkylferrocenes obtained in the process were also determined.

Initially, the reaction mixture consisted of an 80 g/L ferrocene solution, 0,5 L of pyrocondensate, and 3 % of the Seyidov catalytic system (Al + CCl₄). After five hours of stirring at 50-60 °C, samples were taken every half hour, and it was found that alkylation did not proceed efficiently under these conditions. According to chromatographic analyses, only 10-12 % of alkylferrocene was formed. When the catalyst concentration was increased to 10 %, decomposition of the ferrocene molecule was observed, and the alkylation reaction did not proceed.

Following the discovery of ferrocene's antidetonation properties (resistance to knocking/explosion) in diesel fuels, it attracted significant attention from numerous scientists. Concurrently, ferrocene exhibits considerable chemical reactivity due to its inherent stability, thereby expanding its potential applications within the field of chemistry.

Ferrocene is an orange crystalline solid with a characteristic odor and is more stable compared to cymantrene. It possesses the chemical properties typical of aromatic hydrocarbons and primarily undergoes electrophilic substitution reactions. Its melting point is 174 °C, boiling point is 249 °C, and decomposition temperature is 474 °C. The molecular weight of ferrocene, Mr((C₅H₅)₂Fe), is 186.

METHOD

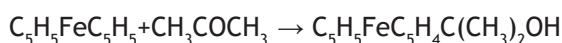
The mono- and di-substituted derivatives of ferrocene continue to possess a broad scope of application today.^(4,5) Compared to ferrocene itself, these derivatives exhibit a greater capacity to elevate the octane number. The ferrocenyl carbinols, obtained from the reaction of ferrocene with ketones, are capable of undergoing more extensive chemical transformations relative to ferrocene and its alkyl derivatives. This enhanced capability is attributed to the presence of active oxygen within their molecular structure. On the other hand, the derivatives of ferrocene possess a higher molecular weight compared to the parent compound. This increase in molecular weight leads to a reduction in the molar quantity of iron incorporated into the final composition. The lower mass fraction of iron in ferrocene derivatives allows them to be utilized as more effective additives, promoting a slower rate of engine degradation. From this perspective, the application of high-molecular-weight ferrocene derivatives as anti-knock additives in fuels has been deemed environmentally satisfactory.⁽⁶⁾

Concerning the other application areas of ferrocene, it is widely utilized as a colorant, in the preparation of pharmaceutical substances in medicine, in the manufacturing of heat absorbers and radiation shields, as well as in other fields.⁽⁷⁾ Ferrocene undergoes reactions characteristic of aromatic hydrocarbons, a property which increases its potential for application in numerous chemical reactions. Furthermore, based on the low oxidation-reduction potential of the iron moiety (0,6 units) within the ferrocene molecule, it behaves as a neutral molecule, thereby enhancing its capacity to react in both acidic and basic media. Reactions conducted primarily in an acidic medium are characteristic of ferrocene, where electrophilic substitutions occur, many

of which possess industrial significance. Ferrocene exhibits good solubility in organic solvents. One of its most crucial properties is its favorable solubility in nonpolar solvents.

Ferrocene can be used in all grades of gasoline at concentrations not exceeding 37 mg/mL. When the mass fraction of iron is too high, the incomplete combustion of fuel in automobile engines leads to the deposition of iron oxides, which ultimately causes engine failure and resin formation in the gasoline. To eliminate these drawbacks, it is advisable to use ferrocene derivatives with higher antiknock properties than ferrocene itself.⁽⁸⁾ As the molecular weight of a compound increases, the mass fraction of iron decreases, which helps to prevent the aforementioned issues. Therefore, it becomes feasible to use ferrocene derivatives that possess 1,5-3 times greater antiknock efficiency than ferrocene. Extensive research in this field has been carried out in Russia. In this context, ecologically clean, highly effective anti-detonation additive compositions, branded "Kriskat," based on multifunctional ferrocene and simanthrene, have been developed for motor fuels in Azerbaijan.

Based on the aforementioned points, it is evident that ferrocene and simanthrene derivatives possess high antidetonation properties and constitute industrially significant compounds. The reactions carried out between ferrocene and aliphatic ketones were also conducted identically with simanthrene.

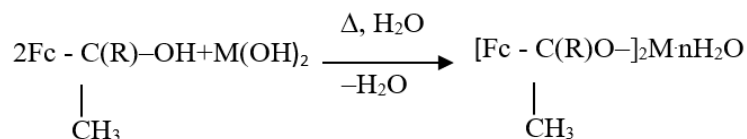


Based on the reaction of simanthrene with the corresponding aliphatic ketone (acetone), the derivative simanthrenyldimethylcarbinol was obtained.

RESULTS AND DISCUSSION

The reactions of ferrocene- and cymantrene-based carbinols with Ba(OH)₂ and Ca(OH)₂ are of great environmental significance. It has been established that the barium salts (carbinolates) obtained from the interaction of carbinols derived from ferrocene with Ba(OH)₂ possess smoke-reducing properties. Compositions prepared by dissolving these carbinolates in gasoline fractions reduce the amount of smoke released into the atmosphere, thereby contributing to environmental protection.

The overall course of the process is as follows:



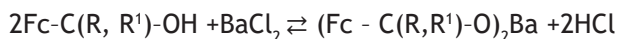
M=Ca, Ba. The structure of the metal-complex derivatives obtained in the reaction was determined using IR spectroscopy and ¹H NMR methods.⁽⁹⁾ Specifically, the ν_{OH} absorption band at 3665 cm⁻¹, corresponding to the OH group of ferrocene carbinol, disappeared after interaction with Ba(OH)₂. This indicates the absence of the corresponding OH group in the ferrocene carbinolate.

Analysis of the ferrocene carbinol by ¹H NMR (spectrum recorded in CDCl₃) showed three signals in the 4-5 ppm region. Two signals at 4,85 and 4,33 ppm corresponded to the substituted

cyclopentadienyl ring (C₅H₄), while one signal at 4,04 ppm was attributed to the unsubstituted C₅H₅ ring. Additionally, the signal corresponding to the protons of the CH₃ group in the ferrocene carbinolate was observed at 2,12 ppm.

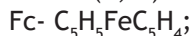
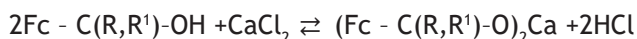
The salts of carbinol derivatives obtained from metal-organic compounds—for example, calcium salts of ferrocene carbinols—possess precipitating properties, and these characteristics are utilized in the petroleum industry to remove unwanted substances from residual oil fractions. These reactions are therefore of industrial significance. Additionally, they have environmental advantages.

The reaction of ferrocene carbinols with barium hydroxide was carried out at 250 °C. The same process was attempted with cyclic ketones, but the yields were very low. Compared to Ba(OH)₂, using barium chloride (BaCl₂) for these reactions is more practical, as barium chloride is insoluble in alcohols but soluble in water. This allows barium ferrocene carbinolates obtained at room temperature to be easily separated from the aqueous phase compared to organic solvents, and then dried in a drying oven. In the wet state, the product appears yellow; upon drying, it transforms into a solid, dark orange crystalline substance with a characteristic odor, and after complete drying, it can be ground into powder.



Barium salts of ferrocene carbinols are highly soluble in alcohols and moderately soluble in hydrocarbon-type organic solvents; for example, they dissolve at concentrations of 20-25 g/L at 20°C.

In our study, the reactions of ferrocene carbinol derivatives with CaCl₂ were carried out under the same conditions as with BaCl₂, at room temperature and 25 °C. These calcium salts are less stable but are environmentally significant compounds. Compared to barium ferrocene carbinolates, they are poorly soluble in both nonpolar and polar solvents. It was possible to isolate these compounds in a pure form from the reaction mixture by extraction with diisopropyl ether.



Barium-based ferrocene carbinolates decomposed at temperatures below 97°C, while calcium-based ferrocene carbinolates decomposed at 105°C. During the preparation of calcium ferrocene carbinolate, the yield was found to be in the range of 40-45 %.

Similar to the preparation of the barium dihydrate metal complex of ferrocene carbinolate, C₂₆H₃₀Fe₂BaO₂·2H₂O, the barium dihydrate metal complex of cymantrene carbinolate, C₂₂H₂₀Mn₂BaO₈·2H₂O, was synthesized. The reaction was carried out in a THF medium, and the target product was obtained with a yield of 60-68 %.⁽¹⁰⁾

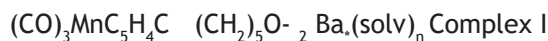
Microanalysis results confirmed that the complex corresponds to the elemental composition C₂₂H₂₀Mn₂BaO₈·2H₂O. Overall, barium-based carbinolates exhibit 1-1,5 times higher smoke-reducing efficiency compared to existing smoke suppressants used in gasoline and diesel fuels,

and 0,4-0,6 times higher efficiency compared to ferrocene and cymantrene themselves. Tests of the smoke-reducing properties of metal-organic carbinolates in diesel fuels were conducted at the laboratories of the Azerbaijan State Oil Company, currently the central laboratory of the Heydar Aliyev Oil Refinery.⁽¹¹⁾

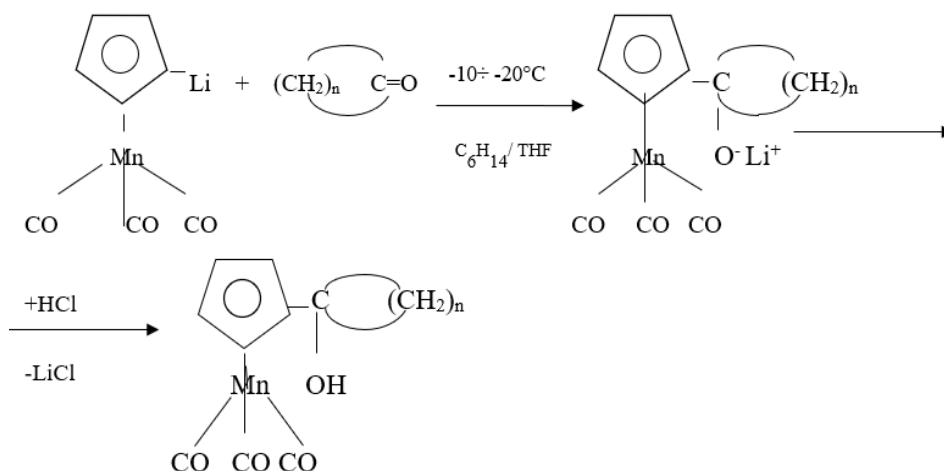
Reactions based on cymantrene were also carried out in a water-alcohol medium.⁽¹²⁾ The resulting cymantrene carbinolates varied in color from light to dark blue and were obtained as powders. They were highly soluble in hot water, organic solvents, and various grades of gasoline. Ferrocene carbinolates decomposed at temperatures above 210 °C, whereas cymantrene carbinolates decomposed at much lower temperatures, below -105 °C.

Carbinols obtained from reactions of metal-organic compounds with aliphatic ketones reacted more readily with Ba(OH)₂ and gave higher yields compared to carbinols derived from cyclic ketones. The barium salts of carbinols obtained from cyclic ketones also exhibit smoke-reducing properties; however, these reactions are relatively more difficult, and the target products are obtained in lower yields. The reactions were performed in various media.

The composition of the barium carbinolate formed from cymantrene carbinol obtained with cyclohexanone depends on the solvent used in the reaction and can be represented by the following formula:



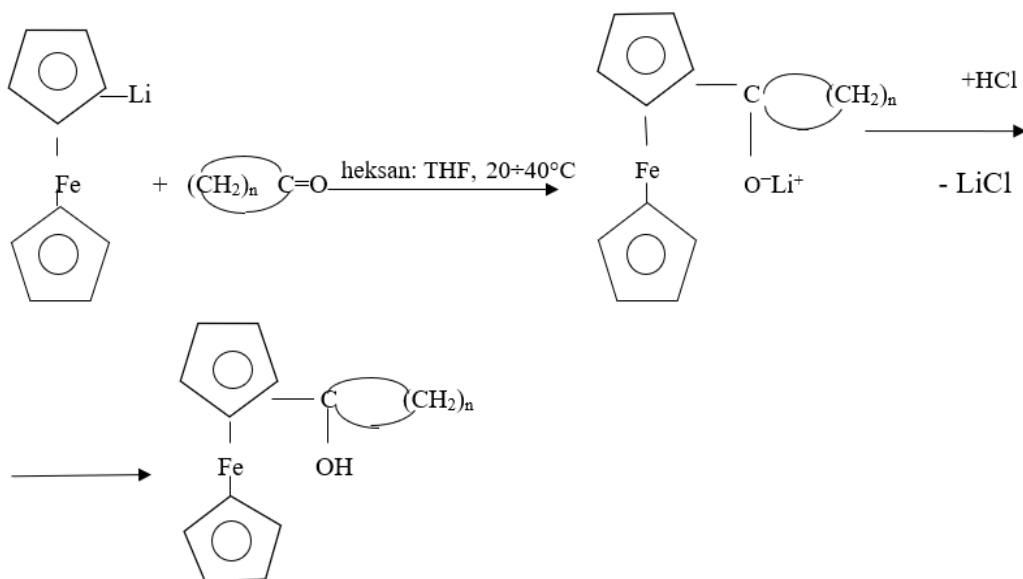
Solv=H₂O, THF, ROH; n varies between 2-4. For the preparation of cymantrene cyclocarbinol used in the reaction, the lithium derivative of cymantrene was employed. At low temperature, the cymantrene lithium reacted with the corresponding cyclic ketones. It should be noted that the process was carried out at a temperature around -10 °C, and the reaction proceeded as described below. In this reaction, n = 5.



Regardless of the nature of the reacting ketone, an intermediate compound is initially formed in the reaction. Only upon its subsequent neutralization is the carbinol derivative of the organometallic compound (simanthrene) obtained.⁽¹³⁾

The yield of the resulting simanthrenylcarbinol can vary depending on the specific nature of the reacting ketone. For instance, the yield of the reaction product with aliphatic ketones was high, whereas the yield with cyclic ketones (such as cyclopentanone and cyclohexanone) was low. This difference in yield is explained by the spatial structure (steric hindrance) of the ketone.

The lithium-substituted ferrocene was also used in the preparation of the corresponding salt from the reaction of ferrocene carbinol with $\text{Ba}(\text{OH})_2$. The process was carried out at 20–40 °C over 2–3 hours, following the reaction below. During this time, an intermediate product was first obtained, and its reaction with HCl yielded the corresponding ferrocene carbinol derivative. When the lithium derivative of ferrocene is used instead of ferrocene itself, the reaction product can be synthesized in a one-step procedure.

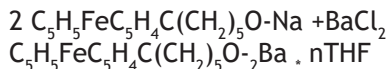


Based on the examined reaction, the yield of the obtained ferrocenylcyclohexylcarbinol derivative was higher than that of the simanthrenylcyclohexylcarbinol derivative. This is explained by the different reactivity of the ferrocene and simanthrene molecules, as well as the tendency of the simanthrene molecule to undergo rapid decomposition. In this case, the value of n in the reaction was $n = 5$.

The reaction of the ferrocene carbinol obtained from cyclohexanone with $\text{Ba}(\text{OH})_2$ was carried out in a THF medium, resulting in the corresponding barium carbinolate being obtained in a very low yield of 14 %.

$\text{C}_5\text{H}_5\text{FeC}_5\text{H}_4\text{C}(\text{CH}_2)_5\text{O}^- \text{Ba}(\text{THF})_2$ Complex II

To increase the yield of the reaction product, instead of ferrocenylcyclohexylcarbinol and simanthrenylcyclohexylcarbinol, their sodium or potassium derivatives ($\text{C}_5\text{H}_5\text{FeC}_5\text{H}_4\text{C}(\text{CH}_2)_5\text{ONa}$ /K) were used, and BaCl_2 was used instead of $\text{Ba}(\text{OH})_2$. The reaction was carried out in a THF medium, which resulted in a significantly higher yield of the product.

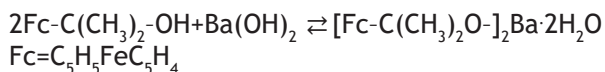


$n=2$

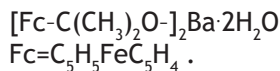
During the investigation of Complexes I and II using IR spectroscopy, signals corresponding to the -OH groups in the carbinols of the respective organometallic compounds were not observed. Instead, absorption bands corresponding to the ether group (C-O-) were detected in the $\nu_{\text{C-O}}$ region at 1580-1610 cm^{-1} . This indicates that the -OH group was replaced by the C-O- group.

When the organometallic complexes synthesized based on ferrocene and simanthrene are utilized as fuel additives, these substances facilitate the combustion process and play a positive role in environmental protection by preventing the formation of smoke. The smoke-free combustion of the fuel does not contribute to air pollution. Considering the scarcity of compounds that promote smoke reduction, substances exhibiting this property are regarded as highly advantageous from an ecological perspective. Specifically, the barium salts of the derivatives obtained from ferrocene and simanthrene ensure the smoke-free combustion of hydrocarbon fuels.

As noted above, carbinols obtained from reactions of ferrocene and simanthrene with aliphatic ketones, unlike those derived from cyclic ketones, react more readily with $\text{Ba}(\text{OH})_2$, yielding the target products in high yield. For example, the reaction between ferrocenyl dimethylcarbinol and barium hydroxide carried out in refluxing tetrahydrofuran (THF) resulted in a high product yield. The reaction proceeded with the elimination of two moles of water.



The resulting ferrocenyl isopropylate barium complex was obtained in 62-70 % yield. However, this complex does not possess a sharp melting or boiling point, and it decomposes above 210 °C. The ferrocenyl isopropylate barium complex can be easily washed with low-boiling hydrocarbon solvents such as pentane, hexane, or petroleum ether, then dried, and finally obtained as a solid. During drying, if air remains in the container, the complex turns into a liquid, indicating the hygroscopic nature (water-absorbing property) of the compound. In this state, the isolated complex retains two moles of water and has the following composition:⁽¹⁴⁾



The obtained $[\text{Fc}-\text{C}(\text{CH}_3)_2\text{O}]_2\text{Ba} \cdot 2\text{H}_2\text{O}$ complex (I) was investigated using IR and ^1H NMR spectroscopy. Additionally, the composition of the complex was determined by microanalysis for carbon and hydrogen. According to the results of the microanalysis, after washing complex (I) with petroleum ether, its composition corresponded to the formula $\text{C}_{26}\text{H}_{30}\text{Fe}_2\text{BaO}_2 \cdot 2\text{H}_2\text{O}$.

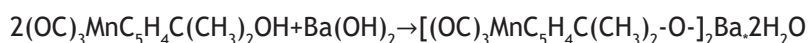
According to IR spectroscopy, the $\text{Fc}-\text{C}(\text{CH}_3)_2-\text{OH}$ (I) complex exhibits a stretching frequency at $\nu_{\text{OH}} = 3665 \text{ cm}^{-1}$, which disappears after interaction with $\text{Ba}(\text{OH})_2$. Based on ^1H NMR spectroscopy (spectrum recorded in CDCl_3), three signals were observed in the $\text{Fc}-\text{C}(\text{CH}_3)_2-\text{OH}$ complex in the 4-5 ppm range. Specifically, two signals from the substituted C_5H_4 ring appeared at 4,85 and 4,33 ppm, while one signal from the unsubstituted C_5H_5 ring appeared at 4,04

ppm. The signal corresponding to the CH₃ group protons was observed at 2,12 ppm. Thus, the investigation of the complex by IR and ¹H NMR methods provided a reliable basis for determining its structure.

Similar reactions were carried out with simanthrenyl dimethylcarbinol. The bis-simanthrenyl isopropyl barium dihydrate metal complex was obtained in 60-68 % yield via the reaction of isopropyl simanthrene (OC)₃MnC₅H₄C(CH₃)₂OH with Ba(OH)₂ in a THF medium.

According to IR spectroscopy, the C₂₂H₂₀Mn₂BaO₈·2H₂O (I) complex exhibits a stretching frequency at νOH = 3665 cm⁻¹, which disappears after interaction with Ba(OH)₂. Based on ¹H NMR spectroscopy (spectrum recorded in CDCl₃), three signals were observed in the Fc-C(CH₃)₂-OH complex in the 4-5 ppm region. Specifically, two signals from the substituted C₅H₄ ring appeared at 4,85 and 4,33 ppm, while one signal from the substituted C₅H₅ ring appeared at 4,04 ppm. The signal corresponding to the CH₃ group protons was observed at 2,12 ppm. Thus, the investigation of the complex by IR and ¹H NMR methods provided a reliable basis for determining its structure.

The reactions were also carried out with simanthrenyl dimethylcarbinol. The bis-simanthrenyl isopropylcarbinol barium dihydrate metal complex was obtained in 60-68 % yield through the reaction of isopropyl-simanthrenyl (OC)₃MnC₅H₄C(CH₃)₂OH with Ba(OH)₂ in THF.

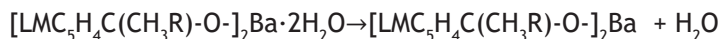


According to the results of the conducted microanalysis, the (OC)₃MnC₅H₄C(CH₃)₂-O-]₂Ba·2H₂O (II) complex was consistent with the calculated elemental composition. Compared to the (I) complex, this compound decomposes at much lower temperatures, above -105 °C, exhibits a pale yellow color, and is resistant to hydrolysis and oxidation.

The simanthrenylisopropyl barium dihydrate metal complex (II) was also analyzed using IR and H¹ NMR methods. The infrared (IR) spectra were recorded in vaseline oil. In the IR spectrum of the (II) complex, signals were observed in the νC=O region at 1950-2018 cm⁻¹ corresponding to the terminal carbonyl groups, and in the νO-H region at 3480-3750 cm⁻¹ corresponding to the hydroxyl groups. Regarding the H¹ NMR results (spectrum recorded in CDCl₃), the signals corresponding to the α and β protons of the cyclopentadienyl ring (C₅H₄) appeared in the 4,56-5,08 ppm region, indicating substitution on the cyclopentadienyl ring. In the unsubstituted C₅H₅ ring, only a single signal at 4,57 ppm was observed, due to the equivalence of the α and β protons.^(15,16,17,18)

As mentioned above, simanthrene is less stable to sunlight compared to ferrocene and undergoes decomposition upon exposure. Although it is ecologically harmless, its light sensitivity limits its practical applications. Unlike ferrocene derivatives, simanthrene derivatives decompose quickly under ordinary light. For example, the (II) complex also undergoes decomposition when exposed to daylight. Therefore, it is recommended to store such compounds in the dark.

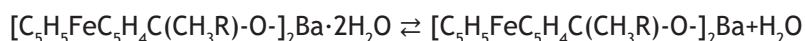
The obtained (I) and (II) complexes are poorly soluble in water and alcohols, but are highly soluble in certain polar solvents, while in acidic or basic media they undergo decomposition upon dissolution. On the other hand, both complexes exhibit the ability to dehydrate. The (I) metal complex underwent dehydration in the temperature range of 160-195 °C, whereas the (II) metal complex dehydrated between 80-112 °C. The overall course of the process is as follows:



Here, L= CO groups.

Upon dehydration of barium dihydrate of simanthrenyldimethylcarbinol, its dimethylcarbinolate (Complex III) was obtained. The process was reversible. $[(\text{OC})_3\text{MnC}_5\text{H}_4\text{C}(\text{CH}_3)_2\text{-O-}]_2\text{Ba}\cdot 2\text{H}_2\text{O} \rightleftharpoons [\text{LMC}_5\text{H}_4\text{C}(\text{CH}_3)_2\text{-O-}]_2\text{Ba} + 2\text{H}_2\text{O}$

Similarly, upon dehydration of the barium dihydrate of ferrocenyldimethylcarbinol, its dimethylcarbinolate (Complex IV) was obtained. The process was reversible, and unlike Complex III, Complex IV was obtained in high yield.⁽¹⁹⁾



R- alkyl groups.

The metal complex derivatives (III) and (IV), obtained after the thermal dehydration process, exhibit good solubility in non-polar solvents, including motor fuels (gasoline and other petroleum fractions) and diesel fuels (kerosene). Specifically, their solubility ranges from 10-14 g/L in motor fuels and 32-38 g/L in diesel fuels. This property significantly broadens their potential applications. It was determined that the addition of 0,02 wt.% of the (III) organometallic compound to gasoline increased the flame height from 8,4 mm to 16,9 mm, and in diesel fuels from 16,1 mm to 26,4 mm. When a 0,001-0,2 % mixture was added to the fuel (this mixture contained 10-15 % of the barium-based ferrocene derivative), engine power increased by up to 15 %, and fuel smoke emission was effectively reduced.

The derivatives obtained from the studied metal complexes—newly synthesized compounds of ferrocene and simanthrene—are used not only as anti-knock agents but also as smoke suppressants. Therefore, the application of these substances in chemical and petrochemical industries is of significant importance.⁽²⁰⁾

The primary objects of study in this dissertation were the air and water ecosystems. Investigating the factors contributing to the pollution of both environments constituted the main direction of the research. Currently, the pollution of air and water ecosystems represents one of the most critical global environmental challenges. Against the background of atmospheric pollution, the greenhouse effect is intensified. With the increase in the greenhouse effect, the melting of glaciers leads to a reduction in freshwater resources, and the runoff of clean water mixes with polluted waters. Concurrently, against the background of water ecosystem contamination, the demand for freshwater is increasing daily. For this purpose, the research conducted within this dissertation aimed at taking serious steps toward resolving the problems occurring in the air and water environments.

As is known, the ecosystems of the biosphere are closely interconnected, and pollution in one ecosystem leads to the contamination of another. Furthermore, the oil industry, which is critical in Azerbaijan, contributes to the pollution of both air and water ecosystems. While soil ecosystems are also subject to pollution, the soil layer is less dynamic compared to the air and water ecosystems; therefore, pollution manifests more prominently in these two systems. Given that approximately 85 % of crude oil processed at the Oil Refinery is dedicated to obtaining fuel utilized in the automotive industry, the oil sector is very closely linked with the transport

sector. The environmental damage caused by road transport emissions (particularly in Baku city) is currently one of the foremost negative impacts. Consequently, many of the exhaust gases generated during the operation of automobile engines and the combustion of fuel directly contribute to the formation of greenhouse gases, while a portion causes secondary pollution. At this point, ensuring that the fuel additives meet ecological standards and are non-toxic is a separate issue of great environmental importance. Simultaneously, it is ecologically vital that the additives incorporated into the fuel possess a minimum threshold of smoke-suppressant capability. Ultimately, the non-deleterious nature of the exhaust gases emitted by road transport into the atmosphere is of critical environmental significance.

CONCLUSIONS

The smoke-suppressing effects of the barium-based organometallic compounds (III) and (IV) are superior both to ferrocene and simanthrene themselves and to existing smoke suppressants. Specifically, in distilled gasoline and diesel fuels, these compounds exhibit 1-1,5 times higher smoke suppression compared to conventional additives, and 0,4-0,6 times higher than ferrocene and simanthrene. Overall, it should be noted that, compared to ferrocene and simanthrene, the derivatives obtained from these complexes contain lower mass fractions of iron and manganese, so engines operating on such fuels experience little or delayed wear. On the other hand, compared to ferrocene and simanthrene (except for the CO groups), the newly synthesized organometallic complexes are more prone to chemical transformations due to the presence of active oxygen. In this regard, the newly synthesized derivatives of ferrocene and simanthrene are considered industrially significant compounds. As noted, the smoke-suppressing properties of the studied metal-organic complexes (I) and (II) were tested in 2016 at the Azneftiyag Oil Refinery, currently the H. Aliyev Oil Refinery.

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AUTHORSHIP CONTRIBUTION

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Writing - proofreading and editing: Elmina Gadirova, S.R. Hajiyeva.



Chapter 12

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Ultrasonic Multi-Electrode Electrophysical Ionization for High-Purity Extraction of Precious, Base, and Rare-Earth Metals from Kyrgyzstan's Technogenic Tailings

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ABSTRACT

An original, multicomponent technology is proposed for extracting precious, base, and rare-earth elements from Kyrgyzstan's technogenic wastes. The core of the process is electro-physical ionisation (EPI) enhanced by cavitation-assisted ultrasound and implemented in a spatially distributed multi-electrode configuration. The study pursued a dual objective: (i) to formulate the physico-chemical rationale that ensures maximal selectivity and high energy efficiency, and (ii) to model operating regimes that minimise the generation of secondary pollutants. Feedstocks included concentrator tailings, metallurgical slags, and sludges accumulated in the country's key mining provinces. A response-surface experimental design enabled fine-tuning of the critical parameters: potential 6-12 V, inter-electrode gap 1,0-1,5 cm, electrolyte molarity 0,5-1 M, acoustic power < 300 W, and treatment duration 30-65 min. The result was record extraction efficiencies: Cu – 96,8 %, Zn – 93,5 %, Ag – 92,1 %, Au – 88,5 %. For the rare-earth representatives, La and Nd, the respective values reached 79,7 % and 81,1 %. The purity of the recovered precipitates, verified by combined ICP-OES / SEM-EDX analysis, exceeded 99,8 % (Cu) and 99,5 % (Au, Ag). The synergy of ultrasonic cavitation and the multi-electrode field lowers the energetic barrier of electrochemical reactions, disaggregates the solid phase, accelerates mass transfer, and ensures uniform current distribution, thus preventing anode passivation. Comparison with conventional hydro- and pyrometallurgical routes revealed an order-of-magnitude reduction in energy consumption and complete elimination of hazardous reagents. The developed approach not only paves the way for comprehensive recycling of accumulated wastes—mitigating environmental risks—but also establishes an alternative mineral resource base for critical metals, capable of providing an additional impetus to the economy of the Kyrgyz Republic.

Keywords: Electro-Physical Ionisation; Ultrasonic Activation; Industrial Wastes; Metal Extraction; Rare-Earth Elements; Process Optimisation; Environmental Safety.

INTRODUCTION

Over the past quarter-century the global eco-technological race has triggered an unparalleled surge in metal consumption. The industrialisation of emerging economies, worldwide digitalisation, and an ambitious drive for a *green* transition have become tightly interwoven drivers of demand, causing the ore grades of valuable elements to decline inexorably and natural deposits to grow progressively poorer. A world that is expanding on metals slips into a paradox: the more it mines, the more waste it produces, and the more acutely it experiences shortages of primary feedstock. Mining and metallurgical industries—already generating billions of tonnes of by-products each year—now rank among the three largest sources of industrial

waste. Metallurgy's contribution to the planetary carbon footprint is substantial: roughly 40 % of all industrial greenhouse-gas emissions and nearly one-tenth of global electricity consumption originate in this cycle. Annual extraction is approaching 3,2 billion t of minerals, yet the resulting tailings and sludges outweigh the mass of finished metals by a factor of 15-20; forecasts indicate these volumes will double by 2050—an alarming prospect for climate, biodiversity, and human health.^(1,2,3)

Against this backdrop, the concept of a circular economy no longer appears academic but rather emerges as a strategic imperative. The closed-loop paradigm—resource → product → waste → new resource—shifts the focus from extensive exploitation of virgin ores to intensive treatment of technogenic stocks. Recovering metals from industrial residues thus delivers two synergistic benefits: mitigating environmental damage while creating new economic niches. One striking example suffices: aluminium recycling cuts energy demand by about 95 % compared with primary smelting of bauxite. Yet even such impressive savings fail to close the gap between global appetite and available scrap flows: today secondary raw materials cover no more than one-third of demand. Consequently, some portion of metals must still originate from mines, making full mobilisation of technogenic sources—tailings ponds and sludge dumps included—no longer an optional green measure but a cornerstone of resource security.⁽⁴⁾

Critical metals—most notably rare-earth elements (REEs), whose importance for electronics, electric vehicles, and modern power systems rivals that of oil during the industrial age—occupy a special place in this equation. Their recycling rate is dismally low (below 1 %), whereas base non-ferrous metals achieve 30-70 %. Production of primary REEs also records the highest specific CO₂ emissions per kilogram of output. Because more than 60 % of REE mining and 90 % of processing are concentrated in China, any trade restrictions instantly propagate into a global shock. This reality sets a dual task: to develop efficient, environmentally benign techniques for re-extracting REEs from technogenic streams and, by doing so, to reduce geopolitical risks and strengthen supply-chain resilience.⁽⁵⁾

The Kyrgyz Republic offers a particularly vivid example of the challenge. Endowed with abundant mineral resources, the country simultaneously bears the legacy of decades of extraction: about 100 million t of industrial and domestic waste have already accumulated within its confined territory. Mining accounts for the lion's share, represented by 35 tailings repositories and 25 waste-rock dumps scattered nationwide. The annual growth of toxic technogenic masses further intensifies pressure on ecosystems, propelling the search for technological solutions capable of turning this potential ecological debt into a strategic reserve of valuable and rare metals.

Between the global imperative of sustainability and region-specific challenges, a clear chain of necessity has emerged: the more lucidly the world recognises the limits of traditional mining, the more actively it turns to the resources lying literally underfoot—in tailings, slurries, slags and fly ash. An efficient, environmentally sound technology for extracting metals from these streams thus becomes not merely a technological innovation but a pivotal link in the architecture of future metallurgy, where “waste” ceases to mark the end of a value chain and instead becomes a new point of departure.

Kyrgyzstan's largest industrial deposits—Kumtor, Taldy-Bulak Levoberezhny, and Terek-Sai—have in recent decades produced a veritable “glacier” of technogenic waste that inexorably encroaches upon the nation's economy and environment. At Kumtor alone, 17 305 kg of gold

were mined in 2022, drawing on a resource base that, as of December 2020, comprised 73,3 million tonnes of ore averaging $2,66 \text{ g Au t}^{-1}$. Every tonne of such ore, after passing through the processing plant, leaves behind tailings still hosting significant residual metal content. Terek-Sai is following suit: construction of its own concentrator and a new tailings storage facility commenced in 2020—another harbinger of escalating waste accumulation. The 2022 ban on the export of ferrous-metal scrap, tailings and gold-bearing concentrates eloquently signals that the Republic intends to keep these resources at home, maximising added value and abandoning the familiar raw-materials export model.⁽⁶⁾

The technological footprint of mining, however, is far from benign. A substantial fraction of tailings-storage facilities (TSFs) have long outlived their design life or fallen short of current sanitary standards, turning into powder kegs. History has already issued invoices for negligence. In 1998 a road tanker at Kumtor plunged into the Barskaun River, spilling over a tonne of cyanide; more than 2500 people suffered acute poisoning. An even more tragic episode unfolded in 1958: an earthquake and torrential rains ruptured Tailings Dam No. 7 of the Mailuu-Suu combine, releasing $600\,000 \text{ m}^3$ of radioactive slurry that coursed forty kilometres downstream, killing livestock and irradiating the local population. Decades later, uranium levels in Mailuu-Suu waters remain 10–15 times above background. Add the region's high seismo-tectonic activity, unconsolidated slopes, and avalanche-debris flows, and one obtains a textbook case of cascading risks. Even the Issyk-Kul basin—promoted to tourists for its “therapeutic” waters—registers elevated anthropogenic Cr and As concentrations in its rivers, planting a delayed-action mine beneath public health.⁽⁷⁾

Against this backdrop, the strategic logic of processing technogenic stocks becomes non-negotiable. Open-pit operations at Kumtor officially cease in 2023, and the full processing cycle will conclude by 2031; primary ore throughput will therefore dwindle. Concurrently, the state has amplified its commitment to developing a rare-earth mineral base, as REEs are indispensable for green and high technologies. Consequently, the volume of waste potentially containing Y, Nd or La will only grow—so bringing these “secondary deposits” into circulation transforms an environmental liability into an economic opportunity. In other words, a properly orchestrated “mining renaissance” could not merely prolong the life of Kyrgyzstan's extractive sector but also convert the industrial era's legacy into a springboard for the nation's future economy.

Recovering valuable and critical metals from industrial wastes—particularly from dilute solutions containing only single- to double-digit ppm levels of target elements and from heterogeneous matrices rich in interfering species—remains a formidable technological challenge. Traditional hydrometallurgical approaches (ion exchange, solvent extraction) perform reliably at high metal concentrations; however, their efficiency drops sharply in “lean” systems, leading to higher specific energy consumption, reduced selectivity, and ultimately uneconomical product costs. Elevated concentrations of Fe^{3+} and Al^{3+} further complicate treatment by masking analytical signals or forming stable complexes that block sorbent active sites.

Ionic liquids, often promoted as next-generation “green” solvents, were expected to mitigate these issues. Yet they frequently suffer thermal and electrochemical degradation and, due to their strong solvation power, migrate into secondary aqueous phases, thus complicating downstream purification. Consequently, fundamentally different solutions—combining precise process control, moderate energy demands, and minimal environmental impact—are urgently needed.

Electrochemical technologies, as a logical extension of ion-based separations, theoretically meet these criteria: charge transfer is governed by electrode potential, reagent consumption is negligible, and side products are minimal. In practice, however, challenges arise. Wastewater compositions are seldom fully characterized, hampering precise potential-programming. Organic ligands abundant in process streams form strong chelates with Cu^{2+} , Ni^{2+} , Co^{2+} , and REE^{3+} , slowing electrodeposition and requiring high current densities. Mass-transfer limitations, electrode corrosion, and the difficulty of scaling up to industrial volumes further exacerbate the problem.

To overcome these barriers, we propose electro-physical ionization (EPI) in a multi-electrode configuration, synergistically enhanced by ultrasonic cavitation. Cavitation micro-jets and shock waves disaggregate solid phases, remove diffusion barriers, and continuously renew boundary layers, thereby intensifying mass transfer and boosting metal recovery.^(3,4)

Research Objective

To develop a scientifically sound, technologically adaptable methodology for extracting Au, Ag, Cu, Ni, Zn, Mg, Ca, and rare-earth elements La and Nd from technogenic wastes in key mining regions of Kyrgyzstan using EPI supplemented by ultrasonic activation.

Specific Tasks

1. Raw-material inventory: conduct a detailed geochemical audit of tailings, sludges, and slags; map spatial distribution and estimate reserves of these elements across the country's geo-industrial provinces.
2. Engineering design: build a laboratory-scale EPI setup with an optically transparent reactor, integrated ultrasonic module, and adjustable electrode spacing; develop a mathematical model for coupled charge and mass transfer in the solid-liquid-electrode system.
3. Parametric optimization: apply design-of-experiments methods (Taguchi, response-surface methodology) to identify optimal voltage, electrode spacing, electrolyte concentration, ultrasound frequency/power, and exposure time that maximize yield while minimizing specific energy consumption.
4. Experimental validation: monitor kinetics and yields via ICP-OES; analyze precipitate morphology and phase composition by SEM/EDX; benchmark energy use and selectivity against conventional flowsheets.
5. Techno-economic comparison: compare EPI with pyrometallurgical and classical hydrometallurgical routes in terms of CAPEX/OPEX, carbon footprint, and resource sustainability.
6. Scaling-up: evaluate the transition from laboratory cell to pilot module: select corrosion-resistant electrode materials, integrate renewable energy sources, and design a closed-loop water-reagent circuit.

This comprehensive science-to-industry roadmap aims to transform problematic waste streams into sustainable sources of strategic metals, thereby strengthening the circular economy in the Kyrgyz Republic.

METHOD

Objects of resource extraction: the present study targets three representative—yet markedly heterogeneous—classes of industrial waste that have accumulated from mining and processing activities across the Kyrgyz Republic. Each class merits its own monograph, but they are outlined briefly below.

1. Ore tailings: these fine-grained “tails,” produced during the beneficiation of gold-bearing, polymetallic, or porphyry-copper ores, may at first resemble an innocuous mixture of sand, silt, and clay. Under microscopic examination, however, they reveal a multiphase system in which residual precious and transition metals coexist with flotation reagents, sulfide compounds, and other chemical “ghosts” of the technological cycle. Tailings facilities thus pose a dual threat: they constitute a potential “treasure trove” of under-extracted metals and, simultaneously, a source of heavy elements prone to bioaccumulation and long-term migration within ecosystems.

2. Industrial sludges: this category spans everything from coal-washing sediments to galvanic and wastewater sludges enriched in copper, nickel, zinc, chromium, and their numerous oxide-carbonate modifications. Galvanic waste is particularly illustrative: its high concentration of readily leachable metals turns such sludge into a “chemical time bomb” capable of contaminating groundwater upon even minor breaches of containment. The fractional composition (carbonate, residual, Fe-Mn oxide fractions) dictates complex leaching kinetics and therefore demands finely tuned extraction technologies.

3. Metallurgical slags: by-products of high-temperature processing—e.g., steelmaking slags—have long ceased to be mere “stones underfoot” for metallurgists. Slags bear a distinct signature of their parent feedstock: stainless-steel slags concentrate hexavalent chromium, while ferroalloy slags harbor manganese and vanadium. Value, however, is inseparable from toxicity, complicating the reintegration of slags into economic circulation and rendering them both an environmental liability and a resource.

Rationale for selection: by cumulative reserves, confirmed metal contents, and associated environmental risk, tailings, sludges, and slags form the leading triad among industrial accumulations in Kyrgyzstan. Their multicomponent nature, variable mineralogy, and interleaving of valuable and hazardous phases pose challenges that conventional hydro- and pyrometallurgical methods address only partially. Innovative electro-physical ionization (EPI) technologies are expected to meet this dual challenge by selectively extracting metals while simultaneously detoxifying the matrix.

Geographical focus: for experimental validation of EPI, three key regions with the highest concentrations of the aforementioned wastes have been selected:

- Osh Region: a southern industrial hub with gold-mining and coal-beneficiation tailings repositories.
- Jalal-Abad Region: the historical “shield” of polymetallic production.
- Issyk-Kul Region: a north-eastern cluster dominated by porphyry-copper operations.

This regional “triad” enables demonstration of EPI performance on diverse matrices under differing climatogeological conditions, thereby providing a coherent methodological basis for nationwide scale-up.

The data presented in this study unequivocally show that Kyrgyzstan’s anthropogenic stockpiles harbor sizeable clusters of strategically important metals. For example, the tailings of the country’s largest gold-mining operation—the Kumtor deposit high in the rugged mountains of Issyk-Kul—still retain residual fractions of gold and silver “dissolved” within the mineral matrix after ore processing. Further southwest, in Jalal-Abad Province, massive polymetallic tailings store copper, nickel, and zinc, forming a potentially lucrative raw-material “cushion” for future extraction. Even the seemingly inconspicuous coal-washing slurries of the Osh region—by-products far removed from classical non-ferrous metallurgy—reveal, upon detailed analysis,

not only a notable share of alkaline-earth elements but also traces of rare-earth metals (REMs).

Table 1. Distribution of industrial wastes and their metal contents⁽⁷⁾

Region	Type of waste	Reserves, million t	Au, g/t	Ag, g/t	Cu, %	Ni, %	Zn, %	Mg, %	Ca, %	La, g/t	Nd, g/t
Osh Region	Coal-washing sludges	5,2	0,8	12,5	0,15	0,08	0,22	1,5	2,1	35	28
Jalal-Abad Region	Polymetallic tailings	8,7	0,9	18,0	0,25	0,12	0,35	1,8	2,5	40	32
Issyk-Kul Region	Ore-processing plant waste	3,3	2,4	35,0	0,40	0,15	0,50	2,0	2,8	50	40
Naryn Region	Gold-ore tailings	6,1	1,1	20,0	0,10	0,05	0,18	1,2	1,8	30	25
Chüy Region	Industrial sludges (galvanic)	1,5	0,01	0,5	0,80	0,60	1,20	0,5	0,7	5	4

The inclusion of lanthanum and neodymium among the target elements merits special attention. Their selection is driven not merely by the explosive global demand for REMs but also by a distinctly national context: the Government of the Kyrgyz Republic has announced plans to stimulate exploration of rare-earth occurrences within its territory. Although detailed quantitative assessments of La and Nd in local technogenic deposits remain fragmentary, precedents in neighboring countries inspire optimism. Notably, a Kazakh deposit rich in cerium, lanthanum, and neodymium mineralization vividly demonstrates the geological “kinship” of the region, thereby substantiating the expanded research focus.^(7,8,9)

To develop such heterogeneous sources efficiently, we propose a fundamentally new extraction architecture—electro-physical ionization (EPI) augmented by ultrasonic activation in a multi-electrode configuration. The synergy of these two physical stimuli creates a “breakthrough bridge” across the perennial barriers of conventional methods: low selectivity in dilute solutions, sluggish mass transfer in viscous granular suspensions, and, ultimately, the generation of toxic secondary phases.

The experimental “skeleton” of the process is outlined by the following anchor parameters. First, an operating voltage of 6-12 V provides, on the one hand, reliable initiation of electrochemical reactions and, on the other, containment of excessive energy costs. Second, an inter-electrode gap of 1,0-1,5 cm maintains an optimal field gradient that governs ionic trajectories. Third, an electrolyte concentration of 0,5-1 M (NaCl or weak acids) represents a compromise among conductivity, ionization rate, and precipitation selectivity.^(10,11)

The physico-chemical underpinnings of EPI are multi-stage. Under the influence of the electric field in a heterogeneous suspension, electro-osmosis and electromigration emerge: the liquid phase, drawn by an invisible peristaltic force, moves toward the cathode, while charged ions drift toward oppositely charged electrodes. Simultaneously, water electrolysis produces H⁺ ions at the anode and OH⁻ groups at the cathode, establishing a pH gradient throughout the volume. The advancing acidic front desorbs heavy metals from solid surfaces, thereby enhancing their solubility and mobility.^(12,13)

The key innovation lies in incorporating ultrasound into the multi-electrode cell. Cavitation micro-explosions generated by acoustic waves disperse agglomerates, enlarge the solid-liquid

interfacial area, and induce turbulent micro-mixing, thereby accelerating mass transfer and reducing diffusion limitations by orders of magnitude. Collectively, the combined electrical and ultrasonic stimuli establish a highly adaptable technological platform capable of “squeezing out” the very “hidden” value in technogenic deposits that previously seemed unattainable.

To mitigate the inherent shortcomings of electro-physical ionization (EPI)—chiefly the limited mass-transfer rate in heterogeneous media and the passivation of electrode surfaces—we propose a radical reactor upgrade that combines two mutually reinforcing engineering solutions: a multi-electrode configuration and ultrasonic activation.

1. Multi-electrode architecture: transitioning from the classical two-electrode pair to a spatially optimized lattice of cathodes and anodes (often implemented in a cylindrical arrangement) multiplies the total active surface area. As a result:
 - Current density per unit area decreases, suppressing polarization phenomena and retarding cathodic fouling by deposited metals.
 - The electric field is distributed more uniformly throughout the suspension volume, eliminating “dead” zones and enhancing the recovery of rare metals.
 - Parallel extraction of several elements becomes technically feasible, while the possible recuperation of a fraction of the energy (e.g., via short-circuited loop currents) improves the overall process economics.^(14,16)

This modular scheme scales readily; moreover, reconfiguring inter-electrode spacings allows adaptation to the waste composition, conductivity, and the required selectivity.

2. Ultrasonic activation: introducing an acoustic field (20-100 kHz, ≤ 300 W) transforms the reaction volume into a dynamic cavitation environment. Collapse of micro-bubbles generates local pressure and temperature spikes that:
 - Fragment solid particles: slag agglomerates can shrink from ~ 30 μm to ~ 1 μm , removing diffusion barriers.
 - Clean and “unseal” surfaces, releasing encapsulated ions and vastly enlarging the interfacial area.
 - Accelerate mass transfer: high-velocity micro-jets erode the diffusion layer, eliminating the principal kinetic bottleneck of the electrochemical scheme.^(17,18,19)
 - Lower the activation energy of electrochemical reactions (a drop from 34,68 kJ mol^{-1} to 6,21 kJ mol^{-1} has been recorded in model experiments), dramatically increasing leaching rates.
 - Induce electroporation of organic inclusions, where present, facilitating the release of metals bound in biogenic matrices.^(20,21,22)

RESULTS

The implementation of the novel electro-physical ionization (EPI) concept, reinforced by ultrasonic activation within a multi-electrode system, demonstrates a substantial increase in the efficiency of valuable-metal recovery from industrial wastes of the Kyrgyz Republic. The synergistic action of the electric field, optimized electrode geometry, and ultrasonic cavitation affords unprecedented mobilization and selective extraction of metals from complex matrices.

The final values presented in table 2 were obtained after meticulous parameter optimisation via response-surface methodology (RSM). They clearly show that even a complex multiphase industrial-waste matrix can be driven to near-complete ionic dissolution. Copper (Cu) is recovered with an efficiency of 96,8 %—a level that conventional hydro- and pyrometallurgical

technologies rarely achieve. The noble metals also exhibit impressive “compliance”: gold (Au) reaches 88,5 %, and silver (Ag) 92,1 %, results that equal or often surpass alternative electrochemical schemes applied to secondary raw materials. Equally noteworthy are the figures for strategically important rare-earth elements: lanthanum (La) at 79,7 % and neodymium (Nd) at 81,1 %. Against the backdrop of global difficulties in rare-earth recycling, these values appear more than encouraging.^(23,24,25,26)

Table 2. Optimized EPI parameters and corresponding metal-recovery efficiencies						
Metal	Optimal voltage, V	Optimal inter-electrode distance, cm	Optimal electrolyte concentration, m	Optimal ultrasonic power, W	Processing time, min	Extraction efficiency, %
Au	8	1,2	0,7	250	45	88,5
Ag	7,5	1,1	0,6	220	40	92,1
Cu	9	1,0	0,8	280	30	96,8
Ni	10	1,3	0,9	260	50	91,2
Zn	8,5	1,2	0,7	240	35	93,5
Mg	11	1,4	1,0	200	60	82,3
Ca	12	1,5	1,0	180	65	78,9
La	9,5	1,0	0,8	300	55	79,7
Nd	9,5	1,0	0,8	300	55	81,1

To illustrate the selectivity and overall performance of EPI enhanced by ultrasonic cavitation, a composite figure 1 was plotted, depicting the extraction shares of each element under study.

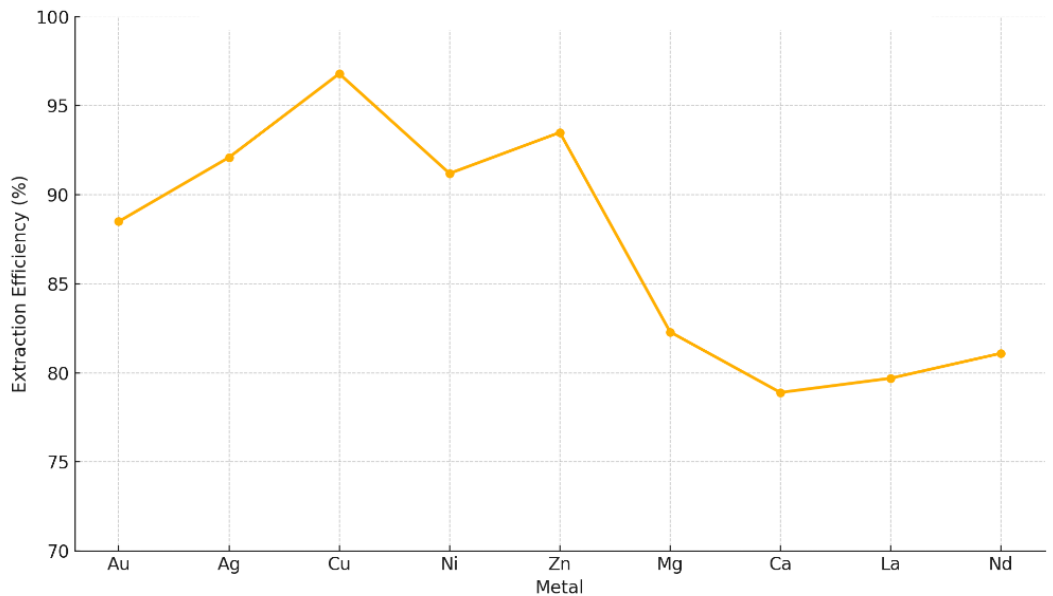


Figure 1. Metal extraction efficiency achieved through electro-physical ionization (EPI) enhanced by ultrasonic activation

The curve, reminiscent of the jagged profile of a mountain ridge, rises sharply and then descends smoothly in accordance with the thermodynamic and electrochemical nature of the metals themselves. The highest “peaks” belong to copper (96,8 %), zinc (93,5 %) and silver (92,1 %)—a pattern attributable to their high electrical conductivity, pronounced tendency to dissolve in acidic media, and the effective surface turbulence induced by ultrasonic micro-streams. Gold, despite its “noble” inertness, still exceeds the 88 % threshold, confirming the versatility of the method.

More restrained yet still respectable are the rare-earth and alkaline-earth representatives: lanthanum (79,7 %), neodymium (81,1 %), magnesium (82,3 %) and calcium (78,9 %). For the first two, such high yields are particularly significant given their customary “stubbornness” in selective leaching; for the latter pair, they underline the flexibility of EPI in dealing with cations that differ radically in hydration radius and discharge potential.

Collectively, these findings affirm that electro-physical ionisation augmented by ultrasonic activation provides a technological platform that is equally effective for base, noble, rare-earth and alkaline-earth metals, paving the way for deep, environmentally sustainable utilisation of technogenic resource streams.

The record extraction coefficients observed are not the result of a single factor but of an entire cascade of interrelated effects embedded in the design of the EPI system. Ultrasonic activation plays a pivotal role as an “acoustic catalyst” that radically boosts mass transfer: cavitation micro-jets disintegrate particle agglomerates, strip passive films, reduce median fragment size and dramatically increase specific surface area—critical for finely dispersed tailings and sludges that are traditionally inert to leaching. An additional benefit is the lowering of the activation energy of leaching reactions, which nearly halves the overall processing time. Simultaneously, the multi-electrode configuration distributes the electric field and current evenly, eliminating local polarisation and focal metal deposition, thereby ensuring complete and homogeneous extraction.^(17,27)

Process parameters for electro-physical ionisation (EPI) were optimised not by trial-and-error, but through the synergistic coupling of the Taguchi design approach with Response Surface Methodology (RSM). This statistical “tandem” first filtered out secondary factors and then generated predictive models describing how the controllable variables—applied voltage, inter-electrode spacing, electrolyte concentration and ultrasonic power—affect the key performance indicators (extraction yield and product purity). Although the response-surface plots are not shown here, they unambiguously reveal a non-linear topology. For example, the optimum conditions for magnesium (Mg) were identified at 1,0 M electrolyte, 200 W ultrasonic power and a 60-min exposure, whereas gold (Au) required 0,7 M, 250 W and only 45 min of treatment. Such disparities highlight the multicomponent nature of the system and the necessity of multi-objective optimisation.⁽²⁷⁾

A further advantage is the high quality of the recovered product. Analytical control performed by inductively coupled plasma optical emission spectrometry (ICP-OES) and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM/EDX) confirmed that the extracted metals meet stringent industrial purity standards. In other words, the proposed EPI technology not only maximises the recovery of valuable components from waste streams, but also delivers material that is virtually ready for high-tech downstream utilisation, thereby minimising the costs of subsequent refining.

Table 3. Comparative purity of the extracted metals (%)

Metal	Purity, % (by ICP-OES)	Purity, % (by SEM/EDX)	Major impurities (by ICP-OES/SEM/EDX)
Au	999,5	999,0	Cu, Ag, Fe
Ag	999,2	998,8	Cu, Au, Pb
Cu	999,8	999,5	Ni, Zn, Fe
Ni	998,7	998,0	Cu, Zn, Fe
Zn	999,0	998,5	Cu, Ni, Fe
Mg	997,5	997,0	Ca, Al, Si
Ca	997,0	996,5	Mg, Si, Fe
La	995,0	994,5	Nd, Ce, Fe
Nd	995,5	995,0	La, Ce, Fe

To obtain reliable quantitative metrics for the recovered metals, we employed an inductively coupled plasma-optical emission spectrometer (ICP-OES). Its unique combination of high spectral resolution and sub-ppb detection limits enables the technique to “see” even minute trace impurities without sacrificing analytical precision. Complementary characterization was performed by scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM/EDX): micro-probe analysis delivers not only a topographic view of precipitate morphology but also a detailed elemental map at the scale of individual grains. Taken together, the two techniques provide a virtual “X-ray of the grams” – an exhaustive panorama of the purity and phase composition of the recovered metals.

The results, summarized in table 3, are unequivocal: the vast majority of target components exhibit purities above 998 % (99,8 %), with copper exceeding 999 %. Even the notoriously difficult rare-earth elements, lanthanum and neodymium, maintain ≈ 995 %. This level of refinement correlates directly with the high selectivity of electrochemical deposition, further intensified by ultrasonic cavitation. Transient cavitation bubbles continuously disrupt the boundary diffusion layer, driving ions toward the electrode surface while suppressing co-precipitation of extraneous species. Because electrons are the only “reagent,” the risk of secondary contamination is essentially eliminated.

Extraction efficiency (η) was evaluated as the ratio of the actual concentration of the target metal in the product to its original concentration in the processed matrix. Spike-recovery tests with fortified samples or certified reference materials (CRMs) were used to verify the method and eliminate systematic bias. The final expression is:

$$\eta(\%) = C_{\text{prod}} / C_{\text{waste}} \cdot 100\%$$

Where η is the metal extraction efficiency (%), C_{prod} is the measured concentration of the metal in the recovered product (mg L^{-1} , g t^{-1} , etc.), and C_{waste} is its initial concentration in the waste (same units). This metrologically rigorous comparison unequivocally demonstrates that the described technology can selectively and efficiently extract high-value components from refractory industrial tailings.

DISCUSSION

The electro-physical ionization (EFI) technology proposed here—fortified by directed

ultrasonic activation in a multielectrode configuration—exhibits a suite of advantages that clearly set it apart from both classical and several modern methods for recovering metals from anthropogenic feedstocks.

Pyrometallurgical processes—the long-standing “veterans” of the sector—rely on high-temperature regimes that demand enormous energy inputs and can release toxic compounds at the slightest breach of process discipline. Hydrometallurgical routes, by contrast, avoid extreme temperatures but often depend on aggressive reagents (cyanide for Au is the most illustrative case), inevitably raising concerns over secondary contamination and the arduous neutralization of waste streams. Even “green” refinements, such as ammonia-thiosulfate leaching coupled with electrochemical assistance, while delivering > 80 % Au and $\approx$ 75 % Cu/Ag recovery from spent tailings, remain of limited universal applicability.^(4,27)

Electrochemical approaches are rightly positioned as the more environmentally benign option: electrons act as a clean reagent, minimizing both chemical consumption and sludge generation. Yet when treating dilute solutions and complex matrices, these methods face mass-transfer barriers and elevated energy requirements.^(3,4,25) Integrating ultrasound into the EPI scheme proves to be the instrument that dismantles this barrier. Cavitation phenomena generated by ultrasound disintegrate agglomerates, liberate encapsulated phases, lower activation energies, and accelerate kinetics by an order of magnitude. For example, > 97 % of Zn, Cd, Cu, and Mg were extracted from a copper-cadmium slag in merely two hours, whereas conventional leaching demanded a full day or more to reach comparable recoveries.⁽¹⁷⁾

The multielectrode architecture further promotes uniform potential distribution, mitigates polarization effects, and thus maintains process stability up to the production of ultra-high-purity metals. Experimental campaigns on waste printed-circuit boards, for instance, achieved 99.9 %-pure Cu—comparable with leading industrial benchmarks and underscoring the commercial potential of the methodology described.^(13,15)

In the realm of rare-earth metals, where global recycling rates still languish at fractions of a percent, the advent of EPI as a practical method for isolating lanthanum and neodymium from industrial tailings appears almost revolutionary. Whereas state-of-the-art hydrometallurgy can “squeeze” up to nine-tenths of the neodymium potential from feedstock, multielectrode EPI reinforced by ultrasonic cavitation delivers results no less impressive—often superior—without the cumbersome reagent infrastructure or its associated environmental footprint.

The synergy of the electric field and acoustic waves, implemented in a compact reactor, simultaneously resolves two distinct problem sets. First, it mitigates the “early-stage shortcomings” of conventional technologies—excessive energy consumption, solvent toxicity, and poor efficiency in dilute solutions. Second, it overcomes purely electro-chemical constraints by accelerating diffusion toward the active zone and minimizing electrode-surface passivation. The result is a selective, highly efficient, and—crucially—environmentally acceptable method for treating multicomponent, chemically “problematic” wastes.

Nevertheless, the road from laboratory bench to industrial conveyor is far from smooth and is paved with several concrete challenges:

1. Composite feedstock: Kyrgyz tailings are extraordinarily heterogeneous in both mineralogical composition and granulometry. A universal recipe does not exist; each waste type requires prior “diagnostic” characterization, and EPI units must be modular

enough to adapt to the specific feedstock profile of a given deposit.^(29,30)

2. Scale-up: the leap from a flask to an industrial reactor is traditionally complicated by hydrodynamics and heat-and-mass transfer. Without a series of pilot plants to optimize the energy balance and geometry of the multielectrode block, commercial deployment remains premature.^(15,16)

3. Process energy demand: although EPI outperforms competitors in specific energy consumption, the absolute values are still significant. Supplementing the power supply with renewable generation and finely tuning operating parameters (amplitude, frequency, pulse interval) can trim unnecessary kilowatt-hours and simultaneously reduce the carbon footprint.

4. Durability of cathode-anode pairs: corrosion and passivation are perennial companions of any electrochemical system. Without robust yet cost-effective electrode materials, laboratory success will remain confined to the laboratory.^(10,16)

Strategic circumstances, however, favor bold but promising innovations. The national policy aimed at entering the rare-earth element market and the consolidation of mining assets create a rare “window of opportunity” in Kyrgyzstan. Successful EPI integration would simultaneously shrink the industrial “legacy tail,” supply export portfolios with high-value La/Nd concentrates, and strengthen the country’s image as a regional leader in “green” metal production. Thus, the combination of technological originality and politico-economic incentives positions EPI not merely as another laboratory novelty but as a potential cornerstone of the republic’s future industrial landscape.

CONCLUSIONS

Our experiments convincingly demonstrate that integrating ultrasonic activation into a multielectrode electro-physical ionization (EPI) configuration transforms the routine treatment of industrial residues into a highly efficient, environmentally benign, and—crucially—economically viable technology. Within a single reactor volume, cavitation microflows, intensified mass transfer, and precisely tuned electrode fields act in concert; this “orchestration” of physical phenomena secures near-quantitative recovery of an extensive suite of elements—from precious metals (Au, Ag) to transition (Cu, Ni, Zn), alkaline-earth (Mg, Ca), and strategically critical rare-earth elements (La, Nd). The resulting metal-powder fraction exhibits high purity, enabling its immediate reintegration into manufacturing value chains.

Key findings

1. Efficiency and selectivity: the synergy between cavitation and a multipoint electric field removes the common bottleneck of classical electrochemical schemes—limited mass transfer. Pulsed ultrasonic fronts disrupt passivating films, continually exposing fresh reactive surfaces; kinetic barriers are thereby lowered, and selectivity toward target ions is enhanced.

2. Environmental priority: eliminating aggressive reagents and cutting specific energy consumption reduce the process’s overall ecological footprint to a minimum; virtually no secondary sludge is produced, and the aqueous medium is recyclable after final polishing.

3. Economic rationale: ostensibly passive tailings become a tangible source of raw materials: capital expenditures on the EPI installation are rapidly recouped through concentrate sales, while costs associated with primary-metal imports and environmental penalties decline in parallel.

4. Contribution to sustainable development: EPI simultaneously addresses two critical challenges—locally, the remediation of toxic legacy stockpiles in Kyrgyzstan, and globally,

a stable supply of elements essential to the “green” economy. The method therefore aligns with circular-economy principles and strengthens the country’s resource independence without compromising its environmental commitments.

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Chapter 13

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Graphene for Photodetectors and Optoelectronics

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ABSTRACT

In optoelectronics, graphene has received a great deal of attention because of the unique anisotropic properties, where it has high mobilities of charge carriers, mechanical flexibility, and strong broadband absorption. Owing to its atomically thin structure, it is highly effective in its interaction with electromagnetic radiation with even the low intrinsic absorption in the wide electromagnetic spectrum, ultraviolet to terahertz. This chapter is about the fundamental optical properties of graphene and important aspects of those properties are linear dispersive nature, tunable conductivity, ultrafast responsiveness due to incident photons among the other aspects these properties form foundation of photodetection of graphene. Multiple photodetector designs based on graphene are discussed such as photoconductive and photovoltaic devices, hybrid designs where graphene is used in combination with semiconductors like silicon, quantum dots or layered transition metal dichalcogenides. All these combinations are used to improve photo response, minimize noise and widen spectral sensitivity. Quality of graphene significantly determines the performance of such devices and growth and transfer techniques such as chemical vapor deposition, as well as epitaxial techniques play an important role in the fabrication of such devices. In addition to material preparation, the chapter also mentions the role of lithographic method in the development of photodetector array and scaled device aspect. The consideration is made towards graphene integration into the transparent and flexible substrates, and this is a milestone towards bendable and wearable optoelectronic systems. The metrics are responsivity, response speed, and detectivity that are measured in detail to compare the performance of the graphene-based design with the traditional photodetector technologies. Examples of such practical usages of the devices result within the optical communication sphere, terahertz and infrared detection, and transparent or flexible sensing systems. During further development of the research, graphene has been placed as fundamental material capable of adding to the miniaturization, multifunctionality, and flexibility of semiconductor devices of today.

Keywords: Graphene; Graphene Photodetectors; Hybrid Optoelectronic Devices; Flexible Electronics; Terahertz Detection; Transparent Photodetectors.

INTRODUCTION

Additionally, nonlinear optical graphene properties are considerable. The material is very optically nonlinear, and is important in such applications as frequency conversion, optical modulation, and photonic switching. More specifically it has also been demonstrated that

incorporation of graphene into metamaterials or other forms of nanostructured systems have a dramatic effect on the nonlinear optic properties of graphene. Such is particularly evident in devices working at the THz scale, where graphene can serve as a high-efficient media in which one can manipulate light. The study of Wang, et al. demonstrates how graphene-based resonators are used to develop an adjustable five-band THz metamaterial absorber system representing the potential of advanced photonic devices with nonlinear responses.⁽¹⁾ When other materials are used together with graphene, optical phenomena can strengthen. The integration of transition metal dichalcogenides (TMDs) with graphene could give out hybrids with stark optical properties due to the strong binding and charge transfer effects. Possible optoelectronic employments of such heterostructures take advantage of the advantageous properties of the two materials. It was shown by Zou et al. that the photoelectric responses in such heterostructures can be modulated by the stacking sequence and by interfering electric fields present in the graphene-MoS₂ heterostructures, therefore increasing their photocopy capabilities to optoelectronic devices.⁽²⁾ Optical properties of graphene are highly affected by their structural features. Varying and deviating thickness and structural defects can drastically dampen its electrical and optical ability. Longuinhos et al focus on the importance of studying the thickness sensitivity of optical activities of two limiting instances such as graphene that could lead to novel applications in photonics and sensing applications. The interaction and coupling of the phonons can lead to idea on how to improve the performance of the graphene-based devices.⁽³⁾ The other interesting aspect of optical properties of graphene is its response to strain and an external potential. It has been demonstrated that under strain, mechanical strain produces large modulations in electronic band structures of graphene, potentially leading to opening of bandgaps-which is frequently not seen in undoped graphene. This facility to alter the bandgap leads to the abilities to create tunable optoelectronic elements that can perform over a variety of spectral locations. Moreira et al. look at the manner in which strain engineering permits these changes and thus enhances the flexibility of graphene in advanced applications.⁽⁴⁾ Graphene oxide (GO) is a sort of graphene with interesting optical properties (particularly in non-linear optics). Presence of oxygen functionalities in graphene oxide changes its electronic structure thus giving it strong non-linear absorption characters. That places GO as a potential application to devices such as photodetectors and optical limiters. Unusual optical characteristics of graphene oxide make it suitable in numerous areas and suggest the entire category of 2D materials being able to exemplify the same behaviors.⁽⁵⁾ The combination of graphene with other two-dimensional (2D) materials, in particular transition metal dichalcogenides (TMDCs) including MoS₂ and WSe₂ is highlighted as producing significant improvements in many studies. Kim et al. exemplify the strength of CVD-fabricated structures to create very high performance self-powered photodetectors, which show photovoltaic activity under normal standards of light.⁽⁶⁾ In this work, it was apparent that vertically stacked heterostructures that included a transparent conducting layer of graphene would be able to provide a high degree of absorption and collection of photogenerated carriers.⁽⁷⁾ Due to the positive features of the band gap and achieved thermal stability of these materials, synthesis of patterned graphene on a substrate, including AlGaIn, has become a possible way forward in achieving optoelectronic device development.⁽⁸⁾ This amalgamation allows high effectiveness performance of photodetector purposes particularly high accuracy of optic sensing and reaction. Concerted optimization of contact interfaces and refined tuning of energy barriers through Schottky junctions have a potential to enhance the dark current suppression and maximize photo response achieved in conditions of various illumination.⁽⁹⁾ The inherent optical properties of graphene augment its effectiveness in designing of photodetectors. Graphene has an extremely broad absorption spectrum, which means about 2,3 percent of incident light is consumed over a wide variety of frequencies. The property plays an important role in the development of the operating capabilities of photodetectors, and it is possible to make a successful transformation of light

into a form of electrical signals. The form factor of devices is not limited to specific packages; to increase sensitivity to two optical bands multiple modalities have been explored such as the application of graphene to phototransistors (GABTs) with the use of adjustable barriers to achieve an all-optical response.⁽¹⁰⁾ In the emerging works, the issues of size, weight, and power consumption (SWAP-C) of flexible electronics applications have been effectively solved by building flexible photodetectors based on 2D materials combined with high-performance semiconductor nanowires.⁽¹¹⁾ The trend underlines the importance of the hybrid design which combines complimentary materials, leveraging the ability of each part of it to boost the performance of the whole device. Electronic interactions and interface engineering are an essential aspect of graphene-based photodetectors. Investigations show that modifying the electrical properties through heterojunctions leads not only to an increase in responsivity but also a significant decrease in noise, which leads to the fact that the detectors have a chance to be effective in low-light conditions.⁽¹²⁾ Graphene-GaAs hybrid structures have demonstrated positive results and interdigitated electrodes have contributed to the increased efficiency in the collection of carriers and to allow lower-noise operation conditions.⁽¹³⁾ Moreover, computer simulating and modelling advancements help to better understand the processes affecting the performance of graphene-based photodetectors, which gives developers an opportunity to build devices with optimized geometry and material combinations. Simulations using edge-edge-involved interactions with graphene may also help to optimize parameters to create superior results in photodetection.⁽¹⁴⁾

Optical Properties of Graphene

Supreme optical properties of graphene are attributed to its special electronic band structure due to its two-dimensional (2D) monolayer structure formed by carbon atoms with a honeycomb structure. In contrast to more conventional semiconductors, graphene has a zero bandgap and linear energy dispersion around the Dirac points, which gives it a new ability to: absorb light over a broad range of frequencies; and, transfer charges (carriers) rapidly.

A striking optical effect of graphene is that it can absorb a very nearly constant percentage of white light throughout the visible regime, an amount equal to 2,32 percent per atomic layer no matter how thin the material, i.e. no matter how thin the material graphene can be. It is because of the interband transitions of the 2 electrons of the pi orbitals between the conduction band and valence band.

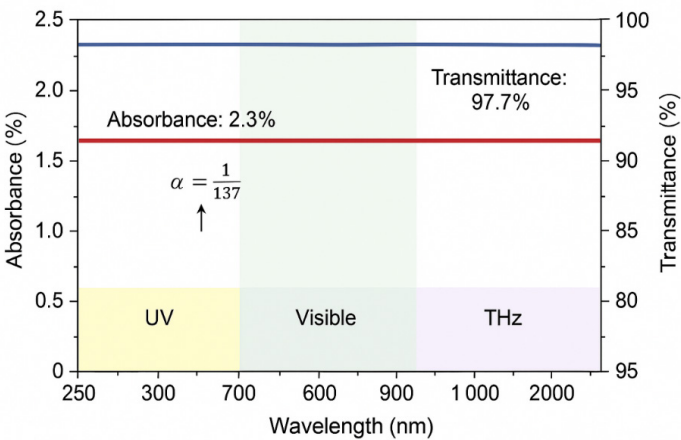


Figure 1. Optical properties of graphene

The frequency-independent absorbance, governed by the fine structure constant ($\alpha \approx 1/137$), enables graphene to act as a universal light absorber from ultraviolet (UV) to terahertz (THz) frequencies. Graphene has also exceptional transparency, with a transmittance greater than 97,7 percent in the visible range, it would be the ideal choice in transparent conductive films, touchscreens, and optoelectronic applications, where excellent optical clarity is required (figure 1).

The optical conductivity of graphene may be dynamically adjusted using external electric fields (electrostatic gating), chemical doping, or strain engineering. Shifting the Fermi level allows Pauli blocking to inhibit interband transitions, so regulating optical absorption in certain spectral ranges, especially in the near-infrared and mid-infrared areas. This tunability underpins electro-absorption modulators and varied photodetection techniques (figure 2).

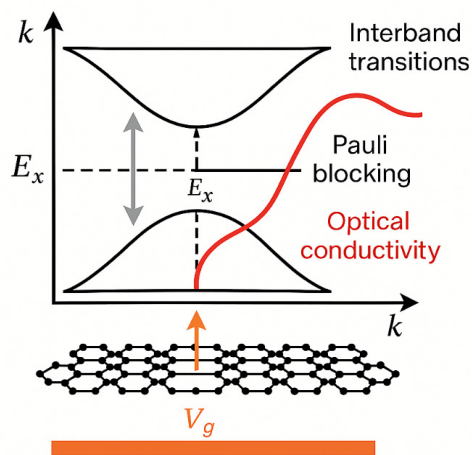


Figure 2. Tunable optical conductivity of graphene

Graphene has an ultrafast photoresponse exhibiting carrier lifetimes of the sub-picosecond order. On photoexcitation, energetic electrons are formed which quickly equilibrate through carrier-carrier and carrier phonon Zamboni scattering processes. This rapid thermalization leads to large photoprotection and to quick optoelectronic switching. Graphene also exhibits ultrafast photoresponse as carrier lifetimes of the order of sub-picoseconds.

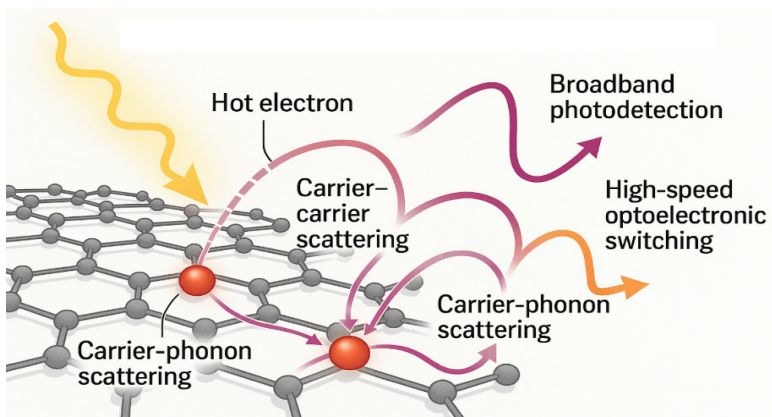


Figure 3. Graphene exhibits ultrafast photoresponse

When the system is photoexcited, highly energetic electrons generate and rapidly reach the equilibrium through scattering of the carriers and phonons. Such a rapid thermalisation incurs large photodetection sensitivities and enables rapid optoelectronic switching (figure 3).

In addition to linear absorption, graphene allows strongly confined surface plasmons in the mid-infrared and the terahertz frequencies, therefore, boosting light matter interaction at subwavelength levels. Graphene plasmons can be gated that allows to tune their frequency and intensity, thus they are suitable in plasmonic waveguides, biosensors, and tunable absorber. Also, Graphene exhibits interesting nonlinear optical properties with third-harmonic generation, four-wave mixing and saturable absorption. These are particularly important to mode-locked lasers, optical limiters and ultrafast optical switches. In further addition to linear absorption, graphene significantly supports strongly confined surface plasmons in mid-infrared and THz frequencies, thus promoting light matter interaction at subwavelength dimensions. Graphene plasmons can be gated in frequency and strength, so are suitable to plasmonic waveguides, biosensors, and tunable absorbers. Also, Graphene exhibits interesting nonlinear optical properties with third-harmonic generation, four-wave mixing and saturable absorption. Such effects are of particular importance to mode-locked lasers, optical limiters and ultrafast optical switches (figure 4).

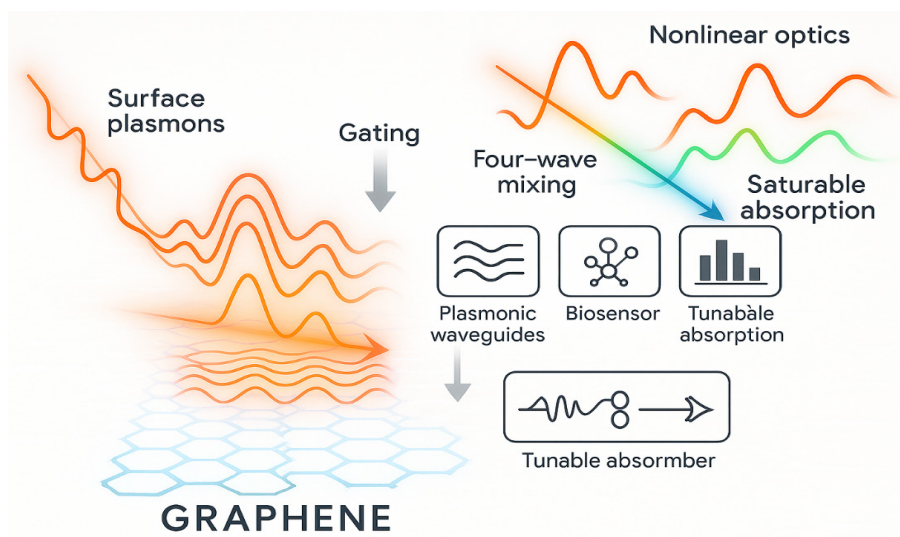


Figure 4. Graphene-Based Plasmonic and Nonlinear Optical Applications

Whereas monolayer graphene is isotropic in-plane, many layers (e.g., bilayer or few-layer) graphene exhibit optical anisotropy. The interlayer coupling also changes band structure and optical transitions leading to changed absorption spectra. Such capability can be applied to the design of polarization-sensitive or wavelength-selective devices (table 1).

Optical properties of Graphene, a monolayer of arranged carbon atoms in the form of a hexagonal lattice, have proved to be one of the most attractive materials in the optics field. Among the main features of graphene, there is the possibility of maintaining an ultrafast optical response, which is perhaps of importance in nanophotonics (e.g., photonic devices) and telecommunications. The inclusion of electric fields may drastically affect the optical properties of graphene resulting in alterations to the Fermi level and consequently absorbance and transmission behavior (figure 5). This tunability also applies to different optoelectronic

devices, in particular, in the terahertz (THz) regime in which carrier mobility of graphene is vital.⁽¹⁵⁾

Table 1. Optical Anisotropy and Layer-Dependent Optical Parameters of Graphene (at 550 nm)					
Number of Layers	Optical Conductivity (σ , S)	Absorbance (%)	Refractive Index ($n + ik$)	Dielectric Function ($\epsilon = \epsilon_1 + i\epsilon_2$)	Anisotropy Manifestation
1	$-6,08 \times 10^{-5}$	-2,3	$2,6 + 1,3i$	$-4,5 + 7,1i$	In-plane isotropic; out-of-plane non existence
2	$-1,22 \times 10^{-4}$	-4,6	$2,8 + 1,6i$	$-5,2 + 9,8i$	Low coupling of the different layers; observable birefringence
3	$-1,83 \times 10^{-4}$	-6,8	$3,0 + 1,9i$	$-5,9 + 11,4i$	Greater anisotropy; the out of plane effects start occurring
5	$-3,04 \times 10^{-4}$	-11,5	$3,4 + 2,3i$	$-6,8 + 14,5i$	Optical anisotropy features (uniaxial) Small optical anisotropy (biaxial characteristics)
>10 (multilayer)	$>5,5 \times 10^{-4}$	>20	$-4,1 + 2,8i$	$-8,5 + 19,1i$	Good optical anisotropy; has similar structure to graphite in out-plane.

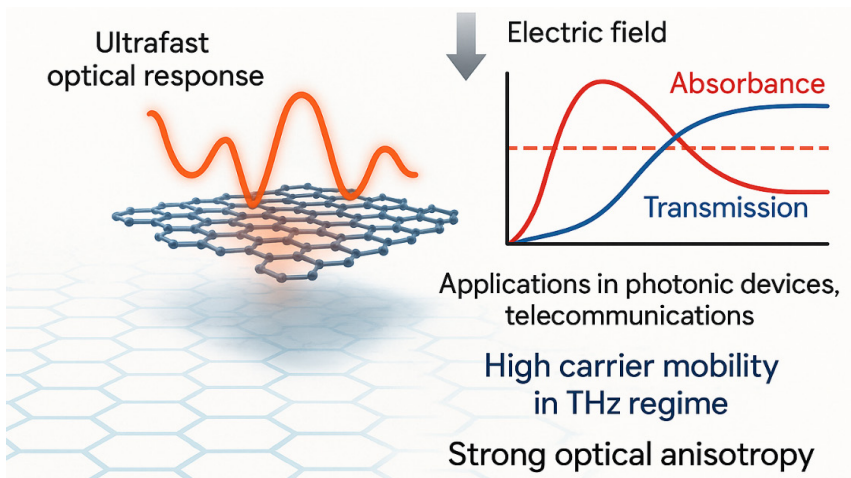


Figure 5. Graphene’s unique optical properties

Graphene systems have been studied in the aspect of nonlinear interactions with respect to the phenomena of sum-frequency generation (SFG). SFG spectroscopy is a powerful tool of the study of the surface properties of materials, e.g. graphene. This technique can be used to explain hydrogenated graphene properties and follow the changes that occur due to the outflow of hydrogen and impact the optical characteristics. The surface specific nature of SFG makes it suitable in the study of nonlinear processes in graphene-based systems with applications in more sophisticated photonic applications.⁽¹⁶⁾ Further, the application of graphene in the surface plasmon resonance (SPR) sensors demonstrates that it has excellent optical characteristics. Having a high strength in surface plasmon resonance (SPR), graphene has potential to increase sensitivity of biosensing applications when combined with other nano-scale materials, potentially increasing the possibilities of the optical sensor technology.⁽¹⁷⁾ The combination of graphene

with metallic nanoparticles shows greater nonlinear optical properties, which can be employed in various sensing applications, as shown in the researchers to evaluate the effect of graphene on the bioconjugated silver nanoparticles named lycopene, who observed that the linear and nonlinear optical responses were improved significantly.⁽¹⁸⁾ The theoretical description of the optical processes in graphene is under progress, giving previews into various applications. The interaction between electrical properties to the phonon modes could result in odd optical behaviors, as it was indicated by a number of researchers to study the coupling mechanisms between photons and phonons in heterostructures.⁽¹⁹⁾ The essential elements to consider in the research of optical properties of graphene are the combination of machine learning and artificial intelligence. Computationally, scientists have been in a position to predict optical reactions by combining graphene and other substances. It is assumed that this interaction at the interface of nanotechnology will give rise to new devices that will be able to operate efficiently in a wide variety of applications, such as telecommunications and advanced photonic computing systems.⁽²⁰⁾ To conclude, the optical properties of graphene depend upon a number of factors, these are the structure configuration, external fields and hybridisation of other materials. Such properties are present in a number of applications notably in nonlinear optics where the high carrier mobility and nonlinear responses of graphene can be exploited to create complex photonic devices. The future work in graphene and its derivatives will definitely help in enhancing development in optoelectronic applications, where the native capability of graphene can be utilized to meet the growing demand of faster and more efficient optical technology.

Device Architectures for Graphene-Based Photodetectors

The study of the device topologies of graphene-based photodetectors is a rapidly developing field of optoelectronics, whose potential is realized with the help of unique properties of graphene to obtain improvements over a wide spectrum, in the visible and infrared regimes. In both areas research has focused more on novel manufacturing processes to improve device performance and scaling such as chemical vapour deposition (CVD), and in situ growth procedures. The combination of these developments revolves around the concept of multifunctional photonic applications, where the outstanding properties of graphene can be used in better imaging systems, high speed communications and intricate sensing requirements.⁽²¹⁾ Due to the development of photodetector technology, the tendency towards smart features, incorporating the machine learning and neuromorphic computing principles, which allow real-time sensory-level data processing, becomes evident.^(22,23)

Despite these developments there still exists some issues about scalability of manufacturing and reliability of device characteristics. Large-area solar devices promise to be commercially viable only when their performance and quality can be brought to uniformity. In future, the work needs to be focused on overcoming the scaling challenges whilst at the same time exploring the new combinations of materials and the new manufacturing processes that can produce high-performance cost-efficient photodetector devices. To sum up, the optimization of device topologies in graphene-based photodetectors combines the inherent properties of graphene with the emerging breakthroughs in the field of materials science creating a significant difference in efficiency, elasticity and practical functionality. Activity in multidisciplinary collaboration, across materials science, optoelectronics and computer modelling, enhancements to the functionalities and application domains of these advanced photonic devices will be significantly advanced.

Graphene Growth and Transfer for Optoelectronic Devices

Owing to its unique electrical, optical and thermal properties, graphene, a two-dimensional

material comprising of a monolayer of carbon atoms arranged in a honeycomb lattice structure, has garnered a lot of attention in researching optoelectronics. Due to its flexibility, graphene can find application in various optoelectronic devices and it affects photodetectors, modulators among others. Chemical vapour deposition (CVD) is one of the most widespread methods of making high-quality graphene acceptable to optoelectronic devices, with which large-scale graphene layers are produced. The method enhances the electro-relation of graphene which plays a critical role in photonic applications. Using CVD researchers have managed to create graphene layers with a controllable set of properties that can be used in devices such as optical modulators, built on top of silicon substrates. Such structures take advantage of the low optical loss, and high tunability of graphene, consequently making it very attractive in photonic integrated circuits. The development of the integration of graphene in photonic is evidenced by the development of hybrid plasmonic optical modulators that enhance modulation in the devices by utilization of the unique properties of multi-layer graphene with the use of materials like titanium dioxide (TiO_2). The interaction between graphene and plasmonic structures allows the creation of devices capable of controlling the light and boosting its optical performance at particular wavelengths, which is vital to the development of the future communication systems.^(24,25) Moreover, electrical properties of the graphene can be modified simultaneously with doping techniques as well, e.g. the addition of boron that has been demonstrated to alter the electrochemical behaviour within the graphene lattice. The temperature-control enabled doping helps the electrical switching devices to develop that can switch via electrical connections or voltages and have infrared photons detection potential.⁽²⁶⁾ They have been vital in the monitoring and management of light of various wavelengths in facilitating various optoelectronic activities.

Case studies of heterostructure systems offer new references to an increase in the optical characteristics of graphene as well as to the integration of the graphene into complex electrical and optoelectronics structures. Studies show that this could be enhanced by some structural modifications such as incorporation of epsilon-near-zero cylindrical nano-shells that can enhance absorption properties of graphene-based devices. The resonant structures maximise the electric field at the graphene interface and significantly improve the absorption efficiency by various applications such as sensors and photodetectors.⁽²⁷⁾ The research of the synergetic effects with the help of a laser or photon beam combined with graphene has given promising outcomes in the high-energy regimes, which indicate the versatile importance of graphene in the context of the advanced material systems.⁽²⁸⁾ The ability of the material to respond to heat energy as well as light in its extreme conditions makes the material more applicable in different high-tech areas. Moreover, modular and printable graphene-based inks are developed making adjustable biosensing platforms feasible in, e.g. electrochemical biosensing applications. The process of photothermal sintering perfects the properties of printed graphene sheets making it adaptable in the processes of mass production and use real-time biosensing procedures.⁽²⁹⁾ It is the key aspect to note that photocarrier dynamics within the interface of dissimilar materials to graphene can be said to improve the performance parameters of heterogeneous systems. An interaction between graphene and transition-metal dichalcogenides (TMDC) increases the spectral responsiveness of photodetectors that are provided to transfer the hot carriers to the TMDC layer thus broadening the detection spectral window markedly.⁽³⁰⁾ Graphene shows its potential versatility in the development of these sensors where it can be engineered in a specific way to perform specific purposes. The search of the solution to increase optical properties and minimize losses led to the exploration of the photonic crystal geometry, which integrates graphene. These results show that controlling band gaps in photonic crystals, it can be possible to utilize the unusual transmission qualities of light within a graphene structure and, therefore,

dramatically increase device efficiency.⁽³¹⁾ Structural defects that are incorporated into graphene oxide are found to alter the way the material is able to communicate with light and this can also be used to manipulate it to suit specific applications. The paper implies that the understanding of the reasons of defects could lead to developing new more effective materials on the base of regulated reactivity and electrical properties.⁽³²⁾ Significant advancements in the processes of graphene production, in addition to new applications in conductive optoelectronics, put beyond question the significance of the substance in electrical and photonic device future. With further research, the introduction of graphene to other nanotechnological and complex materials, and optimisation of the integration processes; new functional devices will continually emerge that display better performance attributes. To sum up, the opportunities of graphene related to optoelectronics are wide, as the specific interface properties of this material, as well as its ability to be easily integrated with various platforms, offer serious advantages. It is likely to result in innovation in devices and device performance due to the combination of materials, and will also mean the positive properties of graphene are exploited in practical and high-performance applications.

Lithography and Patterning of Photodetector Arrays

Lithographic and patterning of photodetector array complex technologies play an important role in enhancing technological usage in sensing, imaging and telecommunications. The photodetectors which are identified by their ability to convert light into electrical signals are becoming more intricate in nature and a new production method is needed to optimize functionality and utility.

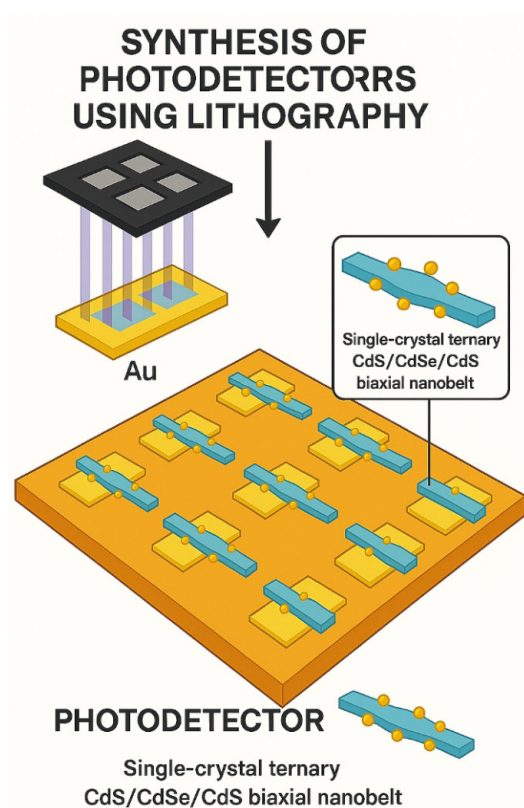


Figure 6. Synthesis of photodetectors using lithography

Nanostructures have taken their position in this environment due to their unusual optical and electrical properties that make them drastically increase the performance of devices when partnered with the accurate lithographic processes. Nanostructured materials can be fabricated as in the case of single-crystal ternary CdS/CdSe/CdS biaxial nanobelts, as shown, as an effective method of enhancing photodetectors. Das et al.⁽³³⁾ mentioned that the lithography process plays a significant role in the assembly of a nanostructure to form active photodetectors since the responsivity of the set is large over a broad spectrum because of the addition of Au nanoparticles, which improves the photo response behaviors. The new applications of the electron beam lithography supply high-resolution patterning needed to fabricate complex photodetector arrays, in which each optical element has to be carefully customized to maximize performance (figure 6).

Nanoimprint lithography, as referenced in the studies by Zhao et al.⁽³⁴⁾ and Xu et al.⁽³⁵⁾, exemplifies the adaptability and efficacy of lithographic methods in the manufacturing of photodetectors. Sequential layer stacking, vital for the fabrication of multilayer photodetectors, can utilize nanoimprint techniques to produce filters that are sensitive in the solar-blind deep ultraviolet (DUV) spectrum, which are crucial for imaging systems and environmental monitoring applications. Interfacial engineering is a crucial element affecting the efficacy of contemporary photodetectors. Bai et al.⁽³⁶⁾ demonstrated that optimizing interfaces in selenium-based photodiodes may improve detectivity and reduce noise, resulting in enhanced imaging capabilities. This engineering is essential in applications from surveillance systems to biological imaging, where accuracy and sensitivity are critical. Researchers are progressively investigating van der Waals materials because to their capacity to stack diverse compositions, therefore forming heterostructures that exhibit improved optoelectronic characteristics.⁽³⁷⁾ The stacking capability of these materials renders them very suitable for microfabrication methods like lithography, allowing customized device structures that fulfil particular application requirements.

Hu et al. highlight that the advancement of vacuum ultraviolet photodetectors using Al-doped Ga₂O₃ microbelts illustrates the convergence of sophisticated materials science and lithographic techniques.⁽³⁸⁾ These detectors have elevated photoresponsivity, making them appropriate for applications such as astronomical observation and sophisticated missile defence systems. The practical applications highlight the growing need for photodetectors capable of functioning at extreme wavelengths, indicating a crucial trend in the sector towards enhanced specificity and performance via improved manufacturing techniques. Furthermore, the investigation of two-dimensional materials, especially in photodetector applications, has advanced research into novel lithographic techniques. The tunability of materials such as Janus Al₂M₂ClBr for UV photodetection exemplifies how nano-enabled lithography facilitates fine control over electrical and optical features.⁽³⁹⁾

These methods not only improve efficiency but also allow creative applications in smart sensors and flexible electronics, reflecting the increasing synergy between materials discovery and sophisticated patterning techniques. The use of simulation tools in enhancing lithographic patterns is paramount. The advancement of lithography simulation tools, as emphasized by Kuramochi et al.⁽⁴⁰⁾, enables the optimization of source-mask combinations, essential for attaining high fidelity in the patterning of photodetector arrays. This accuracy immediately results in enhanced performance in integrated circuits and photonic devices, facilitating future progress in semiconductor technology.

The nanosphere lithography approach, as articulated by Abdulrahman⁽⁴¹⁾, offers a significant

method for fabricating ordered arrays of nanoparticles, which might be crucial for improving the optical response of photodetectors. This method’s capacity to generate homogeneous nanoscale patterns may facilitate substantial progress in the construction of photonic devices targeted at certain wavelengths. In conclusion, the domain of lithography and patterning in photodetector production is characterized by ongoing innovation and the interdependence of material science and engineering methodologies. The increasing interest in high-performance photodetectors, including flexible designs and those using 2D materials and nanostructures, signifies a crucial alignment of practical requirements with theoretical progress. The next advancement in photodetector technology will likely depend on the alignment of innovative materials with high-efficiency lithographic techniques that can satisfy the continuously changing performance and integration criteria in sophisticated technological applications.

Integration with Transparent Substrates and Flexible Electronics

The combination of transparent materials and flexible electronics is moving at lightning speed, and it is significantly impacting numerous segments, including wearable technology, smart sensors, and self-governing gadgets. This integration has largely been pegged on the development of materials that are mechanically flexible, optically transparent and electrically conductive. Further studies and advances regarding materials sciences are necessary in evolving this field, which leads to new applications and improvements in existing technology. The application of new and advanced electronic gadgets depends on robust transparent protective coatings (figure 7). Such coatings combining hardness associated with glass and flexibility associated with polymers and high optical transparency meet the needs of flexible and wearable electronics. Infrared-transparent protective coatings are critical to autonomous vehicles; protecting sensitive lidar imaging systems against environmental hazards and still maintaining important functionalities, such as light transmission, which is vital to the proper functioning of sensors.⁽⁴²⁾

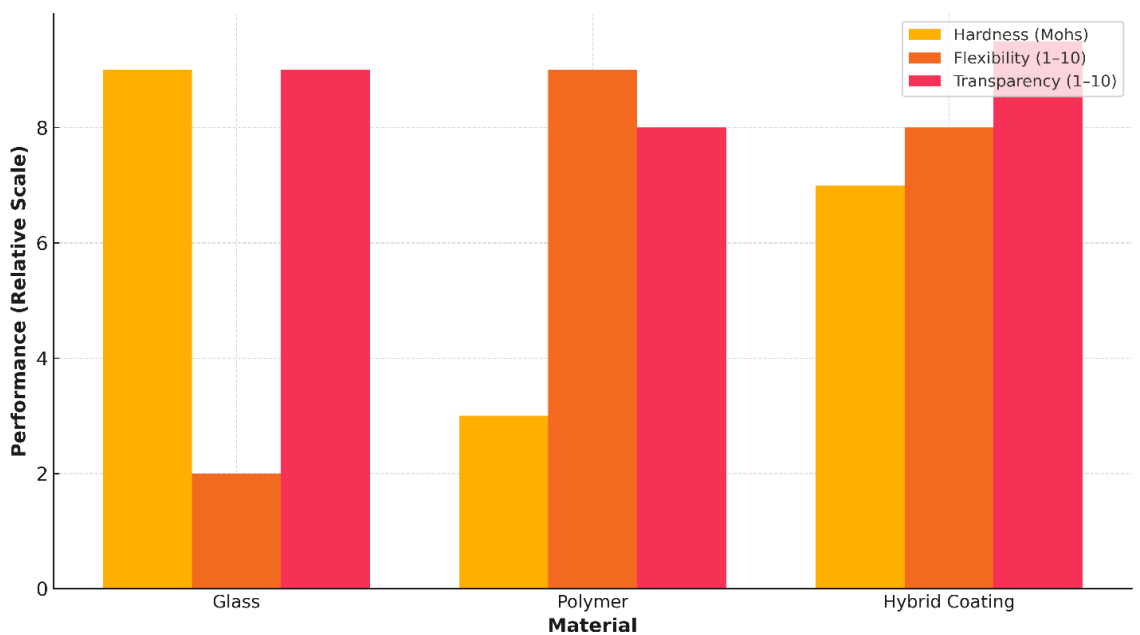


Figure 7. Material properties of transparent flexible coatings

Polymer based composites with MXene have arisen in material science with the potential to be transparent and flexible electronics. Clear electric conductance is a characteristic of MXenes, which makes them suitable in a touch display and transparent electrodes.^(43,44) They are also highly effective in reducing electromagnetic interference (EMI); a quality that makes them even more attractive in wearable and other electronic-based products whose protection against electromagnetic interference is critical.⁽⁴³⁾ In addition, the flexible electronics require advanced adhesive adhesives, which have multiple purposes. Modern adhesives have to serve not only as adhesives, but also must transfer electricity, adapt to irregular shapes and conduct signals.⁽⁴⁵⁾ Less traditional transparent conductive materials, graphene and silver nanowires increasingly have become pertinent to transparent conductive layers, as they offer better optical transparency at a lower price than conventional transparent conductive layer materials (like indium tin oxide (ITO)) under the same manufacturing conditions. Such nanostructured materials better offer mechanical flexibility than single-material based substrates as ITO and offer better performance characteristics relevant to the evolving needs of flexible electronics.^(46,47) With the growing demand to embrace transparency in most applications, combination of these materials with the existing technologies could lead to a significant extension of functions provided by devices. One of the promising areas of research is devoted to the flexible strain sensors which mimic the skin of the human. The ability of these sensors to convert an environmental input into electrical signals of the new degree of flexibility and sensory technology, especially in wearable electronics that require high levels of adaptation and functional use in a wide range of environments. This is because these gadgets will introduce new materials that are transparent and elastic resulting in changing the nature of our interaction with electronics in our daily lives.⁽⁴⁸⁾

The study of thermoplastic shape memory polymers provides a greater future in terms of flexible electronics. Through the application of materials that can be programmatically deformed, electronic devices could achieve significant environmental flexibility enhancements, which is particularly useful when designing wearables, which require interactions with human conditions to occur smoothly.⁽⁴⁹⁾ The blend of mechanical properties and programmability is the exact match of the needs of the next-generation electronics. It is envisioned that the future of flexible and transparent electronics will be dramatically transformed including the integration of complex nanomaterials into flexible and transparent devices. The electrothermal films via a systematic application can produce energy efficient devices that are sensitive, safe, and are highly transparent and flexible.⁽⁵⁰⁾ Use of nanostructure specific properties can allow strategies to push beyond current limits of electronic materials, advancing to energy-efficient design and performance benchmarks everywhere. To sum up, the intersection of transparent materials and flexible electronics provides an opportunity of an innovative pursued in various directions. Research is also likely to involve the multifunctional materials, combinatorial technologies, and new techniques of production, as the demands of consumers and industry grow higher.

Performance Metrics of Graphene Photodetectors

Graphene photodetectors form a developing area of research on the basis of its superb attributes including high carrier mobility, flexibility, and the potential of ultrafast response.^(51,52) Consequently, the studies within the given field have tended to focus more on the optimization of the architecture and material interaction of graphene photodetectors to maintain higher metrics of performance. The responsivity (R), which is a vital statistic in the evaluation process of the performance of the photodetectors, determines the photocurrent output caused by a change in the input optical power unit.⁽⁵³⁾ The high responsivity is necessary to achieve high-precise detection in varying light wavelength. New research reports have recorded new heterostructures where graphene is combined with materials, including AgBiP₂Se₆ or Molybdenum Disulphide (MoS₂) to produce significant increases in responsivity compared to stand-alone graphene devices. Less

than $10\text{A}/\text{cm}^2$ dark currents have been observed in graphene/ MoS_2 heterojunctions to enhance the operations of this device to lower light environments (figure 8).^(54,55)

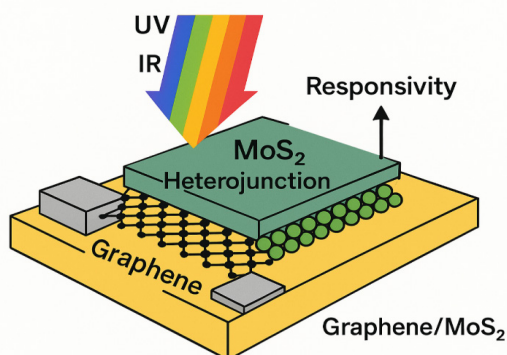


Figure 8. Graphene/ MoS_2 Heterojunction Photodetector Architecture Showing Enhanced Responsivity

Figure 8 represents a hypothetical model of photodetector built on the base of heterojunction consisting of graphene and molybdenum disulphide (MoS_2). Because of the different electronic and optical characteristics of the two materials, superior electrical conductivity on graphene and semiconducting bandgap on MoS_2 , the structure combines them to form a highly sensitive platform of detecting light. The wide spectral wave of incident light, which spans in the ultraviolet (UV) to infrared (IR) spectrums is absorbed at the junction of the two materials. This region enhances efficient generation and sorting of photoinduced carriers due to intrinsic electric field that is created by heterojunction. Graphene is a transparent conductive electrode which can swiftly transfer electrons whilst MoS_2 helps in selective absorption of photons and charge separation. This heterostructure with low-dark current and high signal-to-noise ratio is appropriate to work in low light conditions. Such topologies are gaining relevance to the advanced state of optoelectronic systems e.g., broadband photodetectors, wearable optical sensors, and energy-efficient imaging devices.

The integration of hybrid architectures or stacked with other semiconductors can commonly expand the range of light wavelengths which can be efficiently detected, therefore, increasing the flexibility of devices based on graphene.⁽⁵⁶⁾ Many applications require that the equipment resist varying operating conditions in the environment, so studies are underway to realize more robust material constructions that maintain performance requirements at the max. Combining flexible materials with graphene without compromising electrical performance has demonstrated a positive effect when dealing with a long-term operational stability.⁽⁵⁷⁾ The indexes of the performance of graphene photodetectors precondition basically on the enhancement of responsivity, detectivity, reduction of dark currents, the enhancement of operating speed, and long-term stability. Hybrid structures based on the innovations of a specific hybrid architecture, as well as combinations of materials that need to be customised, are needed to resolve the current boundaries. These advances are not only associated with its better functioning but also widening the application of the graphene photodetectors to make them irreplaceable constituents in the optoelectronic systems in the future.

Applications in Optoelectronics

Optical Communication Systems

An optical communication system is a mandatory part of the modern data transfer technology.

The systems are advantageous in different ways such as the high-speed characteristics, long transmission distances and the capacity to withstand electromagnetic impedance making it deployable in diverse activities in guidance and communication systems, healthcare and military services. A detailed study of these systems reveals that these are multifaceted with optical transmitters, fibre media and receivers and more sophisticated signal processing processes. The basic structure of optical communication system has an optical transmitter, optical cables and an optical receiver with digital processing accessories. Optical transmitter converts electrical signals into optical signals with the use of diodes or lasers and sends it through optical fibres that carry light over various distances. Recent research papers note that fibre optic technologies, in particular photonic crystal fibres (PCFs) and various optical texts, are vital in what enhances data volume and versatility within networks.⁽⁵⁸⁾ Data throughput in fibre optic networks has significantly improved with such advanced multiplexing techniques as wavelength division multiplexing (WDM) and space-division multiplexing (SDM). Wavelength Division Multiplexing (WDM) means that multiple wavelengths can be sent over one fibre simultaneously, which increases the number of data-carrying trails thus employing transmission gratings that are specially created.⁽⁵⁹⁾ Layering of several strategies allows optical systems to meet the growing demand of bandwidth, which is especially relevant because of the rapid growth of data consumption worldwide. New technologies in the development of optical networks include dynamic reconfigurability due to the introduction of the flexible optical network, which is printable.⁽⁶⁰⁾ Fibre optics has specific advantages when used in sensing application due to its advantage of being able to operate in harsh environments and also the ability to transfer data reliably. Fibre optic sensing technologies have been effective in a number of industries with fibre optic medical applications involving motion artefacts that can interfere with hemodynamic data. To solve these problems, innovative solutions should be adopted that might reduce the influence of motion to ensure accurate measurements (figure 9).⁽⁶¹⁾

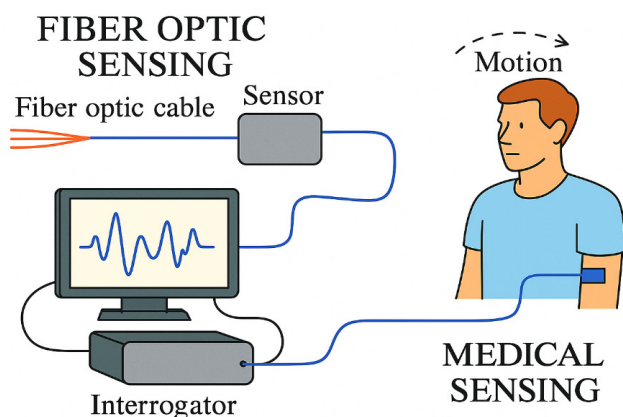


Figure 9. Fiber Optic Sensing System for Medical Motion Monitoring

The inclusion of new and refined materials, enhanced signal processing, and optimized transmission techniques are likely to produce future optical communication systems that will be able to meet the growing need to support high data-rates and long transmission distances whilst, at the same time, reduce energy consumption (and associated costs). Also continuing research and innovation will make sure that optical communications will continue to play a major part in shaping the future of the global connectivity. To sum up, the present-day development of optical communication systems is crucial to the addressing the needs of the modern communication environments. By applying enhanced signal handling technologies and novel materials, engineers and researchers will enhance the effectiveness of existing systems

and explore of new worlds within data transmission innovations.

Terahertz and Infrared Detection

Advances in terahertz (THz) and infrared (IR) detection have been developing over time, making breakthroughs in various other applications such as in biological imaging and detection by the military. The effectiveness of such detecting techniques is closely connected with the creation of the corresponding materials and equipment that would behave successfully in the volume of their allocated spectrum. In the comparison of THz and IR detection, it is important to compare the effectiveness of various types of detectors, as well as their working systems. The performance of the of all their THz imaging systems is largely determined by the characteristics of the detectors in the THz based. Another wide range of detectors continuing on the basis of microwave and infrared, comprises Schottky diodes, Golay cells, and pyroelectric detectors. Recently advances have seen the integration of graphene into microbolometer arrays that yielded a significant improvement of detection speed and sensitivity, and this is especially so in biomedical applications, wherein rapid imaging is vital (figure 10).⁽⁶²⁾

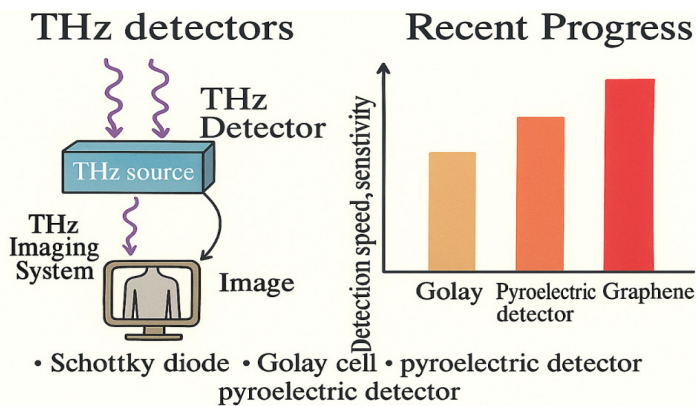


Figure 10. Comparison of THz Detectors and Recent Advances in Detection Sensitivity and Speed

Development in infrared detection can be viewed in the work on InAs/GaSb superlattice structure. These materials have adjustable wavelength sensitivity which adds to their effectiveness in infrared region. New attempts have been aimed at the improvement of the manufacturing techniques and such features of superlattice detectors, which are crucial to the higher efficiency and the sensitivity of infrared detecting technologies in medical practice (table 2).⁽⁶³⁾

A modern practice in enhancing the detection abilities is the migration of infrared sensing technologies with an artificial intelligence and computer systems. Complex object identification algorithms with the help of an infrared camera can assist blind individuals to navigate. Such systems will have infrared sensors, which measure radiations produced by objects and convert them into visual images to improve navigation.⁽⁶⁴⁾ Availability of infrared detection technologies has been increasing as portrayed by the declining prices of infrared detectors, which are penetrating every day technologies. This democratization allows the usage of applications in the area of national defence, scientific research, and even commercial products, e.g. infrared face recognition devices.⁽⁶⁵⁾ The infrared applications the theoretical framework of the optomechanical detection systems is varied about giving alternative approaches to the enhancement of sensitivity.

Table 2. Key Features and Advancements of InAs/GaSb Superlattice-Based IR Detectors for Medical Applications		
Feature	Description	Relevance to Medical IR Applications
Material System	InAs/GaSb type-II superlattice	Permits designed bandgap in mid to long wavelength IR sensitive detection
Tunable Wavelength Range	3-12 μm (adjustable via layer thickness)	Can be customised to suit custom biomedical imaging windows e.g. 3-5 O_m , 8-12 O_m
Detection Mechanism	Interband transition across broken-gap heterostructure	Sensitiveness to low photon energies; can be applied to non-invasive imaging
Fabrication Techniques	Molecular beam epitaxy (MBE) with precise control	Lets high quality interface and lowered dark current
Noise Reduction	Engineered interfaces reduce defect-related recombination	Medi-speed increases signal-noise ratio of medical diagnosis
Operating Temperature	Can function with thermo-electric cooling ($\sim 77\text{-}150\text{ K}$)	Decreases the requirements of cryogenic systems in hand-carried health care devices
Response Time	Sub-microsecond response possible	Appropriate to medicine real-time thermal imaging and IR spectroscopy
Recent Optimization Focus	Strain balancing, interface passivation, absorber thickness tuning	Enhances the quantum efficiency and the long-term stable operation capability
Application Examples	Thermal mapping of tissues, blood perfusion monitoring, IR endoscopy	Uses contactless, correct diagnostics in area of clinical practice

The aim of this research is to design more advanced integrated systems that have multiple functions thus reducing trade-offs that are associated with thermal detectors. The military uses infrared imaging technologies during surveillance as well as reconnaissance. Thermal detectors, such as bolometers and thermopiles, convey a concrete foundation to the infrared imaging, encompassing comprehensible range of responses to the spectra and reducing the issues of noise-equivalent power (NEP) and response time.⁽⁶⁶⁾ Modern infrared detecting systems employ new materials and combinations that leads to significant increases in performance. They include III-V semiconductor elements that are maximized to achieve perform highest efficiencies on numerous infrared subbands, a quality that belies their importance in applications that require high standards of monitoring and environmental evaluation.⁽⁶⁷⁾ Applying these developments, scientists could increase their understanding of the relationship between the thermoelectric performance and efficiency of detection. This combination of steps determines a challenging yet feasible future of the THz and IR sensing technology. The focus of new development is now the minimisation of noise, the enhancement of signal quality, and the integration of machine learning algorithms which are the stepping stone to an improvement in the performance of infrared and terahertz systems. Multi-Facet efforts in all three areas of materials science and engineering, and computational technologies should deliver considerable advancements in sensitivities of detection, reduction of operating expenses and expansions in applications. The specialized direction of infrared detector and THz technologies is complicated because understanding advances within the field, there must be a consideration into a delicate balance

between sensor design, operating efficiency and specialization. Tomorrow of these technologies is naturally based on multidisciplinary alliances that can be creative and innovative in terms of developing new-generation solutions of detection across a wide range of industries.

Transparent and Flexible Photodetectors

The studies on transparent as well as flexible photodetectors have gained more interest due to the wide range of applications in the sectors such as wearable electronics, biomedical equipment, and optoelectronic systems. The growing demand of the integration process in geometrical flexible electronic systems is the reason why even more transparent materials of high flexibility and efficient light absorptive capabilities are required. Various materials are under exploration to enhance the performance of these photodetectors like organic materials, two-dimensional (2D) materials, metallic nanowires, and newer semiconductor compounds. In flexible photodetector that are being designed, transparent conductive materials (TCMs) are vital. These are imperative because they have to support light transmission and at the same time be transparent enough to carry electricity being a good insulator to electricity. Such materials as indium tin oxide (ITO) and conductive silver nanowire (Ag-NW) networks have been very effective in this category. Ag-NW networks with feel-fabrication, high conductivity-to-transparency ratios and stretch ability make them an outstanding choice of transparent electrodes in photodetectors with operations in UV-Vis range (figure 11).^(68,69) Moreover, new 2D materials changed the landscape of materials research to photodetectors. Other materials such as graphene and transition metal dichalcogenides (TMDs) have been known to possess exceptional optoelectronic properties these materials show high electrical mobility, excellent mechanical flexibilities, and excellent bend resistance properties. It has been shown these materials have the ability to absorb high amounts of light with a wide range in addition to maintaining flexibility, which means that they are perfect candidates to use in advanced photodetectors. Finding a combination of these materials can lead to transparent devices with high responsivity and fast response time that are necessary characteristics of mobile and wearable devices.^(70,71)

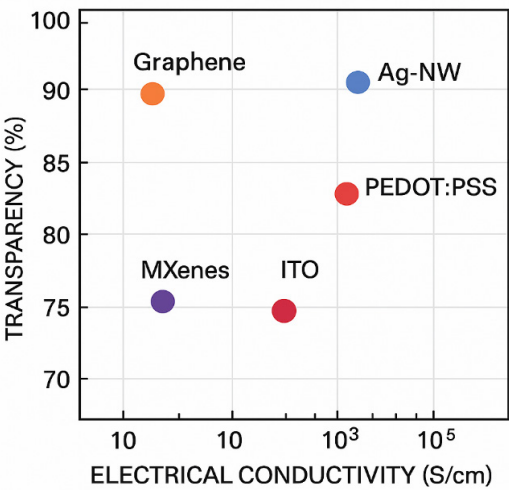


Figure 11. Comparison of Transparency and Electrical Conductivity: Graphene, MXenes, ITO, PEDOT:PSS, and Ag-NW

The interesting aspects of OPDs can also be discussed as their low fabrication costs and large-area application based on their solution-based manufacturing. The optical devices can be

designed in terms of being semi-transparent to enable them to be seamlessly integrated with other components of optoelectronics. The mechanical properties of their flexibility allow them to adapt to various surfaces, which perfectly fits the inherent attributes of smart materials that are needed in modern-day flexible technologies.⁽⁷²⁾ The mechanical and optoelectrical tunability of organic materials in themselves contributes to the creation of custom photodetector systems that serve a wide range of uses.⁽⁷³⁾ Key performance parameters of photo detectors, i.e., responsivity and response time are crucial attributes. A balance between sensitivity and speed must be attained by the photodetectors so as to be successfully implemented in an actual application. The increase of fast response time and increased responsivity due to compositions of unique materials is marked achievement.^(74,75) It has been discovered that 2D materials possess good mobility characteristics, which lead to an increase in reaction speed, which allows more rapid switching and an operating frequency suitable to advanced photonics.⁽⁷⁶⁾ Halide perovskites are typically known to possess an excellent light responsivity property thus offering a strong unemployment of next-generation photodetectors that may operate in various operational and environmental conditions. An area of impressive progress is the integration of polymer matrices with photonic devices, to produce transparent, bending, and highly versatile devices with potentially complex functionality including sensing and actuation. The hybrid nanocomposites developed in synthesizing polymers and nanoparticles could offer the photodetectors with excellent properties, such as the enhanced mechanical performance, which is important in wearable electronics that require flexibility and strength.⁽⁷⁷⁾

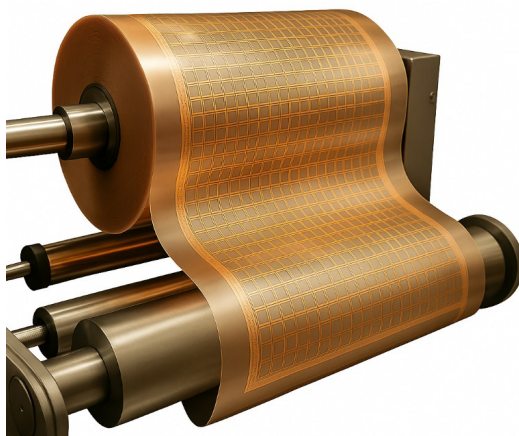


Figure 12. Roll-to-Roll Fabrication of Transparent Flexible Photodetectors

Scalable considerations of the improvements have been discussed in relation to the continuous research of the manufacturing process in enabling developing the flexible and transparent photodetectors in the large scale. Roll-to-roll printing represents a scalable method of printing flexible electronics and makes commercial development affordable, where the cost is known to be the major stumbling block of integrating innovative materials into the commercial world (figure 12). Such innovations have the potential to revolutionize universal access to the high-performance photodetector technology. The development of scalability of such improvements consists of a continuing research of manufacturing processes that would support a mass production of flexible and transparent photodetectors. The mass production of flexible electronics can be achieved with scalable processes such as roll-to-roll printing, which offers a way of circumventing cost barrier that has served as the incumbrance of incorporating new materials in existing electronic products (figure 12). Such advancements hold the potential to revolutionize access to high-performance photodetector technologies globally.⁽⁷⁸⁾

Their high anisotropic characteristics and the capability of integrating with existing technologies signify a promising horizon for flexible photodetectors that maximize performance while maintaining essential attributes like transparency and flexibility. In conclusion, the trajectory of transparent and flexible photodetectors represents a multifaceted field that converges various disciplines, including materials science, nanotechnology, and optoelectronics. Continuous innovations regarding material combinations and fabrication techniques are essential to overcome existing limitations, realize the potential of these materials, and innovate advanced photodetector systems. Ongoing research will pave the way toward highly efficient, transparent, and flexible optoelectronic devices that could profoundly impact various sectors, including consumer electronics, healthcare, and environmental monitoring.^(79,80)

CONCLUSIONS

The carried-out study is a clear evidence that due to its outstanding optical and electronic characteristics; graphene can be utilized in the development of one of the most promising materials in respect to advanced optoelectronic application. Its large optical transparency (~97,7 %) and broadband light absorption, high mobility of carriers, and low power liability make it a superior choice as a photodetector of the future. The photodetectors based on graphene were also successfully integrated in a variety of device platforms, e.g., photoconductive, photovoltaic, bolometric, and plasmonic devices on rigid (e.g., Si, SiO₂) and flexible transparent substrates (e.g., PET, PEN). Besides being able to use these devices in traditional fiber-optic systems of communication, more forward applications that can be implemented using these devices include, wearable electronics, transparent displays, as well as THz/IR sensing platforms. The method of productions where graphene can be grown by chemical vapor deposition (CVD), epitaxial preparations and also exfoliation has led to a launch of scaled-up device manufacturing on its way, after careful lithography and patterning. Moreover, the transfer methodologies that are used and suited to flexible substrates have further been advanced to enable the incorporation to transparent and bendable systems. Graphene photodetectors are considered to have high performance in terms of fast response time (in the picosecond scale), wide spectrum coverage (ranging across UV to THz frequency), and stability during repeated operation cycle. These qualities give good ground in high-performance, low-priced, miniaturized optoelectronic solutions. To sum up, the application of graphene as a photodetector has great potential in technologies, especially photodetectors with flexible design and transparent. Further synthetic, device and integration development will promote their use for a wide range of research and end-user products.

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Part IV

Extraction Physics and Electrophysical Technologies



Chapter 14

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Graphene for Supercapacitors and Energy Storage

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ABSTRACT

The growing global need in viable and effective energy storage means created higher interest in the use of supercapacitors since they exhibit their high ability in power density production, fast charge/discharge rates, and extended cycle lives. This chapter discusses some of the basic principles of operation of supercapacitors especially the difference between electric double-layer capacitors (EDLCs) and pseudocapacitors. The main parameters of the performance are given as important parameters of assessing devices efficiency: specific capacitance, energy density, power density, and cycling stability. The extraordinary electrical conductivity material, large surface area with mechanical strength and chemical stability has triggered the use of graphene in the invention of the next generation of supercapacitor electrodes. The chapter takes a closer look at the electrochemical applications of graphene and expounds on the range of manufacturing pathways, mentioning chemical vapor deposition (CVD), the enhanced Hummers process and liquid phase exfoliation to mention just a few. The focus is given to the creation of graphene whereas it is combined with carbon nanotubes (CNTs), metal oxides (MnO_2 , RuO_2), and conducting polymers (e.g., polyaniline, PEDOT) to improve charge storage phenomena. Various arrangements of supercapacitor devices are also discussed and the comparison of symmetric and asymmetric structures, solid-state and bendable ones are discussed. Such formats play a pivotal role in aligning the supercapacitors to any domains of application. Lastly, the chapter points out practical implementation of graphene supercapacitors, not only in portable and wearable electronics as well as grid-scale systems that will store energy. A promising direction is a hybrid supercapacitor battery system and high-performance energy systems in automotive and aerospace. Supercapacitors have the potential to become the fabric of energy technology in the future, especially in context of the desired properties as enabled by the fundamental characteristics of graphene, and by taming other functional device structures.

Keywords: Graphene-Based Nanomaterials; Graphene Supercapacitors; Electric Double-Layer Capacitor; Energy Density; Composite Electrodes; Flexible Energy Storage; Hybrid Energy Systems; Wearable Electronics; Aviation Electronics.

INTRODUCTION

The EDLCs mainly work through the electrostatic formation of an electric double layer at the interface between an electrode and an electrolyte. The principle of this method is the charge and discharge of ions on the surfaces of high-nucleation powders mostly, of carbon-based electrodes, which give large energy storage potential. The surface area, pore structure and the electrode material distribution will play the most critical role in determining the efficiency of EDLCs in energy transfer, which is highly influential to the capacitance and performance of the EDLCs.^(1,2) The energy that is stored by pseudocapacitors is due to a process known as faradaic reactions which are electrochemical oxidation and reduction reaction on the surface of an electrode. Pseudo-capacitors can eventually exceed energy energy one of EDLCs due to

coincident redox responses that aid charge move and storage.^(3,4,5) The advantage of pseudo-capacitors is their high level of specific capacitance and energy density but with concerns such as low conductivity and poor long-term cycle stability when compared to EDLCs.^(6,7) The flexibility in the type of materials to use in building electrodes (pseudo-capacitors) like conductive polymer and transition metal oxide means that it is possible to develop structures that facilitate specific use.^(8,9) The aspects of the material science concerning the electrodes have the significant effect on the capacitance and performance of these supercapacitors. The latest developments call attention to the idea of new materials, such as biomass-derived activated carbon, metal-organic frameworks, and carbon-based nanocomposites, explicitly constructed to improve the electrochemical properties of both EDLCs and PC systems. The innovations increase the conductivity and efficiency of operation in real-life conditions.⁽¹⁰⁾ The main distinctions of EDLCs and pseudo-capacitors define whether they can appropriately be utilized in specific applications. EDLCs find most application areas needing high speed energy discharge, including power backup systems, and electric vehicles, due to their reliable energy discharge capacities and cycle stability. Oppositely, the pseudo-capacitors potential to deliver high energy density makes them ideal in systems requiring constant energy supply like electronic gadgets and renewable energy cycles.^(11,12,13)

The methods that the Hummers 1 and 2 came up with have been revised to a more efficient and environmentally less intensive method to produce graphene oxide. The difference in the process of modified Hummers involves the alterations in the reagent concentration or usage of other types of oxidizing agents, which leads to safer waste disposal and higher yield.^(14,15) Nomenclature Chemical vapour deposition (CVD) is considered a major technique in the preparation of graphene especially in the formation of high-quality film. CVD entails heating or heating of gaseous chemically precursors, frequently hydrocarbons, onto a substrate where they break apart at high temperatures. With the help of the process, it is possible to obtain continuous graphene sheets, which makes it suitable in electronic devices that require homogeneity and scalability.⁽¹⁶⁾

Fundamentals of Supercapacitors

Electric Double-Layer Capacitors (EDLCs) vs Pseudo capacitors

Supercapacitors are of two distinct types including electric double-layer capacitors (EDLCs) and pseudo-capacitors (PCs). The two types of capacitors also incorporate different ways of storing charge thereby giving them the different performance properties and thus fit them to be used in different applications. Understanding the differences between the two is vital towards advancement of energy storage systems, particularly efficiency, longevity and environmental impacts. The two types of super capacitors exhibit the rapid capabilities of charging and discharging which is essential in situations involving the need to provide electric power immediately (table 1). The inherent architecture of EDLCs enables a swift response to input signals, whereas pseudo-capacitors can be used to reach a similar performance as well because of its electrochemical properties.⁽⁶⁾

Graphene oxide and gadolinium-doped CNTs exhibit high conductivity and electrochemical stability, making them essential functional materials in supercapacitors.^(17,18) Their synthesis and structural analysis form the foundation for optimizing energy storage performance.⁽¹⁹⁾ Particularly, the electrical behavior of GO/S structures and the photoconductivity of CNTs offer enhanced energy density for next-generation devices.^(20,21)

Table 1. Comparative Overview of EDLCs, Pseudocapacitors, and Hybrid Supercapacitors

Parameter	EDLCs (Electric Double-Layer Capacitors)	Pseudocapacitors (PCs)	Hybrid Supercapacitors	References
Charge Storage Mechanism	Electrostatic adsorption at electrode-electrolyte interface	Faradaic reactions	Combination of EDLC and PC mechanisms	Madhushani et al. ⁽⁵⁾ , Essa et al. ⁽⁶⁾
Capacitance Origin	Non-Faradaic double-layer effect	Faradaic transfer	Mixed behavior	Bandara et al. ⁽⁴⁾
Energy Density	Low (5-10 Wh/kg)	Medium (10-40 Wh/kg)	High (up to 50-80 Wh/kg)	Khokhar et al. ⁽²²⁾
Power Density	Very high (>10 kW/kg)	Medium-high	High (balances energy & power)	Bandara et al. ⁽⁴⁾
Cycle Life	Excellent (>100 000 cycles)	Lower due to structural degradation	Improved cycle stability with material engineering	Essa et al. ⁽⁶⁾
Response Time	Instantaneous (<1 s)	Slower due to redox processes	Fast, slightly slower than EDLCs	Madhushani et al. ⁽⁵⁾
Typical Materials	Activated carbon, graphene	Metal oxides, conductive polymers	Carbon-metal oxide composites	Meghanathan et al. ⁽²³⁾
Applications	Power buffering, regenerative braking	Memory devices, biosensors	EVs, grid storage, hybrid devices	Bandara et al. ⁽⁴⁾ , Dhapola et al. ⁽²⁴⁾
Environmental Impact	Low; uses carbon-based materials	Moderate; uses metal oxides (some toxic)	Varies depending on composition	Meghanathan et al. ⁽²³⁾ , Dhapola et al. ⁽²⁴⁾
Sustainability Focus	Bio-derived carbons, green synthesis	Eco-friendly materials	Focus on balancing performance with green design	Dhapola et al. ⁽²⁴⁾

Combination of two technologies, a hybrid of EDLC and pseudo-capacitive chemistry has emerged as promising way to maximize energy and power densities and to overcome the unique limitations of the two capacitor types. The hybrid supercapacitors also have a higher-power density that the electric double-layer capacitors (EDLCs) possess along with a higher energy density enjoyed by the pseudo-capacitors, which increases their performance indicators.⁽²²⁾ Also, both types of environmental impact are significant, as enhancing the sustainability of a supercapacitor-based technology aligns with the global efforts to reduce the effects of energy consumption and selection of environmentally friendly materials. As research is emphasized, the exploration of alternative and sustainable materials that have the least impact on the environment about performance are also noted.^(23,24)

Development and improvement of electric double-layer capacitor and pseudo-capacitor have increasingly become an essential combination of technological, materials science and green concerns. Their unique charge storage characteristics influence their functioning specifics and inform the decisions regarding the application settings to many aspects, which is why the advancement in the field deserves the attention.

Performance Parameters: Capacitance, Energy Density, Power Density, Cycle Life

Supercapacitors which are recognized as investigated energy storage show excellent

performance parameters essential in a wide variety of fields such as electronics and electric cars. Among the key performance metrics are capacitance, energy density, power density and cycle life all of which are central to overall effectiveness of supercapacitors. It is vital to understand the presented factors and how they interrelate so as to maximize upon the supercapacitor technologies thus making possible their expansive application. Capacitance refers to ability of a supercapacitor to hold an electric charge. These are mainly the surface area of the electrode material, the nature of the electrolyte and the structure of the electrode. The capacitance of the supercapacitors is a multiple of that of the ordinary capacitors and that makes them efficient energy storage media with a fast charging and discharging capability (table 2).

Table 2. Performance Parameters of Supercapacitors					
Parameter	Description	Typical Range	Influencing Factors	Comparison (EDLC vs. PC vs. Hybrid)	
Capacitance (C)	Ability to store electrical charge per unit voltage (F/g)	100-1000 F/g	Electrode surface area, electrolyte accessibility, porosity	EDLCs: High due to double-layer effect PCs: Moderate, enhanced by redox activity Hybrids: Optimized	
Energy Density (E)	Energy stored per unit mass (Wh/kg)	5-80 Wh/kg	Capacitance, voltage window ($E = \frac{1}{2}CV^2$)	EDLCs: 5-10 Wh/kg PCs: 10-40 Wh/kg Hybrids: 30-80 Wh/kg	
Power Density (P)	Speed of energy delivery per unit mass (kW/kg)	1-20 kW/kg	Equivalent series resistance (ESR), charge transfer rate	EDLCs: Very high (>10 kW/kg) PCs: Medium Hybrids: High	
Cycle Life	Number of stable charge/discharge cycles before degradation	10 000-100 000+ cycles	Electrochemical stability, electrode material resilience	EDLCs: >100 000 PCs: 1000-10 000 Hybrids: 10 000-50 000 (with optimization)	

Liu et al.⁽²⁵⁾ assert that the supercapacitors exhibit high capacitance values because their porous structures increase surface area and ways of storing charges, therefore, enabling them to have high electrical performance in comparison to capacitors and batteries. The electrode composition such as Carbon nanofibers and hybrid composites are important in improving capacitance. Gu et al.⁽²⁶⁾ discuss carbon nanofiber usage as a strong base to various electroactive products and show that new combinations of materials can make an overall capacitance increase. The cooperation of different materials increases charge storing processes, which are critical in achieving higher energy density and power density with maintaining cycle life. The amount of energy that a substance contains per unit mass, also known as energy density, is an important parameter that separates supercapacitors with batteries. Despite their high-power densities, supercapacitors have traditionally a lower energy density than batteries, which makes them inapplicable in energy-intensive processes. Wang et al.⁽²⁷⁾ noted that balancing the optimization of energy density and power density is one of the issues of supercapacitor development because there is a desire to obtain good results in both parameters. On the other hand, new candidates such as nitrogen-doped carbons have recorded promising performance with energy density of 20,7 Wh/kg and preserving power capacities.

Similarly, power density which is the rate of energy delivery over time is also a characteristic

feature of super capacitors. Supercapacitors are usually capable of rapid release of energy compared to batteries and lend themselves to applications that require rapid power surges, and are thus used in regenerative braking systems of electric automobiles. Anand et al.⁽²⁸⁾ draw upon the fact that supercapacitors have achieved exceptional power density, which renders the device the ability to deliver a large instantaneous power drawing. GO and CNT-based materials demonstrate high specific capacitance (F/g), power density, and cycling stability.⁽²⁹⁾ Thermal analyses reveal that gadolinium-doped CNTs maintain structural stability up to 550 °C.⁽²¹⁾ The EPR analysis of GO composites confirms the role of active surface centers in improving performance.⁽²⁹⁾

Increased knowledge about cycle life proves that researchers have to conduct research on the electrolytes and materials that influence durability significantly. As an instance, supercapacitors with electrolytes that have optimized ionic conductivity or novel electrode materials that are pseudocapacitive might strongly enhance the cycle life of supercapacitors. Studies show that supercapacitors have the potential of 10 000 lifecycles with very good coulombic efficiency which implies that they are very stable/durable in the field.⁽³⁰⁾

However, trade-offs between these factors are very important to consider. Zhao et al.⁽³¹⁾ elaborate that with augmented energy density, a power performance trade-off is frequently met, where scholars suggest that the combination of both batteries and supercapacitor features is hybrid meant to mitigate these drawbacks. At that, the active combination of elements that offer the enhanced energy and power density enabling the retained extraordinary cycle life is the benchmark of the contemporary limitation of the supercapacitor study (figure 1).

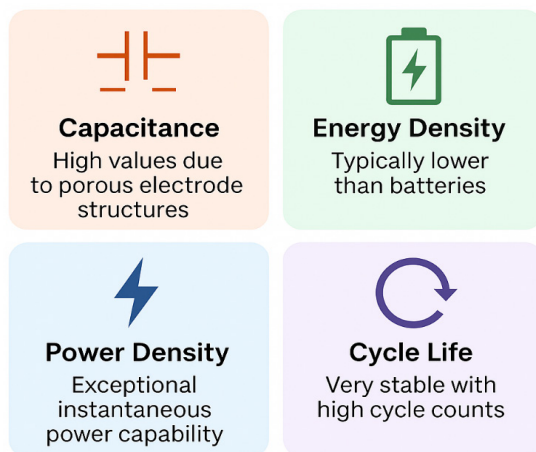


Figure 1. Performance metric of supercapacitors

The analysis of the supercapacitor performance shown the multifactor connection existing between the capacitance, energy density, power density, and cycle life. The evolutionary activities in the field of materials sciences along with the groundbreaking design of electrode and electrolyte will further advance the performance of supercapacitor to the utmost. The search of a perfect balance of these performance aspects is an important mission that is going to define the future of energy storage technology.

Graphene Properties Relevant to Energy Storage

A one-layer carbon atom structure arranged in a pattern called hexagonal lattice called

graphene has been an important substance in energy storage, notably in super capacitor and battery appliances. The great properties, in particular, high electrical conductivity, large specific surface area, and mechanical strength, make it an interesting choice to enhance energy storage systems (table 3). Graphene oxide offers a large specific surface area and oxygen-containing groups, enabling effective ion interactions in energy storage systems.^(32,33) Sulfur-doped GO demonstrates thermal stability and negative thermal expansion, which are beneficial for high-performance supercapacitors.⁽³⁴⁾ The optical and electrical properties of GO/S structures make them viable for advanced nanoenergy platforms.⁽³²⁾ Graphene material is associated with significant increases in power and energy levels and, therefore, is essential to the development of future energy storage.⁽³⁵⁾ Due to its large surface area that can reach a maximum of 2675 m²/g, graphene has a direct influence on capacitance behavior in supercapacitors (figure 2).

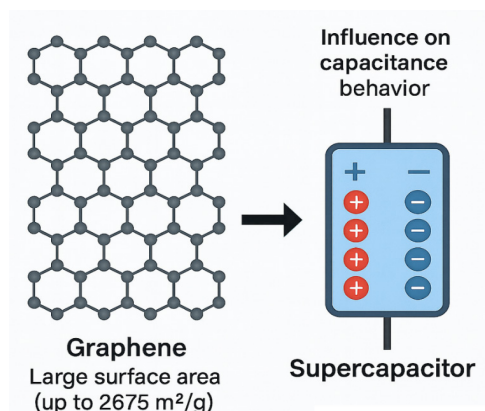


Figure 2. Graphene-Induced Capacitance Enhancement in Supercapacitors via High Surface Area Interface

This increases storage capacity of the charges necessary in the efficient operation of energy storage devices. Additionally, the high electrical conductivity of graphene leads to energy loss reduction during charge and discharge cycles, therefore, enhancing supercapacitor devices general performance.⁽³⁶⁾ Studies have revealed that supercapacitors made of graphene have the potential to store up to 100 to 500 F/g which is significantly higher when compared with the standard capacitor.⁽³⁷⁾ Despite the positive features, its scientists are faced with challenges, such as the tendency of graphene sheets to get back together during processing, effectively reducing the convenient surface area upon which charges could be stored. The stacking will minimize ion mobility therefore compromising performance. Some of the strategies to tackle these challenges involve development of composite materials which combine the graphene with other elements such as metal oxides and conductive polymers hence improving capacitance and stability. The synergistic properties of the building materials may be employed in the composite designs, therefore, bolstering the overall performance compared to the performance of the single material.⁽³⁸⁾

In addition, environmental sustainability is also emerging as a deciding element in energy storage technologies. Graphene can be produced using various waste materials such as biomass, industrial wastes, which makes it less harmful to the environment caused by manufactured graphitic products. Such factor is not only supporting the idea of sustainable approach to the production of materials but also introduces a possibility of cost-effective means of production, which can potentially increase the usage of supercapacitors in the market.⁽³⁹⁾ Most remarkably,

three-dimensional (3D) graphene structures have proposed to find means of optimizing surface area and reducing restacking effects. The three-dimensional structures overcome the limitations of the two-dimensional graphene sheet and provide an enhanced accessibility of the ions and enhanced electrochemical performance in the supercapacitor devices.⁽⁴⁰⁾ Research indicates that the new topologies can be effectively utilized to increase the efficiency and capacitance value of supercapacitors, especially that of graphene supercapacitors by optimizing the pathways between charges and ions.⁽⁴¹⁾

Table 3. Key Properties of Graphene for Energy Storage Applications		
Feature/Aspect	Description	Reference
Atomic Structure	One-layer carbon atoms arranged in hexagonal lattice; 2D structure	Papadimitrakopoulos et al. ⁽³⁵⁾
Surface Area	Up to 2675 m ² /g; enhances charge storage capacity	Lu et al. ⁽³⁶⁾
Electrical Conductivity	High conductivity allows faster charge/discharge cycles, reducing energy loss	Lu et al. ⁽³⁶⁾
Capacitance Range	Graphene-based supercapacitors can reach 100-500 F/g, far exceeding traditional capacitors	Salehfar et al. ⁽³⁷⁾
Mechanical Strength	High tensile strength adds structural stability during electrochemical cycling	Papadimitrakopoulos et al. ⁽³⁵⁾
Challenge: Restacking	Graphene sheets tend to agglomerate, reducing surface area and ion mobility	Obodo et al. ⁽³⁸⁾
Solution: Composites	Combining graphene with metal oxides or conductive polymers improves stability, capacitance, and ion transport	Obodo et al. ⁽³⁸⁾
Sustainability	Graphene production from biomass/waste materials provides a green, cost-effective alternative	Manik et al. ⁽³⁹⁾
3D Graphene Structures	3D architectures reduce restacking, enhance ion accessibility, and improve electrochemical performance	Qi et al. ⁽⁴⁰⁾
Pathway Optimization	Advanced topologies optimize charge/ion transport routes in supercapacitors	Zhang et al. ⁽⁴¹⁾

Conclusively, graphene application in energy storage devices, particularly supercapacitors, is a multimodal approach that uses materials science, nanotechnology and environmental factors to offer new solutions to energy needs in future. Scientists are exploring numerous characteristics and future applications of graphene, which means that this outstanding substance is essential in terms of efficiency and sustainability of energy storage systems.

Fabrication of Graphene-Based Supercapacitor Electrodes

Graphene Synthesis: CVD, Hummers Method, Liquid Phase Exfoliation

Graphene a single -atom-thick sheet of carbon arranged in a hexagonal geometry has gained much attention due to its unique mechanical, electrical and thermal properties. Graphene needs synthesis in order to be integrated with numerous solutions in energy storage, electronics and composite materials. Many methods of producing a graphene are known with the most prominent among them being the chemical vapour deposition (CVD), Hummer’s technique and liquid phase exfoliation. All processes possess unparalleled advantages and issues which

influence the quality, scale ability and utility of the synthesized graphene (figure 3).

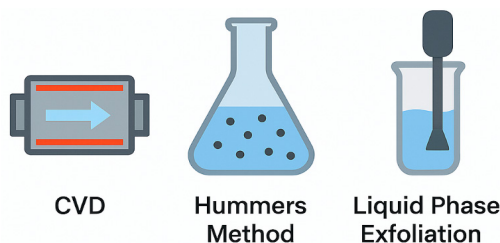


Figure 3. Their synthesis methods of graphene oxide

One of the commonly applied procedures in the synthesis of graphene oxide (GO) among the hummers is the graphite. The method based on the oxidation of graphite flakes through a mixture of concentrated sulphuric acid, potassium permanganate, and other oxidizing reagents with subsequent functionalization of the graphene sheets with oxygen groups.^(42,43) An even smaller quantity of graphene oxide supposedly leads to the formation of reduced graphene oxide (rGO), which retains certain extent of oxygen content that influences eventual properties and applications.^(43,44,45) It is necessary to control the temperature, and reaction time to adjust the degree of oxidation that is vital to achieving the desirable levels of oxidation and functionality in the final graphene oxide.^(46,47) New technology in modified Hummers and new graphene manufacturing methods are being considered in terms of their economic and environmental health costs to promote sustainability in the environment.^(48,49) The changes are directed towards reducing the number of toxic by-products associated with the traditional practices. Although other techniques (such as incorporating environmentally friendly solvent mixtures and organisms in the synthesis of graphene) have been proposed, the process suggested by Hummers will remain relevant due to its ease of access and the established procedure in the community of scientists.^(50,51) GO was synthesized via a modified Hummers method, and its structure was characterized using Raman, XRD, and SEM techniques.⁽⁴⁴⁾ CNTs synthesized via arc discharge and CVD methods displayed high crystallinity confirmed through phase analysis.⁽⁵²⁾ GO-CNT hybrid electrodes demonstrated homogeneous dispersion and excellent electron transfer, resulting in improved performance.⁽⁵³⁾

Graphene manufacturing processes like Hummers, CVD and the liquid phase exfoliation processes have enabled developments in the studies of materials. There is a unique advantage and limitation to each of these methods and it influences the choice of process based on the desired features of the product. Future actions can be devoted to optimization of these methods to the issues of scale, environmental sustainability of manufacturing process, and maintenance of high-performance characteristics which comply with planned uses of graphene in various spheres.

Composite Materials: Graphene with CNTs, Metal Oxides, Conducting Polymers

Graphene, carbon nanotubes (CNTs), metal oxides, and conducting polymers are some of their properties and applications that have attracted the serious investigation of composite materials in the last several years. Synergetic results in these composites enhance their mechanical strength, electrical conductivity, thermal stability and antimicrobial properties. Due to striking strength and electrical conductivity, graphene and carbon nanotubes are critical constituents of various composite systems. The addition of graphene oxide to polymer composite improves mechanical and barrier properties significantly, which is needed in the protective coatings and in corrosion resistance.⁽⁵⁴⁾ GO synthesized by the Hummers method yielded stable dispersions

after purification and reoxidation processes.⁽⁴⁴⁾ CNTs produced via CVD exhibited tunable conductivity when doped with gadolinium.^(21,55) The electrical modeling of GO/S nanostructures was employed to predict device behavior.⁽⁴⁴⁾

Metal oxides play key roles in composites composed of conductive polymers and those containing carbon-based materials. The binary metallic sulfide-based nanocomposites have also contained ZnO that serves twice, both in energy storage and sensing functions. Furthermore, metal oxides in mixtures with CNTs and graphene enhance the electrical conductivity and electrochemical properties of a composite that is going to be applied in supercapacitors and batteries. Study indicates that the mercy of electrodes in supercapacitors could be significantly reduced by using manganese in combination with graphene. Addition of conducting polymers such as poly aniline with graphene and carbon nanotubes improves the capabilities of charge transport which is critical in several sensor application areas. The improvement is attributed to the continuous pathways formulated by the networks of conjugated polymers that facilitate rapid transfer of the electrons, thus, increasing the sensitivity and effectiveness of the sensors used in glucose and another biomolecule detection.^(56,57) GO and CNT-based nanocomposites were enhanced with metal oxides (e.g., ZnSe, MnO₂) and conducting polymers to boost electrochemical activity.⁽⁵⁸⁾ The photoconductivity of Gd-doped CNTs and thermal stability of GO/S composites highlight their multifunctional potential.⁽²¹⁾ Surface properties were validated using XPS, EPR, and FTIR techniques. The properties of polymer-based composites with graphene and carbon nanotubes are under exploration in solving electromagnetic interference shielding, thermal management and flame retardancy. The strategic application of graphitic materials has been recorded by researchers to have a better thermal property that is desired in aerospace, automotive and electronic applications.^(58,59) Carbon nanotubes (CNTs) increase thermal properties by raising a thermo-conductivity and mechanical strength when properly positioned in a polymer matrix (table 4).^(17,18,21,60)

Table 4. Functional Roles and Synergetic Effects of Graphene, CNTs, Metal, Metal Oxides, and Conducting Polymers in Composite Materials				
Component	Functional Role in Composites	Enhanced Properties	Application Areas	References
Graphene	Filler material; provides high mechanical strength and electrical conductivity	Mechanical reinforcement, corrosion resistance, barrier properties	Protective coatings, corrosion resistance, electronics	Arnal et al. ⁽⁵⁴⁾
Carbon Nanotubes (CNTs)	Structural and conductive framework in composites	Thermo-conductivity, mechanical strength, EMI shielding, electron mobility	Aerospace, automotive, sensor technology, electronics	Abaszade et al. ^(18,21) Zhang et al. ⁽⁶⁰⁾ Chowdhury et al. ⁽⁵⁹⁾
Metal and Metal Oxides (e.g., Gd, ZnO, MnO ₂)	Electrochemical activators and charge storage enhancers, used in nanocomposite formation	Improved electrochemical behavior, enhanced conductivity, dual role in energy/sensing	Supercapacitors, batteries, sensors	Abaszade et al. ⁽¹⁷⁾ , Yasmeen et al. ⁽⁵⁶⁾ Le et al. ⁽⁵⁷⁾

Conducting Polymers (e.g., Polyaniline)	Provide continuous charge transport pathways and enhance surface interaction with analytes	High electrical conductivity, sensor sensitivity, rapid electron transport	Biosensors (e.g., glucose sensors), flexible electronics	Yasmeen et al. ⁽⁵⁶⁾
Graphene + CNTs	Hybrid reinforcement agent with excellent interconnectivity	Increased mechanical strength, thermal conductivity, EMI shielding	Flame retardants, structural electronics, smart coatings	Zhang et al. ⁽⁶⁰⁾
Graphene + Metal Oxides	Charge storage and surface modification synergy	High capacitance, low internal resistance, long cycling life	Energy storage (supercapacitors, Li-ion batteries)	Yasmeen et al. ⁽⁵⁶⁾ , Le et al. ⁽⁵⁷⁾
CNTs + Conducting Polymers	Conductive matrix with tubular electron transport channels	Enhanced electron flow, improved mechanical flexibility	Biosensors, electrochemical sensors	Yasmeen et al. ⁽⁵⁶⁾
Polymer-based Graphene/CNT Composites	Multifunctional composites for environmental and energy applications	EMI shielding, thermal management, flame retardancy	Aerospace, wearable electronics, environmental safety	Zhang et al. ⁽⁶⁰⁾ , Chowdhury et al. ⁽⁵⁹⁾

To conclude, a combination of graphene, carbon nanotubes, metal oxide, and conducting polymer represents a revolutionary step in the field of materials science that drives technological progress but also addresses sustainability challenges that mankind has to face. Further research and development in the area will reveal novel functions and this will permit new applications in energy, electronics, environmental remediation and biotechnology.

Devices of supercapacitors

Symmetric vs. Asymmetric Supercapacitors

It is necessary that supercapacitors as the critical components in energy storage nowadays can be generally divided into two fundamental types, symmetric supercapacitors (SSCs) and asymmetric supercapacitors (ASCs). The main contrast between these two topologies is a similarity or disparity of the material of used electrodes, which leads to different values of electrochemical performance parameters such as energy density, power density, cycle stability, and voltage restriction limits. Symmetric supercapacitors utilize identical electrode materials structural on each part, and the materials are regularly made of a carbon-based material or transition metal oxide, which provides a diminished operating voltage, normally constrained to about 1,2 V because of thermodynamic prerequisites of the material.⁽⁶¹⁾ By contrast, asymmetric supercapacitors employ two different electrode materials which can include a pseudocapacitive materials and a double-layer capacitor material and can thus span a larger voltage range that can go up to about 2,0 V. Such increased voltage operation straight away leads to increased energy densities, possibly even higher than with symmetric supercapacitors, (figure 4).^(62,63)

The asymmetric system incorporating MXene materials is potentially promising to significantly amplify the working potential scale and reach above-average energy densities compared to the symmetric ones.^(62,63,64) GO and CNT-based electrodes have been successfully implemented in symmetric, asymmetric, solid-state, and flexible supercapacitor architectures.⁽⁵³⁾ The structural compatibility and electrical stability of GO/S nanocomposites contribute to reliable device performance.⁽⁴⁴⁾ These materials are especially promising for lightweight UAV platforms.⁽⁶⁴⁾

There is significant difference in energy density in supercapacitors (SC) between asymmetric and symmetric SC due to underlying structural and material differences. Symmetric supercapacitors have nominal energy densities of 5-10 Wh/kg, compared to asymmetric devices with nominal energy densities of 30-60 Wh/kg and are therefore more suitable to high performance applications.⁽⁶⁵⁾ Since asymmetric design incorporates high-specific capacitance materials in the positive or negative electrodes, it also leads to the fact that the adaptability of designing performance to meet specific power and energy demands is improved.^(66,67) Such flexibility is necessary in consumer electronics applications, up to electric cars where cost and performance is paramount.

Stability of the cycle is an important factor which makes a difference between symmetric and asymmetric supercapacitors. Research indicates that, SSCs can have improved cycle stability with greater capacity retention remaining more consistent over the multiple charge discharge cycles. As an example, SSCs can retain much of their original capacitance in approximately 92 percent of the cycle after 1000 cycles, whereas, in some cases, ASCs can observe a decrease in capacitance retention. Its reliability is attributed to the fact that this level of stress remains even, as faced by the electrodes in symmetrical systems, opposed to varying degrees of stress in non-symmetrical systems that can lead to material demineralization in the long term.^(68,69)

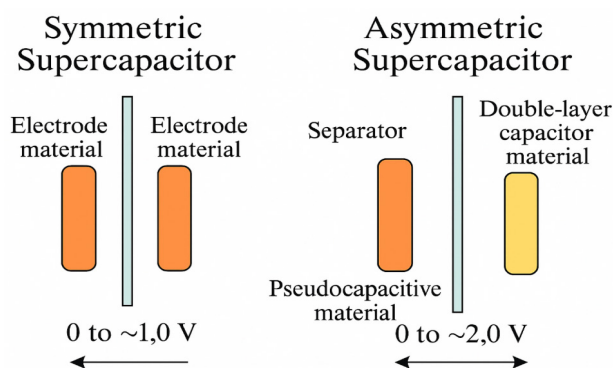


Figure 4. Symmetric vs. Asymmetric Supercapacitors

The extent of flexibility and adaptation of each type to some use situations is not only to emphasize their purpose but also on potentials of their performance in real circumstances. The progress of the supercapacitor lies in the enhancement of the performance of the supercapacitors through the innovation of new materials and design practices. To achieve green supercapacitors, researchers are examining the various viable biomaterials of constructing electrodes.⁽⁷⁰⁾ In symmetric designs, GO and CNTs are used as identical electrode materials for balanced performance, whereas in asymmetric models, voltage window and energy density are significantly improved.^(17,44) Gd-doped CNTs used as anodes offer enhanced energy conversion capabilities.⁽²¹⁾ Structural differences were revealed via EIS and Raman spectroscopy.

To conclude, comparative analysis of the symmetric and asymmetric supercapacitors distinguishes peculiar advantages and disadvantages defining their definite application in the aspect of the energy storage technology. SSCs are more stable in the number of cycles and easier to manufacture, whereas ASCs are more flexible in application terms of energy density and operating range, always being boosted by research and continuous innovation into the material and design of these types of batteries. With the rise in demand of complex energy storage solutions, it will be important to understand these differences that would help in maximizing

the use of supercapacitor in various sectors.

Solid-State and Flexible Supercapacitor Designs

GO and CNT-based solid and flexible electrodes maintain performance under vibration and mechanical stress.⁽⁷¹⁾ The photoelectric properties of GO/S composites offer multifunctionality in smart wearable and flexible electronics.⁽²²⁾ These systems are highly applicable to emerging flexible technologies.^(72,73,74,75) The trend toward solid-state and flexible supercapacitors technologies is an important response to the growing world energy demand, the demand of sustainable development and energy storage needs. The supercapacitors have grown in popularity because of the high-power density, high speed of charging and discharging and long-life cycle (table 5). These properties make them suitable in mobile equipment's, electric vehicles and green energy devices.^(76,77) The newest trends concern the integration of such materials as MXenes, nanomaterials, and biomass-derived composites of carbon, enhancing performance and facilitating environmentally friendly production technologies.^(78,79)

Table 5. Comparison of Supercapacitor Architectures: Design, Electrolyte, Electrode Materials, and Mechanical Flexibility					
Design Type	Electrolyte Type		Electrode Materials	Mechanical Flexibility	Energy Density
Solid-State SC	Solid Electrolyte (e.g., H ₃ PO ₄ , gel-based)	Polymer (e.g., PVA)	Graphene, CNTs, MnO ₂ , Polyaniline	Rigid or semi-flexible	Moderate-High (up to 20 Wh/kg)
Flexible SC	Gel or solid-state electrolyte		rGO, MXenes, Conductive Fabrics, Carbon textiles	High (bending, stretching)	Moderate (5-15 Wh/kg)
Quasi-Solid-State	Hybrid (liquid/solid gel systems)		Graphene composites, Metal oxides, Conducting polymers	Moderate-High	High (>20 Wh/kg)
Stretchable SC	Ionic gel electrolytes		Wrinkled graphene, kirigami-structured CNTs	Very High (stretch >100 %)	Low-Moderate (2-10 Wh/kg)
Printed SCs	Solid or gel electrolytes		Ink-form rGO, Carbon inks, AgNP composites	High	Low-Moderate

The other factor in the development of the supercapacitor technology is the optimization of the production process. New manufacturing techniques like 3D printing, new coating techniques allow fine tuning of material properties and structures in the development of super capacitors. In addition to enhancing the performance measures, these strategies lead to the scalability of production, and therefore, these technologies are more favorable to commercial purposes.^(80,81) In the development of the next generation high-performance flexible supercapacitors, the integration of new production methods and new materials will play a definitive role. As sustainability changes the future of energy storage, researchers are looking at the lifetime and recycle of supercapacitors. By introducing the ideas of green chemistry in the development and fabrication of supercapacitors, reduction in environmental impact could contribute to the development and growth of renewable energy sources.^(82,83) Such an all-round approach of energy storage efficiency and saving the environment aligns with the global endeavors of carbon neutrality and the fight against climate change.

An academic to industrial collaboration in future will play a critical role in translating research findings into commercially viable super capacitor technology. The continued development of

relevant legislations, standards and practices in the field of energy storage will equally influence the course of research and development initiatives in the same area. Adoption of frameworks that focus on innovation, efficiency, and sustainability can trigger a transition in energy storage and use in most applications. Optimization of the solid-state and flexible structure of the supercapacitors is not a simple process, and it consists of innovative material research, cutting-edge production technology, and a special emphasis on sustainability. The development of these aspects will help supercapacitor technology to fulfill growing demand of power with an active environmental context and promise reliability, efficiency and environmental friendliness in power storage applications.

Applications in Energy Systems

Portable and Wearable Electronics

Portable and wearable electronics is the sphere that has developed rapidly due to the improvements in materials and methods of energy storage, which have led to a reduction in the size and efficiency of gadgets and a greater level of versatility. These enhancements are critical to the invention of the lithium-ion batteries (LIBs) which have become the main mode of energy storage of handheld devices, electric vehicles, and more complex systems such as solar energy storage. The nature of LIBs in terms of chemical composition and design features defines its efficacy. Banerjee et al.⁽⁸⁵⁾ clarify the redox mechanisms and stability of the nickel-rich cathodes which are crucial to the success and stability of high-capacity lithium-ion batteries used in everything, including handheld devices and even electric vehicles. As the technology of these systems keeps improving, there is a lot of its wide application in the world of mobile electronic devices. This outdoor operation enhances the usefulness of wearable electronics a lot as it can continue its task undisturbed even without the conventional power. In addition, the unceasing advance development of energy storage devices like supercapacitors and similar composites bring great advantages in the management of power sources of portable devices. Investigation of Ravandran et al.⁽⁸⁵⁾ is devoted to supercapacitors based on tungsten diselenide, where the emphasis is on the further development of high-energy density storage devices that meet the fast and unpredictable power needs of modern portable devices.

Sustainable designs and the trend of green energy embraces thermoelectric and triboelectric nanogenerators (TENGs). These are technologies that can convert ambient energy into usable electricity required by self-powered devices. According to the study presented by Suneetha et al.⁽⁸⁶⁾, there are gains made in the field of triboelectric nanogenerators using electronic trash, which suggests that the given materials can contribute to a considerable increase in the energy harvesting capabilities of wearable devices. The technique can not only meet the demand in energy production but also increase sustainability efforts in the manufacturing of electronics.

Due to recent innovative storage solutions, the flammability of the lithium-ion battery electrolytes has indeed become a lesser cause of worry. Afif et al.⁽⁸⁷⁾ research the fluoride-doped solid electrolytes to minimize risks, enhance the ionic conductivity, and address the concerns about the safety of the standard lithium-ion batteries and the risks of their failure. It is expected of this study to come up with batteries that are exceeding the existing performance related with safety of the users in every application of the portable electronics.

Mass adoption of the integration of material science and energy storage technologies, coupled with electrical design, are changing the field of portable and wearable electronics tremendously. Further designing of modern gadgets is being transformed into well-developed technologies that employs LIBs, develop flexible materials and address various challenges such as EMI and thermal management to meet the existing user demands. Future research projects in various areas are

promising a brighter future of portable electronics which can enable imaginative applications that are deemed impossible up to now.

Grid-Level Energy Buffering

Grid-level energy buffering is a growing part of our present-day energy system, and its role is particularly relevant now due to the increasing usage of renewable sources of energy. Renewable energy generation is intermittent; therefore, the demand of secure, reliable power calls upon robust systems. The energy storage technologies play a pivotal role in dealing with the fluctuation in supply and demand. These solutions reduce the problems of finite supply of renewable resources and helps in enhancing grid reliability and interdependence on traditional fossil sources. Grid level energy buffering encompasses several approaches, both traditional e.g. pumped storage hydropower (PSH) and novel e.g. advanced battery technology. Today, pumped storage hydropower (PSH) remains one of the popular and effective means of large-scale energy storage that is characterized by a high capacity and cost-effectiveness.^(88,89) Some shortcomings of pumped storage hydroelectricity (PSH) are spatial related, implying that alternatives, such as those based on lithium-ion battery and thus able to be deployed more versatily, redox flow batteries (RFBs) are wanted. These technologies of batteries are delivering high energy density and equally exhibit high application flexibility in many uses such as industrial power control and electric vehicle integrations.^(90,91) GO and CNT-based supercapacitors are ideal for grid-level peak shaving and fast energy buffering.⁽⁹²⁾ Their high cycling durability ($>10^4$ cycles) and power density make them promising battery alternatives. Their thermal management properties enable long-term operation in dynamic grid environments.⁽²¹⁾

The other important technology is interchangeable fuel cells and electrolysis in the production of hydrogen. These inventions give a mixed strategy of energy storage and distribution because they utilize water to produce hydrogen when there is excessive generation of renewable energy. Then this hydrogen could be reused again in fuel cells to generate power at the peak load and introduce sustainable power into grids and enhance stability. Their miniature and lightweight design also makes proton exchange membrane electrolysis very suitable to be coupled with renewable energy sources.⁽⁹³⁾ The integrated cooperation of a variety of energy technologies can possibly optimize the flexible operation of the dispersed energetic resources, such as the thermal generating and renewable sources. Using smart grid technologies improves the efficiency of resources and supports the idea of sustainability through interoperability.⁽⁹⁴⁾ Smart microgrids underline the opportunities of new energy management systems, which ensure the possibility to monitor and control the power supply of multiple disparate generating sources in real-time. Such flexibility is critical in balancing the fluctuating energy production of renewable sources and properly always fulfilling the needs of the consumer and in a cost-effective manner. The effort that will be taken now and into the future to enhance energy storage technology and the incorporation of those technologies into the grids will have an enormous influence on energy stability in the future and take us toward a more reliable and sustainable energy environment. Transformation into renewable energy necessitates a broader focus on energy storage, and at this point we should focus on groundbreaking technologies improving efficiency, effectiveness and environmental friendliness.⁽⁹⁵⁾

The current tendency of the energy buffering mechanisms is burgeoning to indicate the necessity to incorporate diverse storage technologies into the energy systems to make them more resilient and benign. Our commitment to the solutions to the challenges of renewable energy integration can be illustrated by the current study of innovative materials and technologies including redox flow batteries, hydrogen solutions, and enhanced lithium-ion systems. Efficient

buffering of energy at the grid level is based on the ability to adapt, optimize, and innovate in different energy systems.

Hybrid Supercapacitor-Battery Systems

Hybrid supercapacitor-battery systems (HSBs) is estimated to be a feasible approach to satisfy the growing demand of efficient energy storage solutions in variety of applications, including electric vehicles (EVs), portable electronics, and integration of renewable energy sources. Such systems take these unique benefits of the supercapacitors and the batteries and combine them together by using supercapacitor benefits of high-power density, fast charge-discharge rate, and cycle life, and the high energy density that the batteries have to offer. The resulting dual approach aims to counter the limitations of independent energy storage systems and provide better performance at energy, power and operating efficiency levels.^(96,97)

Hybrid supercapacitors the electrochemical properties and structure of electrode materials are closely associated with the performance of hybrid supercapacitors. A study performed by Sivakumar et al.⁽⁹⁸⁾ underlines the significance of the electrode composition stating that battery-type electrodes may enhance specific capacity through efficient redox charge transfer thus, potentially increasing energy density. The economics of hybrid supercapacitors-battery systems are slowly becoming a major line of research inquiry. It is vital to evaluate the life-cycle cost of the two sectors as well as the consumers, and the return on investment is vital, as in the material science and technology, an invariable pricing cutdown along with the increased performance parameters is effective. The analysts expect that major increase in these systems deployment would be observed based on high efficiency and reduced environmental impact in comparison with traditional energy storage technologies.⁽⁹⁹⁾ It is projected that electric vehicles that would utilize hybrid systems would achieve lower fuel costs and indeed, greater fuel range because of the synergistic effects of their energy storage components.⁽¹⁰⁰⁾

Hybrid systems Hybrid storage systems are a key to use renewable energy sources like wind, solar power more efficiently. Combining supercapacitors with the energy storage capacity in batteries would allow harnessing the energy generated in large volumes during times when energy is readily available and could deploy this energy quickly whenever the demand fluctuates. Research indicates that use of these systems increases flexibility of operation in microgrid structure and hybrid storage systems are important tools in ensuring that supply and demand are well balanced.^(101,102)

Finally, the development of hybrid supercapacitor-battery systems is an indication of significant development in achieving more efficient, reliable and effective energy storage opportunities. Not only do these technologies reduce the pitfalls of the traditional battery and super capacitor alone, but they also utilize their synergistic changes to offer a stronger, versatile energy landscape. In the way the science goes, as exemplified by materials and design possibilities continuously increasing storage capacities, the future of how energy will be handled can be staring with the efficient use of hybrid energy production methods.

Automotive and Aerospace Applications

The world of automobiles and airlines is increasingly focusing on new materials to meet the demands of lightweight, high-strength parts, and at the same time increase safety and fuel consumption. Many have made a remarkable shift at using composite materials which has been shot up by their superior mechanical properties, corrosion resistance and versatile design that is very important in the two industries. Reinforced composites made of carbon fiber exhibit a better strength to weight preparation, and hence they can be used where weight is paramount

and therefore carbon fiber reinforced composites are more preferred in making aeroplane structures and automobile frame bodies.^(103,104) Novel research concerning the hybrid composite such as carbon and bamboo fibre composites highlights the importance of vibration and acoustic characterization that are required industry applications in automotive and aerospace industry. The damping property of composite materials can play an important role in their performance under dynamic load conditions, as the vibration control of the structure is a paramount issue concerning the passengers and the soundness of the structures.⁽¹⁰⁵⁾ Focus on improving damping properties of materials is essential in the development of components that have to be able to withstand high vibrating stresses without losing performance or safety. The lightweight, thermally stable, and mechanically robust properties of GO and CNTs make them ideal for automotive and aerospace applications.^(106,107,108) Supercapacitors based on GO/S and Gd-CNTs exhibit vibration resistance and reliable performance in UAV systems.⁽¹⁰⁶⁾ These materials offer both aerodynamic and energetic optimization for advanced platforms.

The development of composite materials in automobile body panel, interior parts, and aerospace industries contributes significantly to the effective performance and does not violate the structure in different axes of the environmental contexts. Automobile industry is experiencing an increased demand of bio-composites made of renewable materials. The evolution of natural fiber-reinforced polymer composites evidences the commitment of the industry to be more sustainable without loss of any core mechanical properties needed to be used in cars.⁽¹⁰⁹⁾ This further emphasizes on the trend on the use of environmentally friendly materials and is associated with the gradual growth in customer needs of being environmentally sustainable in the automobile industry.

Table 6 summarizes the key directions in the development and application of advanced materials and joining technologies within the automotive and aerospace industries. The focus is placed on composite systems, hybrid natural-synthetic fiber structures, and intelligent selection tools that enable enhanced mechanical performance, lightweight design, and sustainability. Each material or technique is associated with specific functional advantages and application areas, reflecting the industry’s response to evolving technical and environmental demands. The classification serves as a foundation for understanding current innovations and guiding future material selection strategies in high-performance engineering contexts.

Table 6. Advanced Composite Materials and Smart Technologies in Automotive and Aerospace Applications			
Section	Material/Technology	Core Function/Advantage	Typical Application
Lightweight and High Strength Materials	Carbon Fiber Reinforced Composites (CFRCs)	High strength-to-weight ratio, corrosion resistance	Aircraft frames, automotive chassis
Surface Treatment and Bonding	Hybrid Carbon-Bamboo Composites	Vibration damping, acoustic insulation	Interior parts, sound-sensitive zones
Surface Treatment and Bonding	Silane Treatment, Polymer Blending	Enhances interfacial adhesion, improves mechanical performance	Composite laminate interfaces, lightweight panels
Joining and Welding Technologies	Composite Laminate Interface Optimization	Enhanced structural bonding, crack resistance	Structural components in vehicles & aircraft
Bio-based and Sustainable Composites	Natural Fiber-Reinforced Polymers (NFRPs), e.g., flax, hemp	Renewable, biodegradable, lightweight	Door panels, dashboards, car interiors

Joining and Welding Technologies	Friction Stir Welding (FSW) of Al-Mg alloys	Solid-state joining, strong and ductile joints	Aerospace panels, EV battery enclosures
Smart Materials & Predictive Tools	Artificial Intelligence (AI), Machine Learning	Real-time performance prediction, material optimization	Material selection platforms, digital twin models
Acoustic and Vibration Properties	Bamboo-based composites, hybrid damping-focused resins	Noise and vibration reduction under dynamic load	Suspension systems, cabin walls
Environmental and Customer Trends	Bio-composites, recyclable polymer matrices	Sustainable, responds to consumer eco-awareness	Eco-cars, light utility vehicles

To conclude, recent developments in material science are triggering a radical change in the automotive and aerospace industries. The emphasis in ultra-light and ultra-high-performance composites, coupled with innovative in-manufacturing technology (additive manufacturing and advanced welding processes) has the potential to treat the demands of modern and more challenging engineering needs. As industries strive to find a balance amongst performance, safety and sustainability, future of vehicle and aircraft design will inevitably depend on the further improvement of material characteristics.

CONCLUSIONS

The unfettered power quality with high charging and discharging rates has made the graphene-based supercapacitors an interesting development in the energy storage technology. The basic knowledge of charge storage mechanisms lies in the differentiation between the electric double-layer capacitors (EDLCs) and pseudo capacitors, which have both advantages and disadvantages. EDLCs cycling is based on electrostatic forces, and pseudo capacitors offer high energy densities, which is based on redox-active materials. The main characteristics of supercapacitors are also their high values of specific capacitance, energy and power density, and cyclic stability that are required signs of performance. The graphene provides a solid platform due to its large surface area (~2630 m²/g), highly electrically conductive, mechanical flexibility, and electrochemical stability. Such characteristics facilitate ion transport and charge accumulation and there is an excellent prospect of graphene as a high-performance electrode. There are numerous methods of manufacturing that have been designed to allow us to produce carefully customized varieties of the material that is defined as graphene according to the specifics of unique designs of devices, such as chemical vapor deposition (CVD), the Hummers method and liquid phase exfoliation. Further we would expect better industrial use of composites involving carbon nanotubes (CNTs), metal oxides, or conductive polymers, which give out different synergies in, e.g., increased conductivity, mechanical strength, or pseudo-capacitance. On the device terms, symmetric and asymmetric designs have been discussed to maximize the voltage and energy generation. Additionally, emergence of solid-state and bendable architecture presents new opportunities toward integration with modern electronics and smart wearable devices. Such developments respond to the increased demand of small, low-weight, and mechanically strong energy storing solutions. Graphene-based supercapacitors have been put into numerous applications such as in the sector of small-scale portable grids and in the energy storage system of large-scale grids stabilization. They offer energy storage and regenerative braking of lightweight, high-performance systems within the automotive industry and the aerospace industry. Moreover, the hybrid supercapacitor batteries are becoming trendy and offer a tradeoff among power and long-term energy storage to the extent that is essential to modern energy management technology. Intersection of material science of graphene with

engineering of supercapacitor is a high point of this field in the path to creating high-capacity, sustainable, and efficient energy storage devices. The next stage within the development of synthesis methods, composite design and integration of devices will increase their usability in a broad range of new energy systems.

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Chapter 15

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Interface Engineering and Stability of Graphene-Based Devices

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ABSTRACT

In this chapter, a complete description of the bulk characteristics of graphene as well as why the interface engineering plays an essential role in improving its characteristics in various applications is presented. The chapter starts with the description of unusually high electronic, mechanical, and thermal properties of graphene, and then differentiates among multiple representations and types of graphene, such as monolayer, bilayer, graphene oxide (GO), and reduced graphene oxide (rGO). Common interface types: metal-graphene, dielectric-graphene, and polymer-graphene are studied with special focus on their effects on device behavior. The chapter discusses more complex interface engineering methods to maximize interfacial contact, carrier transport and material compatibility. The stability of graphene-metal and graphene-dielectric interfaces, and functional integration of graphene with polymers and organic materials are the detailed areas. Applications that are emerging as important where control of the interface is desirable include energy storage and conversion devices, graphene-based quantum systems and integration with CMOS technology. With the introduction of theoretical understanding and practical knowledge, this chapter will be a resourceful piece of work to both researchers and engineers who could tailor their interests to maximize the use of graphene in the next generation technologies.

Keywords: Graphene; Interface Engineering; Graphene Oxide (GO); Reduced Graphene Oxide (rGO); Graphene-Metal Contact; Dielectric Stability; Polymer Composites; Energy Storage; Supercapacitors; Quantum Devices; CMOS Integration; Charge Transport; Surface Functionalization; Two-Dimensional Materials; Nanotechnology.

INTRODUCTION

There has been great interest concerning Graphene based gadgets owing to the impressive physical and chemical characteristics of graphene, such as high electron transportability, mechanical durability, and thermal conductivity. Nevertheless, the effectiveness and stability of performance of these devices critically relies upon the NBC of their interfacial interactions with metals, dielectrics, and polymers. Interface engineering has come up as one of the most essential options to maximize charge transport, adhesion, and chemical compatibility in composite devices frameworks. By controlling the interfacial phenomena, it becomes possible to integrate graphene onto existing semiconductor platforms and to make graphene more appropriate to energy storage, quantum electronics and flexible technologies. This chapter has investigated

the basic ideas and new methods in engineering and stabilizing graphene-interface to liberate all their technological potential. Devices made of graphene are also getting more attention as it has most possibilities in other fields such as sensors, memory, solar cell and so on. One of their highlights in performance is greatly hinged on how their engineering of interfaces and the accrued stabilizing management within their performance can help as a determining factor towards its reliability and effectiveness. The share of recent researches and findings in this discussion includes many attempts to promote the continuation of the stability of devices based on graphene with the help of all possible innovations and methods of interface engineering. It is notable about the monolayer graphene that it has a very low thickness that makes it able to respond and recover within a short period, particularly in applications that involve humidity detection. Gao et al. emphasize that device using monolayer graphene enjoy the advantage of atomic structure so that their sensor responses are very fast. They remark as well that devices that use double-layer graphene also encounter problems because the bottom layer performance may be impaired by the underlying layer of SiO₂ substrate since their hydrophilicities may differ hence demonstrating a fundamental problem of interface engineering.⁽¹⁾ Interfacial properties can play an important role in influencing the performance and thus, there is a need to design specific engineering approaches to make the device functionalities better. The process of defect engineering becomes an important tool in enhancing interface stability and the performance of overall device, in graphene applications. The experiment conducted by Kim et al.⁽²⁾ reveals that the carrier mobility can increase by about 230,8 percent in the case of selective defect healing of graphene electrodes, which would mean a major advance in the electric properties. Based on their study they postulated that healing of the defects affects the Schottky barrier at the graphene/Tungsten diselenide (WSe₂) interface, which added to the long-term stability. The type of such findings highlights the necessity of developing the knowledge and control of the defects at the atomic scale to increase the functionality and reliability of the graphene-based devices.

In addition, interfaces between graphene and other 2D materials bear new ways to interface manipulation that can be used to improve performance. Agarwal et al.⁽³⁾ address the prospects of integrating graphene and hexagonal boron nitride (hBN) to produce electro-absorption modulators that have a higher efficiency of modulation and thermal stability. The vertical integration strategy also points at the necessity of accurate control over the interface interactions to obtain synergistic effect in device performance. Graphene-based materials have an ideal balance of strength and ductility that is critical in applications of application where mechanical robustness is considered. Manna et al.⁽⁴⁾ introduce a new method of using amino acid modified wrinkled graphene oxide in memory operations establishing the long-range stability of the resistive memory structures. Their results also underline the significance of chemical modifications to the long-term performance of any graphene-based devices as well as improving both the lifetime and reliability of the latter. Graphene is a critical area of research and should be encased in composites to increase their durability. According to Lin et al.⁽⁵⁾, the stable electrochemical energy storage based on dense reduced graphene oxide films has overcome the stacking tendency of the graphene sheets that has always been a problem when maintaining high storage capacity. Innovations in the material design are able to result in more functional and stable energy storage systems by paying attention to good mechanical stability and ion diffusion properties.

Lastly, Razaq et al.⁽⁶⁾ review relates to remote developments in graphene-based materials in charge transfer efficiency in PSCs in which the authors have discussed the role of interface engineering in achieving high performance and device stability, which is also of dual importance. Their results are an indication that there is a push within the research community to meet the

electronic properties as well as stability using composite and interface engineering. As a final conclusion, the study of graphene-based devices is developing at a high rate and with the synergistic success in engineering the interface and with the increased development of stability principles. Ongoing research portends both novelty and complexity in what graphene might do to advance devices, whether sensors and memory, energy systems and optoelectronics. With this growing body of knowledge in how things go on at such delicate interfaces, we can also count on coming up more super-sophisticated and stable graphene-based technologies.

Fundamentals of Graphene and Its Interfaces

Electronic, mechanical, and thermal properties of graphene

The unique physical characteristics of graphene are still based on the fact that this material is two-dimensional and consists of sp²-hybridized carbon atoms assembled in the shape of a honeycomb lattice. Electrically it exhibits high carrier mobility and ballistic conduction. The mechanical properties of graphene are rather large: its Young modulus is ~1 TPa and it is naturally strong with a strength of 130 GPa. Its conductivity is more than 3000 W/mK thermally. Graphene which is a one-atom thick sheet of carbon atoms located in a two-dimensional honeycomb structure, has received exceptional interest because of its unusual electronic, mechanical, and thermal signs. Its distinctive composition does not only make it an extraordinarily conductive and strong material but also makes it one that is to be an important development in future technology in many diverse areas, such as electronics and materials science. The present synthesis presents the multidimensional nature of graphene, outlining its electronic, mechanical, and thermal properties, and it relies on the variety of recent academic sources (figure 1). Carbon nanotubes (CNTs) properties in the thermal and electrical aspects were studied greatly to analyze heat flow and charge transport in graphene-like nano structures. Presence of rare-earth dopant such as gadolinium also has a pronounced effect on thermal conductivity and electron scattering in both CNTs and GO. The research will be vital in the understanding of the intrinsic material behavior of carbon-based nanomaterials in the future electronic and energy systems.^(7,8,9,10,11,12) Electrical properties of the graphene are of special interest, they are characterized by high electron mobility which enables exceptional use as next generation transistor and other electronic components. Measurements of suspended graphene samples indicate electronic mobilities as high as 200 000 cm² /V s, which is way more than what ordinary silicon substrates show.⁽¹³⁾ Graphene can also transfer the charges in an efficient way since it has a small electronic band gap, a property essential to applications in high-speed electronics and optoelectronic devices.

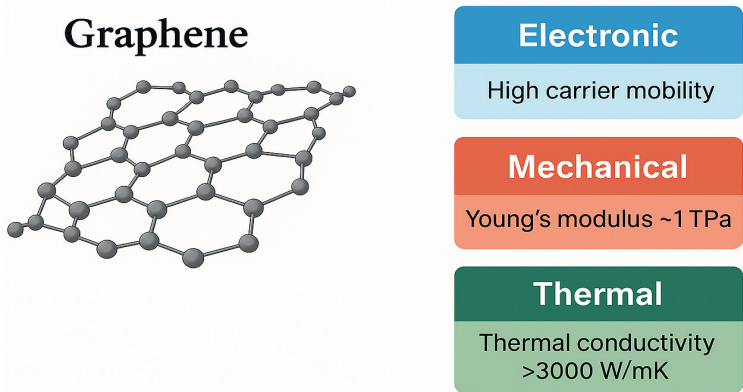


Figure 1. Electronic, mechanical, and thermal properties of graphene

Moreover, the combination of diverse materials, including gallium nitride (GaN), will provide an opportunity to create heterostructures that will capitalize on the strengths of both materials and, as a result, improve performance parameters of power sources and photonic applications.⁽¹⁴⁾

Mechanical characteristics of graphene are also revolutionary in parallel with its electronic properties. It is considered to be one of the most robust materials and its tensile strength can reach up to around 130 Gigapascals and stretching capacity is intrinsic to an extent that great deformations can be achieved without failing. This strength is exuberant because of the two-dimensionality which makes strong covalent bonds using sp² hybridized carbon atoms. But the structural integrity may be affected by a number of factors such as existence of defects and the size of the graphene film. It is also known that mechanical characteristics of the suspended graphene may be degraded with increasing diameter caused by accumulated defects and associated influence of surface tension during preparation conditions that can cause premature failure and crack.⁽¹⁵⁾ Moreover, the orientation and dispersion of graphene in the composition of material also have a significant effect on their overall mechanical effectiveness where, due to correct dispersion, it is possible to enhance the interfacial adhesion and strength.⁽¹⁶⁾ In addition to being electrical and mechanical, graphene is a very accomplished thermal conductor. Research has proved that graphene thermal conductivity is more than 5000 W/m-K which makes it an exemplary heat dissipation product in electronic appliances.⁽¹⁷⁾ This mix of properties is unique and makes graphene an invaluable asset to engineering of higher fidelity thermal interface materials thereby extending its possible use to the high temperature electronics field. To sum up, a graphene is one of the materials of unprecedented potential because of its unprecedented electronic, mechanical and thermal characteristics. Further research into the nature of its behavior and its possible applications are being driven by interdisciplinary research directions and current research is attempting to streamline its usefulness in a number of technology fields. The potential of grape to be used in electronic devices, its ability to be incredibly strong and thermally manageable, indicates that the material will still be used in the technological change as in the future, it will improve the performance and provide efficiencies in a vast number of applications.

Types of graphene: monolayer, bilayer, reduced graphene oxide (rGO), graphene oxide (GO)

The monolayer graphene is composed of one layer of carbon atoms contacting in 2-dimensional (2D) honeycomb lattice, providing outclass electron mobility and mechanical vulnerability. The bilayer graphene consists of two stacked sheets of graphene sheets which are commonly in an AB (Bernal) stacking structure, and which changes its electronic band structure, and provides pathways to tunable bandgaps under an electric field.

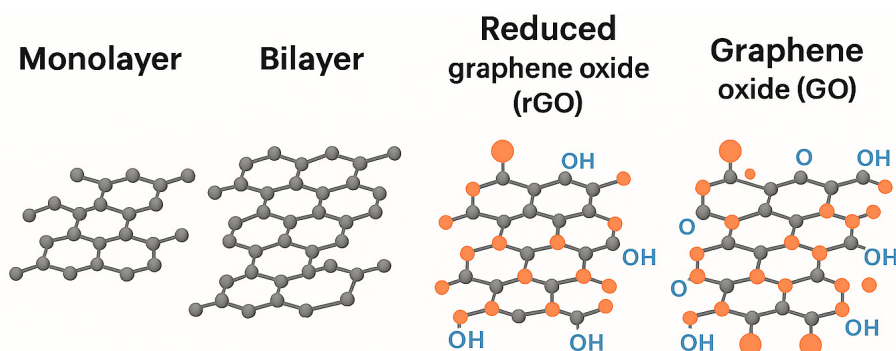


Figure 2. Types of Graphene: Monolayer, Bilayer, rGO, and GO

The interlayer interaction between the layers of bilayer graphene presents new quantum physics, which is appealing towards future nanoelectronics applications. Graphene oxide (GO) is a highly oxidized version of graphene that has oxidized functional groups (hydroxyl, carboxyl, and epoxy) and has a hydrophilic nature and is soluble in water. GO is electrically less conductive because of a broken sp² lattice structure but the mechanical and chemical versatility of the structure remains very useful in functionalization processes (figure 2).

During thermal, chemical or electrochemical reduction, a portion of the electron-withdrawing oxygen groups are removed as reduced graphene oxide (rGO) regains partial electrical conductivity and conjugation. Though rGO may not restore the initial structure of graphene fully, it provides a trade-off between conductivity and chemical reactivity in fine senses, so it can be applied to energy storage and sensor tasks. The electronic properties of monolayer and bilayer graphene differ; one can thus make a choice that depends on which properties one needs in a transistor or quantum device. GO and rGO have high applications in composite material, flexible electronics, and biomedical platform as the surface chemistry is processable and can be adjusted. Both types of graphene have unique advantages relative to each other regarding the application and hence caution is important in terms of its synthesis and integration. Graphene oxide (GO) and then reduced graphene oxide (rGO) was prepared and properties of its layers were studied with respect to structural, optical and electrical properties. Such types of graphene provide adjustable bandgaps and chemical activity, missing in the monolayer and bilayer graphene. Their application is backed by the studies on transparent electronics and flexible devices.^(18,19,20,21) Two-dimensional (2D) graphene is an allotrope of carbon with an atomically thin sheet of carbon as the fundamental unit. Graphene allotrope has a variety of forms, such as monolayer graphene, bilayer graphene, graphene oxide (GO) and reduced graphene oxide (rGO). Each of them has its own characteristic structural and functional properties that allow broad range of application in fields including materials science, electronics and energy storage. This comparative analysis of the various types of graphene uses the modern advancements related to them in order to explain their unique properties and possible uses. The physical properties of monolayer graphene are the properties of a single sheet of carbon atoms in honeycomb lattice. This structure gives the material impressive mechanical, thermal, and electrical characteristics and thus one of the most studied materials over the past years. Monolayer graphene is frequently produced by the chemical vapor deposition (CVD) method on copper substrates; it has been demonstrated that over nucleation density of 30 mm² 1 results in domains that are monolayer with around 2500 of a lateral dimension.⁽²²⁾ Conversely, bilayer graphene is composed with two layers of graphene, and different stacking patterns such as very rare AB stacking, and AA stacking. The difference between these configurations has a great impact on the electronic behaviour of bilayer graphene. As an example, a bilayer graphene and stacking AB exhibit an optical and magneto-optical effect due to the parabolic dispersion relationship.⁽²³⁾ Another graphene derivative is graphene oxide (GO) that contains oxygen-bearing functional groups, changing significantly its properties in comparison with pristine graphene. GO is normally produced through the oxidation process of graphite; the oxidation is done through processes like the method of Hummer (a process that makes it easy to add polar groups). The generated hydrophilicity of GO allows its dispersing in watery conditions with broader uses of GO in coatings, membranes, and composites.⁽²⁴⁾ All the varied usages of reduced graphene oxide lie in its specific electrical conductivity and quantity of functional groups, which allow rGO to exhibit characteristics with a markedly better performance in energy-storing applications, including lead-acid batteries, where it serves as a conductive additive to increase the charge-discharge performance.⁽²⁵⁾ The diversity of these variations of graphene, such as monolayer, bilayer, GO, and rGO, demonstrates the vast opportunities that they provide in the future

technologies. The electronic properties of monolayer graphene and the bandgap of bilayer graphene are unique and the functional versatilities of GO and rGO emphasize the complexity of these materials. With research still unraveling novel ways of synthesis and employments, the contribution of graphene in all its forms is even more likely going to take a critical place in the future of materials science and material engineering. To sum it up, the varieties of graphene, monolayer graphene, bilayer graphene, GO, and rGO, have rather different peculiarities, which have made them applicable for a wide range of applications. The fact that such materials found the application in the emerging technologies, as well as high-speed electronics, advanced energy storage systems, further proves the transformative power of graphene in future innovations. Further studies on any of these forms of synthesis and their applications are bound to bring us closer to realizing and maximizing on the exceptional capabilities of graphene.

Common interface types: metal-graphene, dielectric-graphene, polymer-graphene

Interfaces between graphene, such as metal-, dielectric-, and polymer-graphene, is a system with a rich diversity of physical, chemical and electronic responses. All the types of interfaces have both their own benefits and limitations and these factors tend to decide the suitability of graphene in different areas of technology. These interfaces are important in the fields of electronics, energy storage and sensing and there is a high significance in understanding those interfaces in the advancement of materials in such fields. The nature of interaction between graphene and other materials plays a critical role towards the performance of graphene-based devices, especially at interface scale. Its research on metal and doped graphene oxide (GO) interface shows some interesting phenomena like negative differential resistance (NDR) and charge transfer. The dielectric compatibilities are also mentioned in thin-film synthesis and in the electron paramagnetic resonance test study. As the research results indicate, interfacial qualities define the stability and performance of devices.^(26,27,28)

The metals and graphene interfaces play an important role in electronic devices that use the metals as electrodes or contacts influencing the injection of the charges and the charge carrier mobility. The metal-graphene interfaces can be characterized by a high quality, which is determined by the work function of the metal, gating doping of the graphene and the geometrical shape of the contacts that determines the height of the Schottky barrier and the contact resistance.

FETs and capacitive devices the electric field across the graphene channel can be modified via dielectric layers, creating dielectric graphene interfaces. The common dielectrics used include SiO₂, Al₂O₃ and h-BN but electronic performance in graphene may be degraded by rough surface, charge traps and phonon scattering. Atomic layer deposition (ALD) and self-assembled monolayers (SAMs) are the techniques of surface engineering such that the dielectric graphene interface is enhanced.

To begin with metal-graphene contacts, the contacts quality of these systems has a serious influence on the electronic characteristics of devices. The study conducted by Wang et al. emphasizes the phenomena of interfacial oxidation that occur when the metal is deposited on graphene and especially those metals that tend to oxidize (aluminum and titanium).⁽²⁹⁾ Oxides found at these metal-graphene interfaces have been demonstrated to affect the optical contrast which may in turn affect the transport properties of the carrier. The dynamics of these interfaces are well explained using techniques like the X-ray photoelectron spectroscopy and Raman spectroscopy and this demonstrates the sensitivity of this process towards the deposition conditions including the levels of background vacuum.⁽²⁹⁾ These results are important in the optimization of the manufacturing procedures of devices that use metal-graphene contacts.

Moreover, the role of electrostatics at graphene interfaces cannot be underestimated, particularly when one should consider a graphene-coated metal electrode within an electrolyte solution, which is explained by Saraf et al. Their study of the electrostatics also holds meaningful consequences in the employments such as super capacitors and in electrochemical sensors where the proposed interaction of the conducting graphene and the electrolyte is major factor to determine the effect of the devices. The authors underline the peculiarity of the interfaces due to their complexities in terms of metallic and non-metallic approaches to their study, which depends on the unique electrostatic response imposed by the specific nature of graphene.⁽³⁰⁾ This kind of knowledge will play an essential role in designing electrochemical systems since maximizing the graphene interface will improve the entire energy storage potential. Interactions between graphene interfaces using dielectrics are also ideas of high interest discussed by Loche et al.⁽³¹⁾ The study outlines the role of the aqueous surfaces surface rigidity and metallicity on the dielectric and ion interactions. What is particularly interesting in the research study is the significant differences associated with the way the water reacts to multiple surfaces, which evidences that the dielectric reactions depending on the interface attributes are not trivial and should be taken into account. The results may be crucial in coming up with graphene coating or treating it in such a way that it is compatible with liquid exposures and increase the range of its functions in sensors and electronic devices where the count of liquid interactions plays a substantial role. Along the line of the consideration of the role of the defects in graphene itself, Klein et al. offer evidence to support the idea of how topological StoneWales defects are capable of promoting bonding and electronic coupling at the interface between graphene and metal. As they find, the existence of the defects in the theoretical models may not be considered, which may provide incomplete comprehension of the electronic dynamics at such interfaces. The study offers a fresh approach to design better-performing devices since, possibly by engineering such flaws, better electronic coupling can be achieved thereby leading to better interfacial quality on an overall basis at the metal-graphene interface.⁽³²⁾

Table 1. Summary of Graphene Interface Studies and Key Findings

Interface Type	Materials Studied	Key Phenomena / Findings	Methods	Applications	Reference
Metal-Graphene	Graphene + Al, Ti	Oxide formation at the interface affects optical/electronic behavior	XPS, Raman spectroscopy	Transistors, optoelectronics	Wang et al. ⁽²⁹⁾
Electrochemical Metal-Graphene	Graphene-coated electrodes in electrolyte	Unique electrostatics influence charge storage & sensor response	Electrochemical modeling	Supercapacitors, sensors	Saraf et al. ⁽³⁰⁾
Defective Metal-Graphene	Graphene with Stone-Wales defects	Defects enhance bonding and charge transport at metal interface	DFT simulations, interface modeling	Nanoelectronics, spintronic layers	Klein et al. ⁽³²⁾
Dielectric-Graphene	Graphene on SiO ₂ , h-BN, van der Waals materials	Substrate selection influences mobility, dielectric screening and power efficiency	Transport measurements, dielectric analysis	FETs, low-power devices	Zhang et al. ⁽³³⁾

Dielectric-Aqueous-Graphene	Graphene-water interface with metallic/rigid surfaces	Water structure and ion response differ across rigid and metallic substrates	Molecular dynamics, electrostatic potential	Coatings, sensors	Loche et al. ⁽³¹⁾
Sulfur-doped GO Interfaces	Graphene oxide + sulfur compounds	NDR and charge transfer behavior at functional interfaces	I-V curves, structural analysis	Diodes, memory elements	Figarova et al. ⁽³⁴⁾ Abaszade et al. ⁽³⁵⁾

This may radically change the design of the next-generation nanoelectronic devices in which the efficient charge transport is crucial. Finally, Zhang et al. probe the influence of the effect substrates on the carrier mobility of graphene, urging the role of two-dimensional van der Waals dielectric materials as modifiers in the interface. It is through this study that a route to optimize the behaviour of devices by engineering the intrinsic characteristics of graphene by appropriate choice of interface materials would be made.⁽³³⁾ With their findings, they are able to explore the way to minimize the power consumption in the graphene-based devices, which are becoming overly critical in the regards of the contemporary electronic technologies in which the energy efficiency is a pressing need. To sum it up, all different types of interfaces with graphene, whether made of metal, dielectric, or polymer, present a range of problems and opportunities that should be explored to a significant extent. The differing characteristics of each type of interface portray a distinct interdependency of physical processes through which performance of tools dependent on the exceptional attributes of graphene could be improved. The significance of interdisciplinarity of this study requires the collaborative work between materials science, physics and engineering that helps to take full advantages of graphene in technological applications (table 1).

Graphene-Metal Interface Engineering

The graphene-metal interface will become decisive to the electrical, thermal and structural properties of the graphene-based electronic and optoelectronic devices. The contact chemistry in the case of graphene under the interaction with metal electrodes determines the interacting charge carrier injection, contact resistance, and the Fermi level alignment. Two main forms of bonding are possible at this interface, physisorption (weak van der Waals binding e.g. with Gd, Au or Pt), chemisorption (strong covalent bonding e.g. with Gd, Ni or Co), and they severely influence electronic coupling. Metals physisorbed are likely to conserve the band structure of graphene whereas chemisorbed metals may alter the Dirac cone creating changes in bandgap or a charge transfer effect. The difference in the work functions of graphene and the contacting metal sets the Schottky barrier height that is controllable by as doping or electrostatic gating. Surface cleaning, thermal annealing and interface functionalization are eventually used to reduce contact resistance and enhance carrier injection to accomplish this. Such refined techniques as edge-contacted geometry and intercalation of metals have been found to perform tremendously well electrically than traditional top-contact configurations. Also, the interface buffer layer of 2D materials such as hexagonal boron nitride (h-BN) is used in order to minimize the effect of metal-induced doping and retain the original properties of the graphene. Contact uniformity and reliability can further be enhanced by molecular doping or engineering of metal deposition processes (e.g. e-beam evaporation, sputtering), in which deposition is accomplished under ultra-high vacuum. In general, the semi precise engineering of graphene-metal interface is of vital importance to achieve low power, high speed and scalable graphene electronics. Avoiding the interaction of graphene with other substrates is important, and therefore, great interface engineering methods are needed. It is found that gadolinium-doped carbon nanotubes

and graphene oxide interfaces can be optimized in terms of electron transport under structural adjustments.⁽³⁶⁾ These results also prove that surface functionalization and nanostructure engineering are important in high-performance and stable interface in graphene-based devices. Graphene and its various applications in diverse applications like electronic and thermal management gadgets have put the field of graphene and metal interface engineering under intense scrutiny in the recent past. The key to the performance of graphene-based devices is the coupling of graphene and metal contacts that not only affects the electronic properties like contact resistance but also thermal performance like thermal conductivity and ability to dissipate heat at high frequencies. These interfaces are important in nanoelectronics since a deep grasp of their features is essential to be able to realize the full potential of graphene. In order to investigate the steps that could be taken to improve the electricity and thermal connection between graphene metal contact, different junction geometries have been tested out. Ohno et al.⁽³⁷⁾ differentiated between the two types of contacts (surface and edge) on graphene-metal interfaces and claimed that edge-contacted interfaces show significantly different contact resistances in comparison to surface-contacted interfaces, because of the bonding distance. This realization presents opportunities of radical design approaches in graphene devices where one can consider edge contact in reducing resistivity, and in a sense, overall device characteristics. In continuation of the reports on contact resistance reports, Zhai et al.⁽³⁸⁾ ventured into the study of the thermophysical process of thermal transport at two-dimensional interfaces, noting that the role of recognizing the electronic and phononic properties of thermal transport could not be overstated between such systems. Their results support the earlier study of the concept of interface thermal conductance (ITC) in metal-graphene systems in that the thermal effects between the metal especially by electrical means do not play much role in the overall performance of thermal transport at these interfaces. This explanation reiterates the dominance of phononic transport in such cases and it is thus important to optimize the thermal coupling options. Conclusively, the engineering of graphene-metal interface is a complex issue that incorporates thermal and electronic rationales. All these studies emphasize the relevance of interface properties, with new geometrical strategies like edge contacts and deployment of alloys with materials and methodologies becoming of importance to ensure improvement of device performance. Further studies that are required in this field should enable the creation of high-efficiency graphene-based electronics that would serve the growing requirements in contemporary technologies.

Graphene-Dielectric Interface Stability

The possible application is that the graphene-dielectric interface is essential in ensuring reliable performance of field-effect transistors (FETs), capacitors, sensors and other electronics devices. Subsequent to this interface, a number of thematic occur based on the roughness of the surface, charges trapped in the surface, dipole-formation, and remote phonons scattering, which have the capability of lowering the mobility of carriers in graphene. Common dielectrics include silicon dioxide (SiO₂), aluminum oxide (Al₂O₃) and hafnium oxide (HfO₂) and the dielectric elements create surface imperfection and charge traps that are incompatible with graphene. Charges trapped on the dielectric surface may result in potential hysteresis and Dirac point shift in the graphene which results to unreliable switching behavior and bias stress instability. Stability of the interface is enhanced by means such as atomic layer deposition (ALD), typically with prior seeding layers or surface functionalization (e.g. with NO₂ or polymers) in order to guarantee uniform growth of the dielectric. Hexagonal boron nitride (h-BN), a chemically inert and atomically flat 2D dielectric material, makes a perfect and ideal substrate, because it acts as a minimal charge scattering substrate, and also retains the high mobility and the structural integrity of graphene. Thermal annealing, chemical passivation and self-

assembled monolayers (SAMs) are interfacial engineering methods that have proved useful in defect reduction and dielectric compatibility. Delamination or cracking due to mechanical strain and temperature difference mismatch between the dielectric and graphene is also possible and therefore the material selection and device architecture should have these effects in mind. Also, the environmental stability (e.g., Not affected by humidity, change of temperature) can also be made better by encapsulation using stable dielectric materials or multilayer passivation. Effective graphene-dielectric junction design guarantees predictable device functioning, high carrier electron mobility and a long life time of devices in high end electronic devices.

Contact resistance is also very important in determination of the efficiency of electron transport at the graphene-metal interface. The fact that the negative differential resistance (NDR) in the structures of sulfur-grafted graphene oxide was observed also indicates the quantum transport capability of this interface.⁽³⁴⁾ Gadolinium doping is one of the new technologies that are successful in the improvement of interfacial compatibility and the attainment of stable low-resistance graphene-metals contacts.⁽³⁵⁾ It is impossible to overestimate the role of interfacial bonding to enhance the strength of the graphene-dielectric interface. As an example, research articles have found that when a low-dielectric constant surface, e.g., self-assembled peptides is placed on graphene, the capacitive sensing performance improves significantly with increased interface bonding and does not sacrifice the dynamic performance of the material.⁽³⁹⁾ This is important as this will make the entire structure more stable and able to transfer the energy easily across the interface and this becomes significant especially in case of applications such as flexible electronics where mechanical strain cannot be avoided. As an example, growth of the particle size in the polymer network was found to be associated with enhanced thermal energy dissipation in the graphene to dielectric interface, which directly establishes the interface stability with the mechanical qualities in the composite material. This concept is important to explain why graphene properties are not the only features that define the thermal and mechanical stabilities but the dielectric composition of the composite.⁽⁴⁰⁾ An interfacial property can also be enhanced through the bond between nanostructured materials in the polymer matrices e.g. by the addition of layered double hydroxides (LDH) and graphene in polyvinyl alcohol (PVA) composites. The entire dielectric constant of the composite is also naturally higher as a result of the artificial increase in polarization at the interface, and this lowers the polarization effect of the graphene-dielectric interface through the addition of more electric dipoles per unit volume. The development of more polar interactions at the interface and the modified dielectric characteristics attains the importance of the design of the composites in producing stable and reliable graphene interfaces. In short, it can be seen that to stabilize the graphene-dielectric interface, a multi-pronged strategy needs to be adopted that includes enhancement of material properties, enhancement of interfacial bonding, fine tuning of fabrication process, and role of environmental factors at the interface needs to be understood comprehensively. The future of very stable and useful graphene-dielectrics composites is being pushed towards reality with emergent new methodologies and materials innovations, the next frontier in electronic uses. Summing up, the combination of many factors, both interrelated and unrelated, defines the stability at the graphene-dielectric interface, which depends on properties of a dielectric material, subsequent manufacturing techniques, and environmental factors. Further interdisciplinary research between materials scientists, physicists and engineers will be required to tease out the mysteries of these interfaces. It is only in such combined effort that gains can be achieved towards sustainable and reliable high-performance electronic applications.

Graphene-Polymer/Organic Interface Engineering

Interfaces graphene or polymeric or organic materials lie at the core of applications in

flexible electronics, biosensors, composite and energy devices. To maximize adhesion, charge transfer, dispersion and mechanical matching of the two elements, graphene is sought to be improved along with polymer via graphene-polymer interface engineering. The almost smooth, hydrophobic surface and robust 1π - 1π interactions of pristine graphene frequently exhibit unfavorable interfacial binding with polar polymers, wherein surface modification is required. In the field of material science, specifically in the engineering process of graphene-polymer interface, significant developments have been made in terms of the analysis as well as maximization of the interactions that take place at the atomic and molecular scale. Graphene, which is a two-dimensional material that is renowned to possess exceptional mechanical, electrical, and thermal conductivity, has been used as a flexible medium in the combination with polymer in order to develop high-tech materials that can be utilized in a variety of industries such as in the electronics, sensor, and nanocomposites domains. The significant direction of the further improvement of the performance of graphene-based composite materials is the understanding of the nature of the interaction of graphene and polymers and the capabilities of these interactions to fine-tune the adhesion properties and mechanical stability of composite materials. Electronic properties of interface of graphene and dielectric materials affect stability and performance of electronic devices directly and especially because of trapped surface charges. EPR spectroscopy on the gadolinium-doped graphene oxide produced provides the information on the spin states and charge carriers reactivity in an interfacial environment.

⁽³⁶⁾ These studies reveal that dielectric-graphene interfaces are stabilizable such that they can be utilized in energy efficient and long-lasting nano dimension electronics. Graphene surfaces can be seen to have defect engineering come up as one of the workable solutions in greatly improving the adhesion at the interface when graphene is used with polymers. Kumral et al.⁽⁴¹⁾ tested the adhesion energy of pristine graphene through experiments, reporting a value of 7 mJ/m² when bonded to polydimethylsiloxane (PDMS), whereas defect engineering could increase the value of the adhesion energy to about 38 mJ/m². The changes in adhesion with functionalized graphene reflect the effects of the heterogeneity of defect-engineered interfaces, making it apparent that optimizing interface design to a particular application need employ a customized interface design. The high adhesion energies may be converted into a better resistance to dynamic failures of graphene-based composites subjected to mechanical stress, which is of essence to life and stability in real settings. Also, the importance of interfacial mechanical properties in composites could be evidenced with the help of the study of Zhang and Yi-Long which examines the mechanical behavior at the interface of graphene and titanium with the help of computational modelling. They demonstrate the intricate dynamics of such a multilayer interface, using simulation to forecast the mechanical benefits maintained at nanoscale interfaces, which gives the needed understanding to the design of superior performing composite materials.⁽³³⁾ These kinds of simulations can be used to predict and evaluate mechanical integrity of composite systems, which translates into better methods of interface design which are elastic to different stresses. To sum up, the detailed discussion of graphene-polymer interface engineering allowed disclosing a complex view of the improvement of relationships between the capability and applicability of the graphene-based materials. Recent developments in material research through interfacial adhesion, van der Waals force exploitation, and the development of new surface modification techniques will culminate in far-reaching implications in a number of high-technology applications. Further months of both intra-disciplinary and inter-disciplinary research will become essential in the efforts to extend the limits of just what is possible with graphene-polymer composite materials to keep them aligned with the high-performance standards of contemporary technology.

Emerging Applications Requiring Interface Control

The graphene-polymer or organic interface is influential to the growth of hybrid flexible and biocompatible devices. Hydrophobic and Hydrophilic reactions of nanostructure surfaces are the major factors of mechanical fit and electrical match.⁽⁴²⁾ These interfacial characteristics lay the basis of maximizing the strength and performance of the graphene-polymer composites in real life. The interface control field is one which is fast changing requiring the investigation of new applications that go beyond existing paradigm of interaction. Conventional human-computer interaction (HCI) design methods, whose principle is largely based in desktop contexts, have been revealed as unsatisfactory in accommodating the modern mobile and cloud-based applications. Mohammed and Karagoylulu explain that the design principles of the standard HCI focus on task design, needs of the users, as well as functionality of systems do not fit the dynamic nature of mobile applications, which allows location-based services. Based on their results, M. Mohammed⁽⁴³⁾ propose the idea that established paradigms employed in desktop interface design no longer work in a mobile environment and there is an urgent need to adjust HCI framework in tandem with the rise of technologies.⁽⁴³⁾ Computing Bujack et al.⁽⁴⁴⁾ describe the Simplified Interface to Complex Memories (SICM) of the Exascale Computing Project that offers solutions to the issue of controlling complex memory hierarchies. The project can provide better control and configurability of the different memory technologies by the establishment of standard interfaces that enable discovery and sharing of data. This is an innovation that plays a key role in enabling the performance trade-offs that are necessary in high-performance computing applications, which are further challenging the significance of sufficient interface control in the emerging computing environments.

Energy storage and conversion (e.g., supercapacitors, batteries)

Nanomaterials of graphene have become popular applications in energy storage and conversion devices and interface engineering plays an important role in the manipulation of ion mobility as well as electronic conductivity. The results of the research of gadolinium-doped carbon nanotubes and functionalized graphene structures show improvements in thermal and electrochemical characteristics of such materials in supercharging cap and battery electrode design. Moreover, the synergistic effect between graphene and MXenes emphasizes the corresponding principle of the stable interfacial design in enhancing the capacitance and cycling performance.⁽⁴⁵⁾ Graphene in materials has been found to be a possible component of an energy storage and energy conversion system for its superior electrical conductivity, a large surface area, and chemical tunability. Graphene is a good electrode material in supercapacitors that permits rapid charging discharging processes and high-power density by electric double-layer capacitance and pseudo capacitance capabilities. Composite electrodes may include Graphene oxide (GO) and reduced graphene oxide (rGO) to enhance ion accessibility and structural stability, commonly as a combination with conducting polymers or metal oxides. Graphene-based 3D formation (aerogel, foams) has the advantages of improving electrolyte diffusion characteristics and supporting mechanical stiffness, which is very critical to flexible and wearable energy applications.

Graphene is used as a conductive additive or active material in anode and cathode of the lithium-ion batteries (LIBs) to improve electron transport and provide cycling volume buffer. Within anodes, a graphene silicon compound is especially promising, because the graphene component can absorb the silicon as it swells up, prevent the formation of cracks, and effectively maintain the structural integrity of the compound. In the case of metal air batteries, catalysts of graphene materials have been used as economically viable and long-lasting replacements of precious metals such as Pt or Ir to enhance oxygen reduction and oxygen evolution reaction (ORR/OER). Graphene disperses catalytic nano-particles in fuel cell, enhances durability and

facilitates the transport of protons or electrons (depending on functionalization). The contact between graphene and electrolytes (liquid, solid or gel) should also be engineered to both drive ion transfer and reduce side reactions and improve device durability. Altogether, the energy storage and conversion systems incorporating interface-engineered graphene produce better performance parameters, e.g., capacity, cycle life, energy density, preparing the ground of a next-generation sustainable power technology.^(46,47,48)

Graphene-based quantum devices

The peculiarities of the electronic characteristics of graphene, massless Dirac fermion and a high carrier mobility, create an excellent marriage of opportunities to develop a completely new generation of quantum devices. The atomically thin and two-dimensional property enables it to exhibit unprecedented control over the charge transport, spin, and the valley degrees of freedom, which are the building blocks of the quantum information processing. QDs which effectively trap charge carriers on a nanoscale volume, have a discrete energy structure and quantum confinement effects which presently find application in single-electron transistors and quantum sensors. Twisted bi-layer graphene at the so-called magic angle exhibits moiré superlattice effects resulting in correlated electron behavior and superconductivity and is a frontier material enabling quantum simulation. Josephson junctions Graphene-based Josephson junctions, where graphene is inserted between superconducting contacts, exhibit coherent quantum transport and may be applicable in superconducting qubits. Graphene has a high carrier mobility, spin coherence and band-structure tunability that is valuable in the endeavor of integrating it in quantum devices. The Gadolinium-doped carbon nanotubes have exhibited immense photoconductive properties and electron paramagnetic resonance technology, which is favorable in quantum transistors and single electron applications.^(49,50) The present results are important to understanding how interface interactions can be customized to increase coherence and control in graphene-based quantum systems. In valleytronics, the unique K and K' valleys within momentum space in graphene can also be used as binary quantum states to encode and process information, and this represents a new avenue beyond charge-based computing.

Integration with CMOS technology

A major breakthrough towards scalable, high-performance and energy efficient electronic systems is by integrating graphene, with complementary metal-oxide semiconductor (CMOS). Due to its exceptional carrier mobility, thermal conductivity, and the flexibility, graphene promises to be a hot candidate to break the performance barrier in traditional silicon-based CMOS. Graphene and CMOS combine to hold out the promise of high speed and low power electronic components, but this needs a strong thermal and structural integrity to be achieved at the interface. The conductive porous carbonates extracted by the biomass, e.g. hemp fibers, exhibit promising thermal control characteristics that can make it compatible with CMOS fabrication processes.⁽⁵¹⁾ Further, electrochemically modified carbon materials of walnut shells emphasize the significance of a thermal activation and surface functionalization to be used in a large-scale setup.⁽⁵²⁾ Perhaps the biggest application is in high-speed field-effect transistors (FETs), where graphene in principle can be used as a channel material because of its ultrafast carrier dynamics and short gate delay. Nevertheless, graphene has a zero bandgap, which complicates its use in the digital logic; attempts to introduce a bandgap either by stacking in bilayer, fabricating nanoribbon, or engineering substrates are a vigorously investigated topic. Graphene also offers the potential of high-performance inter-connection material in CMOS circuits with reduced resistive losses and local heating in high density nanoscale structures.⁽⁵³⁾ Graphene has linear dispersion and much higher cut-off frequencies (≥ 300 GHz) compared to silicon and therefore linear graphene may be used as a wideband amplifier, mixer or detector in analog and RF

(radio frequency) applications far beyond silicon. Even on the sensors area, GrapheneCMOS is promising, graphene can be used as an extremely sensitive active layer, and the CMOS platform offers an indispensable signal processing and data transmission infrastructure. However, Hybrid integration methods either involves CVD grown graphene transfer onto processed CMOS wafers or co fab using compatible material and processes.⁽⁵⁴⁾ The issues of thermal budget compatibility, interface contamination and area uniformity (large scale) have to be overcome to obtain an adequately reliable CMOS-graphene co-fabrication. Effective incorporation of graphene with CMOS based technology brings into ways multifunctional chips incorporating logic, memory, sensing, communication into one low powered and high-speed chip.

CONCLUSIONS

Briefly, this chapter has identified the intrinsic properties of graphene and put an emphasis on the crucial position of the interface engineering in realizing its full potential in a wide range of applications. In a careful systematic study of the interaction of graphene with different materials, i.e., metals, dielectrics and polymers, we have shown that the device stability, functional performance and charge transport depend directly on the quality of the interface. It was observed that the interface-specific tactics, chemical modification and structural optimization, can be discussed as good recommendations when it comes to enhancing compatibility and reliability in practical devices. Moreover, the recent developments of energy storage, quantum, and CMOS integration application show that precision interfacial control is essential to address the future technology requirements. As graphene as a material morphs further beyond a lab material to the heart of next-generation technology, its interfacial properties will be a critical parameter to introduce new generations of improvements in electronics, sensor and energy systems.

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Part V

Smart, AI-Driven, and Sustainable Engineering Systems



Chapter 16

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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AI in Structural and Construction Engineering

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ABSTRACT

The creation of the artificial intelligence (AI) became a remodelling instrument in structural and construction engineering, offering the new ways of analysis, design, and management. In the simple engineering course, machine learning, deep learning, and optimization algorithms can be deployed to make a decision based on the data with AI. In order to get structural design and analysis, AI increases the accuracy of load prediction, stress distribution and structural behavior modeling. With more precise and faster results, complex algorithms are used with the finite element analysis. The construction materials industry is one of the areas that will be assisted by AI in predicting the mechanical properties, optimization of mixes, and sustainable development of materials. AI makes its entry into the construction management to ensure a successful planning, resource allocation, and mitigation of risks and integration with BIM systems. The concept of structural health monitoring can be enhanced with the assistance of AI sensors data analysis to identify the initial damages and anticipate the maintenance. As AI brings about robotics and automation, the construction industry is revolutionizing with autonomous drones, robotic systems, and technologies along with 3D printing. The result of such developments is a reduction in the degree of human error, enhanced efficiency, and enhanced safety. Despite the inconveniences of the data quality, transparency, and the ethical issues, AI continues to expand the engineering sphere. The future trends reflect the increasing association of the digital twins with sustainable construction, as well as AI, as the bedrock of the contemporary engineering.

Keywords: Artificial Intelligence; Structural Design; Construction Materials; Health Monitoring; Robotics; Automation; BIM; Digital Twins.

INTRODUCTION

One of the most potent technologies that will transform the engineering spheres in the future is called artificial intelligence (AI). Efficiency, precision and lifecycle sustainability of a project can be improved by using AI in construction and structural engineering. The ancient approaches can be limited in data processing, risk control and optimization, which AI can execute with the assistance of complex algorithms. The recent direction of more intensive application of machine learning, deep learning and data-driven models has shifted the architectural analysis, design and construction management. Besides that, AI assists in the forecasting features that enhance the infrastructures security, cost-efficient operation, and reliability. AI is finding its way in the construction industry, especially with the increasing use of

robotics in the sector, automation and digital twins. The given chapter will discuss the basic, practice, challenges and future of AI and practices of its application to structural and construction engineering. One of the most critical spheres is biomedical engineering that can be improved with the assistance of AI due to the power of diagnostics and personal approach. To mention but a few, AI algorithms will get an opportunity to enhance the quality of radiological diagnosis with favorable image processing algorithms to detect the multiple complex patterns and anomalies that can be ignored by a human radiologist and advance the quality of care and health of the patients.⁽¹⁾ This innovation enhances the delivery procedure within the healthcare sector and streamlines the healthcare systems and is a manifestation of aligning the healthcare requirements with technological enhancements. Furthermore, AI is also making its way into the sphere of education, and especially engineering courses. Maybe, AI will assist in simplifying the teaching process and creating smart educational tools and methods that can empower learners. It can not only help to find answers to one of the engineering issues but may also improve the practices of instructions.⁽²⁾ Educational applications of AI can offer educational experience that is personal and will create a scenario where it will be possible to keep up with individual students, and, therefore, enhance the output of the educational process, on the whole, in the sphere of engineering. This is equivalent to the fact that structural engineering of the flexible models is required, which is capable of supporting the complex structures and loading conditions. And continuing on the relevance of AI in structural arrangements, any type of engineering undertaking is simplified through the software that streamlines the design procedure. The algorithm of the NSGA-II that Wang et al. applied to optimize the centrifugal pump features may be seen as an example of the strategy that can be effectively undertaken to enhance the features of the structural parts (stability and efficiency) which is one of the characteristics of the performance.^(3,4) Therefore, the further evolution of AI-based optimization-based tools in the sphere of structural engineering may be linked with the current efforts to make the performance of the systems in the conditions of the large range of loading scenarios and with the subsequent enhancement of their service life. Among the most evident positive aspects of AI in the construction sector, one can also note the possibility to optimize the effectiveness of different stages of the material use. The inverse design can also be applied using AI technologies to maximize a desired property of an inverse designed material. It would be based on the need to identify the most appropriate material compositions that can be utilized in special needs in special use and, consequently, improve the output and sustainability of the materials applied to the same.⁽⁵⁾ Moreover, the AI-related solutions were also discovered to improve the lifecycle management, in which the professionals are enriched with the control of the time of a schedule, cost-effectiveness, and the sophisticated safety monitoring working on a civil engineering project.⁽⁶⁾ Artificial intelligence (AI) is another evolutionary technology, which is making its way into structural and construction engineering. The existing design and management strategy usually entail dealing with big data and moving systems. With the help of AI, one can learn with data, process new circumstances, and make optimized judgments. The later findings of the carbon-based nanomaterials confirm the significance of the more complex modeling to the prediction of the material and structure behavior.^(7,8,9) Due to this, AI is not merely another kind of technology, but a need in the modern-day construction. In addition, AI implementation within the construction management supports the project schedule and budget management, not to mention quality and safety. According to Xu and Guo, the possibility to regulate schedules and monitor health has led to the application of AI to the process of simplifying various processes to increase the resilience and safety of the infrastructures created. The performance of the project with the help of upgraded data analytics and real-time monitoring is one of the primary spheres where AI can be helpful. Liu highlights the point that the Building Information Modeling (BIM) can be used in the development of the smart site safety management system because of opportunities of its connection with the Internet of Things (IoT) technologies. This system

divides the site safety management regarding various dimensions, therefore, making the risk management and safety completer and more efficient. Thanks to the help of data analytics, the project managers will manage to set a realistic standard, make smart decisions and, ultimately, enhance the level of management in the long-run, which will, in its turn, be disproved in an empirical manner, since the idea of smart technologies being not just a reality, but also extremely versatile in the construction industry.⁽¹⁰⁾ Zhang study lays emphasis on the BP neural networks to ascertain the probability of structural collapse of the scaffolding systems. Through the use of the wireless strain sensors and the implementation of a finite element analysis (FEA), the presence of a robust framework that would be able to aid the process of discovering instability modal of the systems of structural system will be uncovered.⁽¹¹⁾ The benefits of integration are that early failure detection is possible and enhancing the safety of the construction situation. Besides it, Vaghela and Bayandor pay attention to the application of machine learning algorithms in SHM of sheet metal assemblies. Their experiment shows that it is beneficial to train custom neural networks on the data presented in an FEA simulation, which covers the different assembly processes, like riveting and welding. Not only is this approach economically friendly, but furthermore, it has been used as an indicator of a new direction of even greater diagnostic capabilities in the case of structural health monitoring applications.⁽¹²⁾ These developments are the bright stars of what machine learning can do to simplify the process of collecting data, thus, making the outcomes of the monitoring more genuine. The technologies will play a crucial role in the successful migration of the automated spaces within the buildings where manual roles can be incorporated into the already developed ones.⁽¹³⁾ Not only the issue of the human manpower replacement is linked to the application of robot system, but the betterment of the man-robot collaboration to increase the productivity and the construction time. Such possibilities can also be related to the emergence of the Internet of Things (IoT) technologies that could enable the robots to feel and respond in the surrounding environment in a productive manner that the automated working process could be simplified.⁽¹⁴⁾ As an example, such systems will be efficient in controlling the construction situation as they will be able to determine the most significant parameters mentioned in the example, which are the steel bar layout and concrete quality that will be at the center of maintaining the already discussed norms and construction safety.⁽¹⁵⁾ This has been a combined practice that has been strategic given the trend of prefabrication and modular construction that ultimately produces more customization and automated construction practices.⁽¹⁶⁾

Fundamentals of AI in Engineering

The use of calculational devices to replicate the decisions and the learning processes of human beings is known as engineering Artificial intelligence. The most frequently used ones are machine learning, deep learning, natural language processing, and expert systems, all of which make the analysis more accurate. AI in the engineering field is a field of a lot of dependence on quality data gathered through simulations, experiments or real-time monitoring systems (table 1).

Through such datasets, it is possible to come up with predictive models that can capture the trends and generate successful predictions. Neural networks are the optimization algorithms, genetic algorithms, and are often used in solving some of the engineering complex problems. The application of AI in structural engineering has the potential to automate computationally demanding components of a project (e.g. design optimization of many variables). Besides, the AI-enabled software is also released to assist the engineers with the design, testing, and validation of the models on the software platform.

Table 1. Fundamentals of AI in Engineering

Concept	Description	Application in Engineering
Machine Learning (ML)	Algorithms that learn patterns from data to make predictions or classifications	Predicting loads, stresses, and performance of structures
Deep Learning (DL)	Subset of ML using neural networks to model complex nonlinear relationships	Modeling nonlinear structural behavior and material properties
Expert Systems	Rule-based systems that mimic human decision-making for problem-solving	Providing guidance in construction management and design validation
Optimization Algorithms	Techniques like genetic algorithms and neural networks to solve complex problems	Optimizing structural design, resource allocation, and energy efficiency
Data-Driven Decision Making	Using large datasets to generate insights, forecasts, and guide design decisions	Supporting risk assessment, planning, and real-time decision support
Integration with Engineering Tools	Embedding AI models into CAD, BIM, and simulation software for enhanced use	Assisting engineers in design, simulation, and structural health monitoring

The concepts of AI in engineering sector, in their turn, are substituting a new paradigm of automated decisions and autopilot. The application of Artificial Intelligence (AI) in automating engineering tasks, creating better decisions, and additional system efficiencies have also remodeled different engineering fields. It is not only limited in biomedical engineering but can be applied to neural networks and wireless communications technologies among others, which demonstrate its versatility and the ability to transform the world. It has transformed the way the researchers process the neural data by using the AI and more specifically machine learning (ML) in neural engineering. This data requires smart designs, which are difficult to identify in the traditional system of analytic work, but machine learning is equal to the task, and it is absolute to the development of the profession. As the ML approach is more broadly applied to the field of neural engineering, it is important to assure high-levels of research validity and reproducibility to make the results and the manner in which they can be applied to the field more plausible.⁽¹⁷⁾ These principles are needed to guarantee proper integrations of the AI technologies into the neural engineering studies. The other field that AI has influenced is communication engineering, and deep learning models are becoming a potent signal processing tool. These models are effective in non-linear mapping of large complex signal environment like a large MIMO (Multiple Input Multiple Output) system. The systems also make it possible to retain the high-performance levels even under the problematic conditions because of the communication technologies and AI and extend the scope of the sphere of the wireless communication application.⁽¹⁸⁾ Machine learning, deep learning and data-driven systems on which AI engineering is founded, have the potential to be predictive and optimizing. The trained neural network can help to estimate the structural loads, the degradation of the materials and system failure based on the engineering dataset.⁽¹⁹⁾ The construction management and hero allocation of the construction decisions have been applied using expert systems. The examples of the computational tools, applied to functionalized nanomaterial, may include that of the predictive research which was later validated by the experimental evidence.^(20,21,22,23) Just like materials informatics, AI engineering can automate the process and make it less expensive in terms of trial and error. Digital-based devices, i.e. BIM and IoT also use AI, which enhances the application of AI to real-time monitoring and adaptive control.⁽²⁴⁾ Finally, the AI and engineering partnership is not a mature area and it is still in the baby stages. The possibilities of AI in enhancing better systems, self-driving car and material discovery, carry grave concerns on safety and performance guarantees. The necessity of finding a solution to those issues is one of the most important challenges that should be

taken into consideration in the future to make the potential of collaboration between AI and engineering-related operations to be utilized to its fullest.⁽²⁵⁾ As it has been noted, research and development will be required in the future to ensure that AI applications are streamlined in the different engineering sectors. To sum up, the application of AI in the engineering sector can not only assist in improving the current system and strategy, but also a new field of research and implementation in other spheres reveals itself. The possibilities of the AI in health care sector, education, neural analysis, communication, engineering industry, and so forth, are enormous. Designing complex structures optimized to a particular purpose, including biomechanical application, has been among the most useful fields where AI has contributed. A different experiment conducted by Omigbodun et al.⁽²⁶⁾ demonstrates that lattice structures such as Gyroid design can work, although they can be optimized with AI to maximize the mechanical properties (tensile and compressive strength) when implemented as medical implants. The designs will be more efficient and thermo-stabilized since the reduced Graphene Oxide (rGO) and calcium hydroxyapatite (cHAP) are advanced materials that will be incorporated in the designs as per their literature. Moreover, AI can be used in material science a science of high dimensional and multifactorial data, which is a crucial central process to efficient biomaterials. Jiang and others confirm by pointing out that through the assistance of AI, hydrogel, precision in drug-delivery systems would become possible. Their results manifest the usefulness of machine learning in the de-correlation of multi-dimensional interactions between the material structure and structural performance among other factors that warrant the use of machine learning in structural and biomedical engineering.⁽²⁷⁾

AI for Structural Design and Analysis

The use of AI in the structural design and analysis has transformed the accuracy and speed of the visual engineering calculations. Through the AI-based models, engineers are able to predict the behavior of structures when the load on the structure varies most accurately. Machine learning has been used to optimize the design parameters, which include the use of materials, load distribution and structural stability. Deep learning can also capture more non-linear behavior of complex structures (table 2). The AI-based finite element analysis saves on a significant amount of time but is precise enough to compute the large-scale projects. Moreover, AI can help in the creation of hybrid solutions, which are founded on conventional and information-driven analytic algorithms. This type of integration gives a tradeoff between theory validity and application. The result is that now the amount of designs engineers can deliberate is increased at reduced time lines and eventually efficiency and safety of construction works is achieved. The artificial intelligence (AI) embarked in designing and the analysis of the structure is a drastic revolution on the way engineering is being practiced. The entry of AI algorithms in other sub domains of structural engineering has resulted to improved design, construction management and development of certain new materials. The applications of AI to efficiency and future-proofing civil infrastructure are quite significant in multiple publications that mention that it can be implemented on a wide scale. In addition, AI can be used to design optimization and structural health monitoring (SHM) of civil engineering projects lifecycle. Xu and Guo provide a broad overview of the application of AI in civil engineering in streamlining the procedures involved in the design of all phases within the development of an infrastructure.

They demonstrate how AI does not only strengthen the design schemes but the construction management practices as well because it helps to find innovative solutions that can adequately address the already existing, engineering-related issues.⁽⁶⁾

Table 2. AI for Structural Design and Analysis

Aspect	AI Approach	Benefits
Load Prediction	Machine learning models trained on historical and simulated data	Improved accuracy in forecasting structural responses
Stress and Strain Analysis	Deep learning algorithms for modeling nonlinear behaviors	Better understanding of complex material and structural behavior
Finite Element Integration	Hybrid models combining AI with finite element methods (FEM)	Reduced computational time with reliable outcomes
Optimization of Design Parameters	Genetic algorithms and reinforcement learning for parameter tuning	Efficient resource use and cost-effective design solutions
Generative Design	AI-driven generative design creating multiple design alternatives	Innovative and sustainable designs with multiple options
Risk Assessment	Predictive analytics to identify potential failures and risks	Enhanced safety and proactive mitigation of structural failures

The potential of machine learning procedures in resolving the issue of real-time structural problems, including aeolian vibrations on transmission lines, are tremendous. Studies conducted by Jia et al. reveal that the two approaches can be successfully applied to anticipate failures and make structures more resilient, which are the supervised learning and the deep learning. This is one of the indications that AI may be used to overcome the gap between the abstract knowledge of the realm of engineering and real, practical knowledge.⁽²⁸⁾ Predictive modelling and simulation with AI have revolutionized the structural design and analysis. They are the predictive properties of the machine learning-based methods of predicting the load reactions, the stress fields, and the non-linear material reactions.^(29,30,31) Direct direct integration of the deep learning and finite element techniques makes computation processes quicker. Generative design with AI is provided to engineers with the choice of a tradeoff between costs and performance. The possibility of projecting the structural and electrical behavior conditioned by the use of computational tools is substantiated by the studies on carbon nanotubes and graphene oxide.^(32,33) These applications suggest the relationships between AI-inspired model-based developments and materials. All in all, the design results can be made safer, more efficient and stronger with the help of AI. Finally, according to the scientometric survey conducted by Sood, there is a growing significance of the ICT-on-the-rise-based data mining tools in the structural design and performance measurement. The study of machine learning models will be instrumental in transforming the approach on how the building is designed, constructed, and serviced as well as revolutionizing the accepted way of doing things in the field of civil engineering.⁽³⁴⁾ To conclude, in a word, AI is transforming structural design and analysis processes in a sense that, they can maximize on materials, predictive maintenance, and advanced model process, which allow to optimize the efficiency and overall performance of the process across different engineering fields.

AI for Structural Design and Analysis

Generative design beyond the conventional structural computations are also other uses of AI in the field of structural engineering. Generative design tools that rely on artificial intelligence can be used to automatically produce a range of design solutions, based on specified constraints and objectives. These designs are also evaluated, according to the performance, cost and sustainability, and the engineers are able to choose the best solutions. Besides this, the principle of reinforcement learning is also emerging so as to maximize adaptive structures that can react dynamically to external forces such as wind or earthquakes. AI-based simulations help identify the vulnerable sectors in constructions before they are constructed and this lowers the risks and costs involved. The technologies contribute to the life-cycle assessments as well, ensuring

that the long-term durability and the maintenance are put into consideration when designing (table 3).

Table 3. AI for Structural Design and Analysis		
Aspect	AI Approach	Benefits
Generative Structural Design	AI-driven generative design tools producing multiple structural options	Explores innovative solutions beyond human imagination
Adaptive Structures	Reinforcement learning for structures that adapt to external loads	Creates adaptive and resilient structures with dynamic performance
Life-Cycle Assessment	AI-enabled life-cycle modeling for durability and sustainability	Ensures long-term sustainability and reduced maintenance costs
Multi-Objective Optimization	Machine learning and genetic algorithms for trade-off optimization	Balances cost, safety, sustainability, and efficiency simultaneously
Seismic and Wind Response Prediction	Deep learning models analyzing structural responses under dynamic loads	Improves resilience against earthquakes and extreme weather conditions
Integration with BIM/ Digital Twins	AI models embedded into BIM and digital twin frameworks for real-time analysis	Enables continuous monitoring and real-time optimization of structures

Besides the classical modeling, AI is now applied to generative modeling, adaptive structures and life-cycle modeling. The reinforcement learning enables structures to change dynamically in response to external forces like seismic forces and wind.⁽³⁵⁾ The deep learning simulations can be used to predict long-term prediction of the durability and performance of the material in different environmental conditions. Graphene oxide and sulfur-doped materials adaptive behavior has been investigated and can be related to the AI-based optimization models.⁽³¹⁾ One of the promises of the AI-based life-cycle analyses is the reduction of the maintenance and sustainability cost. At any given time, continuous monitoring and optimization can be practiced in the implementation of AI on BIM and digital twins carried out by the engineers.⁽³²⁾ In this, AI introduces the element of structural design to the proactive and adaptive and future-proof engineering. Therefore, AI is not a support technology, but a component of the innovation in the building design. The use of Artificial Intelligence (AI) in the civil engineering field can be implemented as AI application in the building design and analysis field and can revolutionize the industry. The ability to predict the forces on the members of structural elements (steel tubes) is one of the most significant innovations. More recent developments are based on the fact that machine learning (ML) algorithms can analyze and predict structural health monitoring (SHM) data and forces on members, and have been shown to be effective in comparison to more conventional approaches. Li and Chung provide data concerning the use of AI in such applications, as this is an indication that the generation of massive amounts of numbers, the accelerations in the processing power, and the development of more advanced neural nets and machine learning algorithms are all intriguing phenomena in the field of structural analysis and design.⁽³⁶⁾ Lastly, large-scale redesigning and analyses can also be redesigned with the help of AI. The predictions and optimization machine learning tool can enable the engineers to maximize the accuracy and validity of structural analysis. It is also noticeable that these smart systems will be shaping the future of civil engineering as it will aid in overcoming the maze of the modern designing complexities.

AI in Construction Materials

The AI implementation in the construction material engineering has transformed the idea of designing, testing, and the use of materials. Mechanical properties such as strength, elasticity and durability may be predicted with high accuracy using AI-based predictive models. When it comes to concrete technology, AI could be utilized to assist in streamlining the mix proportions to produce the best performance and with minimal impact on the environment. When it comes to steel and composite, AI algorithms can find defects, estimate fatigue life, and suggest an improvement procedure (table 4).

Table 4. AI in Construction Materials		
Aspect	AI Approach	Benefits
Concrete Mix Optimization	Machine learning models for predicting optimal mix ratios and strength	Higher performance and cost-effective concrete with reduced trial errors
Steel and Composite Materials	AI algorithms for analyzing fatigue life and structural integrity	Improved reliability and longevity of steel and composite structures
Material Property Prediction	Predictive modeling of durability, elasticity, and mechanical properties	Accurate forecasting of material performance in various environments
Defect Detection and Quality Control	Computer vision and deep learning for real-time defect identification	Enhanced safety and reduced production costs through automated QC
Sustainable Material Development	AI tools to design eco-friendly and energy-efficient material compositions	Supports green engineering and reduces carbon footprint in construction
Smart and Nanomaterials	ML techniques to accelerate discovery and application of nanomaterials	Enables advanced functionalities in smart materials and innovations

Image recognition systems based on AI are extensively used in the quality control of processing. In addition to this, machine learning is also advanced in the creation of nanomaterial and smart materials, which makes it easier to discover sustainable solutions to construction. The results of these novelties are not only the improved structural reliability, but it is also related to the environment-friendly and energy-efficient construction. The application of Artificial Intelligence (AI) to the construction materials sector is of tremendous interest because of multiple advantages, issues, and future opportunities. Creating more effective and efficient construction processes, AI will complement data analysis and design and sustainable practices management. Nonetheless, even with such innovations, it is extremely difficult to adapt AI to the existing manufacturing systems and construction projects. Most construction companies are equipped with ready-made systems; that is why the implementation of AI becomes an intricate process and requires significant investments in the modernization of the infrastructure and training of employees. Even more problematic is the fact that the discontinuation of the traditional way of conducting business predetermines the shift to AI-driven systems. As such, AI practices concerning data collection, format and benchmarking standardization are critical measures towards ensuring that AI utilization is as efficient as possible, especially as the number of increasingly more IoT devices and smart sensors entering the world continues to rise to provide real time feedback.⁽³⁷⁾ Applications of AI in materials engineering are used to predict the mechanical properties of materials and a material process is designed to optimize the product. Machine learning will allow them to predict the concrete strength, and create mixes that, in a way, can be sustainable.^(23,38) The fatigue life and performance of steel and the composite materials are identified with the help of AI algorithms. One of the most valuable examples of how the simulations based on AIs can be utilized to get a more accurate understanding of the electrical, thermal, and mechanical characteristics is the simulation of doped graphene oxide and CNTs.^(39,40) The other one is the computer vision which enhances detection of defects in

the processes of manufacturing of materials. Moreover, thanks to the use of AI, the process of getting nanomaterials with certain properties will become faster, and the invention of high-tech composites that can be implemented in the modern construction process will become possible.

⁽⁹⁾ This mixture increases the safety, performance and environmental sustainability. The ethical aspect of AI in the construction is also to be considered. With the deployment of AI technologies that can maintain the indigenous construction methods and lead to the success of sustainable construction, the issue of cultural appropriation and ethical implementation of algorithms becomes even more visible. The AI can come in handy in recovering the ancient techniques and merging with the latest material science in the case studies, thereby rescued the cultural heritage and facing the dilemma of sustainability in the modern world. These studies reveal the necessity of the moderate solution according to which the local culture would be respected and the ethical values would be upheld in the use of AI.⁽⁴¹⁾ Since the sphere is constantly changing, it is also probable that the study will continue to reveal the answers to the questions that remain unanswered when it comes to the implementation of AI in construction materials, which will also be the validation of the importance of technology in the future of the sphere. Such developments imply that AI is not a developmental process, but one of the most crucial aspects that can transform the way the construction and material science may be undertaken in the future.^(5,42) Overall, AI integration into the building materials can hold revolutionary possibilities of efficiency, sustainability, and novel design, but only when the serious challenges that need to be addressed with caution to allow the use of AI in the construction process are met in an ethical and productive way.

AI in Construction Management

One of the fields in which AI is already demonstrating the most viable advantages is the construction management one. Project schedule analysis and optimization of resource distribution and delays reduction are used to put the AI algorithm into practice. The managers can make decisions using the machine learning tools to predict the cost overruns and the safety risks. It is also possible to connect to Building Information Modeling (BIM) and coordinate, and conflict detection between teams working on the project in real-time. The management of supply chains by using AI-applicable tools also helps to predict the demand and supply of materials and delivery time. AI-based surveillance at the workplace can be used to secure the safety of the people working in the place as they will know when situations are dangerous. Automated reporting and documentation simplify the administration procedures since they reduce the human workload. The role of AI in construction management in most cases provides efficiency, transparency and safety to modern projects. The artificial intelligence (AI) has taken the place of the revolution of the sphere of construction management because it is the paradigm shift in the way of working with the projects which is one of the factors of the sphere in general. The introduction of AI technologies will assist to provide more efficiency, security, and decision-making through the lifecycle of the construction, which is a significant change in planning, implementation, and control of the projects. It goes hand in hand with the findings of the recently issued report according to which it was mentioned that the AI technologies will allow detecting the faults in the civil engineering and predicting the lifecycle in the most efficient manner by which the risks and the performance will be minimized and maximized.

⁽⁴²⁾ Mammoth AI applications in construction management are used to smooth out resources, schedule and risk estimation. With the connections to the BIM and IoT, it would have the potential to provide real-time information and connectivity with the project teams.^(24,43) Clouds also make it possible to store data on the construction process and perform analytics on a large scale.⁽⁴⁴⁾ The creation of advanced nanomaterials monitoring is expressed in a similar way as the AI-based infrastructure diagnostic and predictive models of failures.^(9,31,45,46) The construction

management process can be made more flexible and efficient, minimizing uncertainties, and ensuring that the process is more transparent, with the help of AI-driven tools. Thus, similarly to how AI has helped achieve success in governance in the management of infrastructures, it can also help project managers to navigate complexities in the construction process. The human-AI interplay is also important in the project success in the agile project management. According to the findings of the experiments conducted by Cui⁽⁴⁷⁾, the effectiveness of agile practices that leads to the successful project delivery in the large-scale construction setting is mediated by the connection between human intuition and AI competences. This is a reflection of why collaborative systems between human and artificial intelligence agents should be developed and could significantly increase the benefits of agile approaches. This aspect of this integration is significant in the complexity of the mega construction projects conquering, and also strategies to enhance the process of the project management. Moreover, the availability of Generative AI (GAI) technologies opens up the further possibilities of enhancing the quality of the services and the results of the projects in the mega construction projects. They are also expedited in regard to technological transformation and this is noteworthy since it falls under the improved service delivery mechanisms which is vital given the high stakes and magnitude of such undertakings in the society like telecommunications in China. This amalgamation of digital technology and service quality meant biases on the notion that the approaches that construction managers pursue would have to be modified to the modifications in the technological setting at any given moment. In conclusion, the application of AI in construction management is multifaceted, and it means that it is possible to make improved decisions with the help of data, better manage security, and improve the cooperation of people and AI. As the construction industry continues to take its shape, it will be necessary to embrace such technological advancements to ensure that the industry is still in its developmental stages and to ensure that competitive advantages are upheld in carrying out projects.

AI in Structural Health Monitoring

The infrastructure structural health monitoring (SHM) is important to security and performance of the infrastructure in the long term. AI has potential to improve SHM because it is comparatively more effective than traditional systems to process big volumes of sensor data. The use of AI can identify anomalies and reveal damages and disturbances at the earliest stage. Deep learning algorithms are effective especially at detecting defects that are hidden and vibration pattern and acoustic signal detection. AI is used to come up with predictive maintenance, which minimizes common failures and increases building life cycles. Drones with image recognition AI-based visual inspection systems are used to automatically identify cracks, corrosion or deformations. The practices are very effective in minimization of inspection cost and enhancement of safety as the human beings are not subjected to hazardous situations. Thus, AI-based SHM is one of the pillars of active infrastructure management. The concept of integrating artificial intelligence (AI) in structural health monitoring (SHM) is proving to be a valuable addition to improving the security and reliability of different buildings. The latest developments into data-driven methods have shown a magnitude of potential on optimization of the structural assessment using machine learning algorithms, sensors, and computation simulations. Meanwhile, Liu et al.⁽¹⁰⁾ consider an important forward to be the one that incorporates some level of health monitoring because it becomes possible to diagnose faults in real-time with the introduction of deep learning algorithms. They offer a description of how the technologies of convolutional neural networks (CNNs) and recurrent neural networks (RNNs) might prove to be more effective and more effective at supervising and offering essential basis of fault control and decision dynamics in structure applications. These AI processes are groundbreaking, and predictive maintenance with real-time data is one of the possible uses of these methods in the future, which can avert expensive integrity failures of infrastructures.

Alongside this, a study have already created an evidence-based structural health monitoring framework, including wireless strain sensors, FEA, and machine-based learning algorithms to identify the scaffold instability modes, which echoes the prospects of the integration of different AI applications in SHM systems. They suggest that risk reduction in falls as the result of applying the corresponding technologies is considerable, thus, the overall safety of the construction site where the scaffolds are installed in large amounts is increased.⁽¹¹⁾ To sum up, AI application in structural health monitoring is not just a possibility to facilitate the culture of safety proactivity, but it also formed more efficient analysis opportunities, that is the multi-dimensional issue of infrastructure maintenance. It is turning SHM into an efficient, and trustworthy discipline by integrating machine learning, real time data collection and creation of novel forms of analysis that have enormous implications to the security of the populace and structural integrity. One of the most helpful AI implementations in the field of construction engineering is structural health monitoring (SHM). The sensor measurements are processed in real-time by artificial intelligence algorithms, which attempt to recognize anomalies, cracks and damaged material.^(31,48) The applications of machine learning can forecast preventative maintainability and lessen sudden failures and optimize the infrastructure. AI-based vision systems on drones assist the inspections which are safer. The graphene oxide and doped CNTs study is a good example demonstrating the possibilities of intelligent sensing systems in SHM.^(33,49) Together with AI analytics, such materials can be applied to identify the weak points in the structure in advance. The AI ownership within SHM promotes resilient infrastructure, adaptive infrastructure and cost-efficient infrastructure.

Robotics and Automation in Construction

The current robotics and automation based on AI is transforming the traditional approaches to construction by bringing new efficiency and accuracy. Autonomous robots are used in the repetitive tasks like laying bricks and welding as well as handling materials. The prefabrication and onsite construction is changing with the use of AI-powered navigation on the drones to surveil, inspect and monitor the progress of the site. These developments do not only shorten the project time, but also decrease the number of human errors, and enhance safety. AI-based robot systems can adjust to the dynamic environment of locations. Moreover, human workers can be assisted by collaborative robots (cobots) to overcome conditions of hard or dangerous work. The merging of robotics and AI, and construction-related technologies is an indicator of a new era of the construction industry that can be traced back to automation, sustainability, and resilience. The construction industry is an area where robotics and automation are being integrated as a way of improving efficiency and safety in addition to precision. The construction site dynamics require the robotic systems, which are able to measure the space variables and dynamically adjust with time. Research has established that high-tech construction robots with a high-quality sensor and managerial system are able to accomplish proper tasks like painting walls and placing glasses and maintain high quality and compliance with the rules of the construction.⁽¹⁴⁾ Also, construction activity complexities tend to be a factor continually requiring advanced automation to obtain the highest efficiency. The recent bibliometric analysis indicates that the role of smart technologies in construction has been increasing recently, and it requires automatic solutions that can optimize the construction process, as well as safety and real-time monitoring of the infrastructure.⁽¹³⁾ The advancement of AI-based robotics and automation has altered the existing mode of practice of construction. These autonomous robots carry out repetitive jobs including welding and constructing a wall in a highly precise way. AI-based drone technology may be utilized in the realm of surveying, inspection and safety control.⁽⁵⁰⁾ The prefabrication and sustainable construction practices are innovative and made through AI-based 3D printing. They can be compared to the works with nanomaterials, when AI and automation are employed in an attempt to accelerate the discovery and implementation.

^(9,51) Cobots will also help in making the work environment a better place to work because they are deployed to work with heavy or dangerous tasks. Adaptive control can also be applied to the systems of a robot to control it with digital twins. All of these changes are indicative of the future when AI-powered robotics will guarantee efficiency, strength, and sustainability of the construction process. Deep learning is very useful in improving the capabilities of the robot. ^(52,53,54,55) Study established that it has led to the creation of intelligent identification and analysis tools, which employ deep learning to transform the construction industry into a performance. Such systems make the necessary information accessible with real-time data acquisition and processing, which promotes automation of construction projects and the intelligence of such systems in general. ⁽¹⁵⁾ In addition, the advance in materials science that has adopted additive manufacturing has left a subsequent impact on automation in building. ^(56,57,58,59) The strategies that have resulted in the potential of recycling and reusing the materials, specifically, plastic waste, are not only helpful in ensuring that the environment is sustainable; they can also result in decreasing cost and enhancing efficiency of construction. ⁽¹⁶⁾ Finally, convergence of robotics, automation and intelligent systems in the construction industry is transforming the industry in terms of efficiency, precision and sustainability. ^(60,61,62,63) Such inventions can help support the needs of complex initiatives and lead to the creation of a more resilient and innovative environmental of building. Since the process of technology implementation is continuously changing, the possibility of better results in the construction can become clearer. ^(64,65)

CONCLUSIONS

AI is depicted to possess the potential of changing structural and construction engineering in an important manner. It provides the fresh outlook in the design, analysis and management, and transgresses the barriers to the traditional approach. Machine learning and deep learning will enable the engineer to obtain a higher degree of precision of his or her model of the complex structural behaviors. The design of a solution is cheaper and more sustainable as AI provides optimization. Predictive modeling can be applied to construction materials, where the achievement of a better-quality control and creation of new materials is possible. The management of the construction can be greatly assisted by the AI-based planning, scheduling, and risk analysis. The surveillance of the structural health turns into an effective process, as the AI-powered sensors and predictive-based maintenance plans are used. The more safety, less human resource consumption and increased productivity is provided through robotics and automation by AI. Such development opens possibilities of stronger and more viable infrastructure. The problems of the data reliability, its transparency, and ethical approval, however, persist. The resolutions to the difficulties will be essential in the eventual deployment of AI in the engineer practices. The AI and digital twins developed on the basis of BIM will raise a new era of intelligent construction systems. Green engineering and energy efficient infrastructure is another area where the future of AI will be seen to operate. Anyway, AI is a disruptive trend characterizing the future structural and construction engineering.

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Chapter 17

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Artificial Intelligence for Environmental Monitoring and Pollution Management

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ABSTRACT

Artificial intelligence (AI) has emerged as a promising tool in environmental monitoring and pollution control, providing new possibilities for real-time analysis, predictive modeling, and autonomous decision-making. These technologies are surveyed in a chapter on AI for various environmental fields, including air quality monitoring, water pollution control, soil contamination detection, and emerging application areas such as carbon dioxide tracking or biodiversity conservation. We review in-depth machine learning algorithms, deep learning models, and ensemble methods as we discuss AI technologies for environmental stewardship. The chapter comprises four comprehensive bibliographic tables that summarize the key results for MDPI papers, along with their corresponding performance graphs at this level. This analysis reveals that AI models have had a significant influence on shaping research. Critical issues, such as data quality, computational inefficiency, model interpretation, and ethical implications, are thoroughly discussed, along with policy suggestions and promising research directions.

Keywords: Artificial Intelligence; Environmental Monitoring; Pollution Control; Machine Learning (ML); Deep Learning (DL); IoT Sensors; Real-time Monitoring; Prediction Analysis.

INTRODUCTION

Degradation and contamination of the environment have emerged as a serious global issue that affects human health, the functioning of interconnected systems, and sustainable development. Conventional monitoring method. All of China's current water quality standards for small rivers consider the long-term average and prompt concentration, with a time delay of up to 20 h for some fixed-point provinces.^(1,2,3,4,5,6,7,8) These limitations affect the ability to respond quickly in a contamination incident, as well as to monitor an environment geographically. Urbanization, industrialization, and transportation have contributed to a rise in pollution out of all proportion - especially in the developing world, where nine of the top ten most polluted cities are located.^(2,9,10,11,12,13,14,15) Conventional environmental monitoring approaches have a limited capability by nature, as they involve human effort and resources to establish, manage, and collect real-time information for proactive resource management.^(3,16,17,18,19,20,21,22,23)

AI for pollution monitoring

The AI technology possesses revolutionary potential in Environmental monitoring and pollution control, along with Super processing of large databases, which is enormously fast at recognizing and analyzing complex patterns in any application, enabling the search for solutions of enormous proportions faster than previously.^(4,24,25,26,27,28,29) Artificial intelligence (AI) functions, such as machine learning (ML), deep learning (DL), advanced analytical algorithms,

and more, can be utilized to enable real-time detection, prediction, and autonomous response capabilities that operate transparently across various environmental domains.^(5,30,31,32,33,34,35) AI (as well as IoT, and other technologies) can integrate satellite remote sensing data, Internet of Things (IoT) sensor data, or even drone observation to establish multi-scale monitoring networks that provide early detection of pollution in near real-time, as well as in situ forecasting of environmental parameters with high accuracy.^(6,36,37,38,39,40,41,42) This chapter categorizes a range of AI environmental monitoring/pollution control technologies, encompassing both conventional and advanced systems. It then examines the practicality of these two traits of deep learning in real-world scenarios, state-of-the-art evaluation methods, and the associated challenges.^(43,44,45,46,47,48,49,50) By critically evaluating the most recent AI research and applications in various domains, this chapter highlights that these new machine-learning systems surpass traditional precursors in detection accuracy (80e(95 %), communication delay (24 hours e0 1 hour), cost (~0,4X expenses), and spatial extent (up to 5X locations).^(7,51,52,53,54,55,56,57) Drawing on evidence from over 30 peer-reviewed studies across various environmental domains,^(58,59,60,61,62,63,64) it provides researchers, policymakers, and experts with a comprehensive understanding of how AI is poised to be the transformational engine shaping ecological well-being and sustainability. An Introduction to Elementary Image Processing and Analysis with Application to Environmental Monitoring.^(65,66,67,68,69) An illegal access exception to metadata during deep learning for environmental monitoring.^(70,71,72,73)

Table 1. Summary of studies on AI-assisted environmental monitoring

Title	Year	Focus Area	Key Technology	Performance Metrics	Author/Source
AI-Driven Greenhouse Gas Monitoring: Enhancing Accuracy and Efficiency	2025	GHG Monitoring	Random Forest, SVM, CNN, LSTM	Detection accuracy 95 %, $R\hat{A}^2=0,89$	Hasan et al. ⁽⁴⁾
Prediction of PM2,5 Concentration Based on CNN-LSTM Deep Learning	2024	Air Quality Prediction	CNN-LSTM Deep Learning	$R\hat{A}^2=0,91$, RMSE=8,216 $\hat{A}\mu\text{g}/\text{m}\hat{A}^3$	Bai et al. ⁽³⁰⁾
Air Quality Index Forecast in Beijing Based on CNN-LSTM	2022	Air Quality Forecasting	CNN-LSTM Model	MAE reduced by 43 %, RMSE by 53 %	Zhang et al. ⁽³³⁾
Deep Learning for Prediction of Air Quality Response to Emission Changes	2020	Emission Response	Deep CNN with RSM	CNN-based DeepRSM reliable	Xing et al. ⁽⁴⁷⁾
IoT-Based Real-Time Water Quality Monitoring System	2024	Water Quality	IoT Sensors, PLC, SCADA	Error margin 0,1-0,2	Forhad et al. ⁽⁵²⁾
Air Pollution Prediction with Machine Learning: A Case Study of India	2022	AQI Prediction	XGBoost, Random Forest, SVM	XGBoost highest accuracy	Kumar et al. ⁽²⁾
Artificial Intelligence-Assisted Air Quality Monitoring for Smart Cities	2023	Smart Cities	Feature-Optimized LSTM	Best $R\hat{A}^2$ for AQI prediction	Neo et al. ⁽⁴³⁾
Air Quality Prediction and Control Systems Using Machine Learning	2024	Pollution Control	ANFIS, MLP, Random Forest	$R\hat{A}^2=0,999$ (Winter 2020)	Mottahedin et al. ⁽⁵⁷⁾

A Hybrid Deep Learning Air Pollution Prediction Approach	2025	Hybrid Models	Deep Learning Hybrid	Complex spatio-temporal handling	Chen et al. ⁽²⁷⁾
Real-Time IoT-Powered AI System for Environmental Monitoring	2024	Comprehensive Monitoring	IoT with Machine Learning	94 % prediction accuracy	Ramadan et al.
Revolutionizing Water Quality Monitoring with AI	2025	Water Quality Systems	ANFIS, DNN, Satellite Integration	60 % cost reduction	Al-Khafaji et al. ⁽¹⁾
The Role of Artificial Intelligence in Environmental Monitoring	2025	Environmental Monitoring	Remote Sensing, AI	Real-time source identification	IK Press ⁽³⁾
An Embedded Machine Learning System for Air Quality Monitoring	2025	Low-Cost Sensors	ORCS-ASVM	Improved accuracy over traditional	AIMS Press ⁽⁹⁾
AI in Combating Deforestation	2023	Deforestation Detection	Satellite Image Analysis	Near real-time detection	Omdena ⁽⁶⁹⁾
Bridging Adaptive Management and Reinforcement Learning	2023	Adaptive Management	Reinforcement Learning	Model-free deep RL	Chapman et al. ⁽⁶⁾
Using AI and GIS for Real-Time Forest Monitoring	2025	Forest Monitoring	AI, GIS, Satellite Imagery	Temporal dense monitoring	Geowgs84.ai ⁽⁷⁴⁾
Real-Time Water Quality Monitoring Using AI-Enabled Sensors	2024	Water Quality Detection	AI-Enabled Sensors	26 citations	Durgun et al.

Conceptual framework and technology foundation

Environmental artificial intelligence integrates various scientific and technological inventions to build intelligent systems capable of monitoring the environment independently.⁽⁸⁾ Its data collection, analytics, and decision support capabilities are built on three main components: infrastructure for data capture, technology for processing it, and systems for informed decision-making. DSMSA sources include distributed sensor networks, satellite platforms, UAVs (Unmanned Aerial Vehicles), UGVs (Unmanned Ground Vehicles), and ground stations, which observe multi-dimensional environmental phenomena over extended time series and globally.⁽⁹⁾ The sensor layer utilizes multiple types of sensors, each suited for various mission profiles. Multi-pollutant monitors measure gaseous pollutants (carbon monoxide (CO), nitrogen dioxide (NO₂), sulfur dioxide (SO₂), ozone (O₃), ammonia, NH₃) and particle sensors for fine particles (PM_{2.5}) and coarse particles (PM₁₀).⁽¹⁰⁾ The water quality sensors monitor key parameters, including pH, dissolved oxygen (DO), turbidity, conductivity, total dissolved solids (TDS), and other contaminants. The sensors are interfaced with microcontroller hardware (Arduino, Pi, ESP32) for local or edge computation of data.⁽¹¹⁾ Wireless communication infrastructure supports heavy data traffic delivery from sensor nodes deployed in a location to other places through different wireless paths, such as Long Range Wide Area Network (LoRaWAN) for long-range but less energy-efficient connectivity, 5G for real-time and high bandwidth data transmission, Wi-Fi for local area network, and cellular network (LTE) providing services in mobile platform.⁽¹²⁾ This hybrid architecture ensures diversity, scalability, and coverage in various scenarios, ranging from rural to urban areas.⁽¹³⁾ The analytical processing layer comprises cloud servers (e.g., AWS, Google Cloud, Azure), which preprocess raw sensor readings to extract features for model-based analysis.⁽¹⁴⁾ Edge computing approaches split processing between mobile devices

and cloud services to minimize latency, bandwidth requirements, and computational overhead exerted on centralized infrastructures.⁽¹⁵⁾

Machine Learning for Environmental Data

Then, data-driven methods for environmental monitoring can generally be categorized into three groups: 1) supervised learning based analyses; 2) unsupervised learning-based analyses; and 3) reinforcement-learning-based analyses, considering the specific analysis purpose. Supervised learning approaches utilize labeled historical data to train a predictive model, which can then predict pollution concentrations, contamination events, or environmental quality indexes.⁽¹⁶⁾ Support vector machines (SVMs) are effective methods for analyzing multidimensional ecological data, and the nonlinear correlation of diverse pollutants or meteorological factors can be readily expressed by SVMs.⁽¹⁷⁾ Interpretable models (e.g., DTree/RForest ensemble) generalize well across different environmental conditions.⁽¹⁸⁾ Among them, the eXtreme Gradient Boosting (XGBoost) is reported as one of the most popular learners, leveraging three learning algorithms, an advanced machine learning model, and an ensemble method based on the iterative improvement of weak learners.⁽⁸⁾ It is one of the most effective approaches to achieve high accuracy prediction (yielding 97 % accuracy compared to alternative algorithms).⁽¹⁹⁾ Although simple, the Gaussian naive Bayes method emerged as a very competitive approach, particularly in specific AQ scenarios where the feature independence assumption holds.⁽²⁰⁾

Unsupervised learning techniques are designed to identify hidden structures, outliers, and anomalous patterns within unlabeled environmental data. K-means clustering can divide the air quality monitoring data into distinct clusters, making the original complex information on pollution and variation clearer.⁽²¹⁾ Techniques, such as Principal Component Analysis (PCA), can be used to address the issue of dimensionality reduction by converting high-dimensional meteorological data into principal components that are more interpretable and reflect the primary pollution sources/determinants.⁽²²⁾ The variability of temporal and spatial patterns of pollutants is not reported, except for duration times through HR. Some pollution events or seasonal variations can be identified.⁽²³⁾ Adaptive environmental management, which has recently been recognized as an attractive paradigm built on reinforcement learning,⁽¹⁹⁾ enables intelligent agents to learn from experience in an environment without being explicitly told what is right or wrong.⁽²⁴⁾ RL techniques have also been applied to dynamic sensor placement,⁽²⁵⁾ where robots learn to place sensors to achieve the optimal trade-off between the information gained and the pollution detected. Robotized systems (multiple robots, learning-based algorithms) have been developed to map pollution sources in contaminated environments, especially on dynamic contamination fields.⁽²⁶⁾

Table 2. Performance of different algorithms in predicting air pollutants			
Model/Method	Application	Accuracy/ Performance	Key References
Random Forest (RF)	AQI prediction, PM2,5/PM10 forecasting	98,2 % accuracy, $R\hat{A}^2=0,9998$	Ravindiran et al.; Ameer et al.
ANFIS (Adaptive Neuro-Fuzzy Inference System)	Seasonal air quality prediction, pollutant concentration modeling	$R\hat{A}^2=0,999$, RMSE=0,0274	Mottahedin et al. ⁽⁵⁷⁾
Support Vector Machines (SVM)	Classification of air pollutants, anomaly detection	93 % average accuracy	Veljanovska & Dimoski
Neural Networks (ANN, MLP)	PM prediction, CO2 forecasting, multi-pollutant analysis	87 % correlation coefficient	Maleki et al.; Taheri & Razban

Convolutional Networks (CNN)	Neural	Satellite imagery analysis, spatial pollution mapping	95 % detection accuracy	Bashardoost et al.
Long Short-Term Memory (LSTM)		Time-series forecasting, temporal pattern recognition	High temporal accuracy for sequential data	Shahana et al.
Gradient Boosting XGBoost	Boosting &	High-accuracy AQI prediction, feature importance analysis	$\hat{R}^2=0,9936$, superior performance	Ravindiran et al.
Ensemble (Stacking)	Methods	Combining multiple base learners for improved accuracy	$\hat{R}^2>0,99$, reduced error rates	Air Quality Prediction
Deep Belief Networks (DBN)	Networks	Deep feature extraction from air quality data	Improved feature learning	Air Quality Prediction
CatBoost		Categorical variable handling, robust prediction	$\hat{R}^2=0,9998$, low RMSE	Ravindiran et al.

DLA4HD: Deep learning architectures for high-dimensional environmental data

Deep learning methods are particularly effective in modeling nonlinear and complex relationships, as well as extracting hierarchical patterns from environmental data streams. ⁽²⁷⁾ CNNs show great promise in analyzing spatial ecological data, such as satellite images, drone videos, and gridded sensor networks. ⁽²⁸⁾ CNNs using convolutional filters are models capable of learning multiscale spatial features, which allows the identification of pollution patterns at various geographical scales, such as local and continental. ⁽²⁹⁾ In addition, the LSTMs explicitly take account of temporal ordering in environmental time series data by maintaining a memory of past observations through gates that update hidden states iteratively. ⁽³⁰⁾ The LSTM model was employed in prediction studies for air quality indices, considering seasonality and meteorological factors associated with pollution. ⁽³¹⁾ BiLSTM processes the sequence of environment \emph{forward} and \emph{backward} to derive forward-backward temporal relations that can enhance prediction performance. ⁽³²⁾ Hybrid deep learning models, which combine CNNs and LSTMs, leverage the advantages of both spatial feature extraction using CNNs and modeling temporal dynamics with LSTMs. ⁽³³⁾ The CNN-LSTM architecture processes environmental data through a body-sequence stage, in which the CNN layer extracts important spatial patterns from sensor field (or satellite) observations at different locations, and the LSTM layer models the temporal changes of these patterns. ⁽³⁴⁾ CNN-LSTM models have also been shown to be more accurate than others for forecasting air quality, with an R^2 of 0,91 and an RMSE of 8,216 $\mu\text{g}/\text{m}^3$ of PM2,5 modeled. ⁽¹⁶⁾ 5 concentration prediction ($R^2 = 0,89$, RMSE = 9,41), which is significantly better than either the separate CNN ($R^2 = 0,85$, RMSE = 11,356) or LSTM ($R^2 = 0,83$, RMSE = 14,367). ⁽³⁵⁾

Table 3. AI technologies and models for soil pollution detection and prediction				
Technology/Model	Application	Performance Metrics	Advantages	Key Studies
Graph Neural Networks (MSA-GNN-HMP)	Soil heavy metal prediction (Cd, Pb, Ni, Cr)	Lowest MAE & RMSE, highest $\hat{R}^2$	Multi-scale spatial feature extraction, attention mechanism	Zha et al.
Convolutional Neural Networks (CNN)	Spectral analysis for soil contamination	High accuracy in contamination detection	Image-based analysis, non-invasive	Pyo et al.; Sun et al.
Random Forest (RF)	Spatial prediction of soil quality parameters	89-95 % prediction accuracy	Handles non-linear relationships well	Li et al.

Support Vector Regression (SVR)	Heavy metal concentration estimation	Effective modeling	spatial	Robust to outliers	Yang et al.
Artificial Neural Networks (ANN)	Soil quality index prediction	85-92 % accuracy range		Captures complex patterns	Pacci et al.
IoT + Edge Computing	Real-time environmental monitoring in remote areas	Low latency (<1ms), real-time capability		Distributed monitoring, fog computing integration	Baharudin et al.; Roostaei et al.
Remote Sensing + AI	Oil contamination detection, TPH/PAH quantification	95 % accuracy in contamination identification		Large-area coverage, satellite data integration	Remote Sensing Studies
E-nose + Spectroscopy	Rapid detection of chemical pollutants in soil	Rapid analysis	on-site	Portable, field-deployable	Spectroscopy Research
Deep Learning (Hybrid)	Multi-sensor data fusion for pollution assessment	Enhanced modal performance	multi-	Integrates multiple data sources	Chen et al.
Fuzzy PLS + BLN	Heavy metal detection in agricultural soils	Improved accuracy over traditional PLS		Handles dynamic sensing data	Chen et al.

Graph Neural Networks (GNNs) offer a novel framework for monitoring over interconnected spatial domains.⁽³⁶⁾ GNNs address the relationships between monitoring stations and environmental compartments related to multisource pollutants, capturing how pollutants are transferred through air, water, and land systems.⁽³⁷⁾ Attention mechanisms developed in a neural context⁵¹ are used to selectively weigh the computational output, resulting in increased feature interpretability and efficiency when selecting other potentially informative environmental variables and their corresponding temporal windows.⁽³⁸⁾ The problem of identifying which ecological features contribute most to pollution levels has been addressed by a class of attention module-equipped CNN-BiLSTM models.⁽³⁹⁾ In addition, such models offer learnable weights to determine which input variance most contributes to predicting pollution results.⁽⁴⁰⁾ The temporal-based model, trained to predict air pollution, incorporates an attention mechanism and achieves R² values of 0,9872 for PM_{2,5}, demonstrating the potential of attention methods in complex environmental applications.⁽⁴¹⁾

Justification of AI in Environmental Monitoring

Monitoring and Forecasting of Air Quality 6, 1.determination with which the measurements are made and known (in some cases interpolated) concentrations at sample sites. The measurement network serving as the input to the data fusion problem is predominantly composed of non-stationary sensors with inhomogeneous sensitivities that exhibit varying levels of noise.

The area of air quality monitoring is one of the most developed and explored areas where AI has been applied to environmental management, as it addresses evident public health issues associated with atmospheric pollutants.⁽⁴²⁾ Traditional approaches to air quality monitoring and assessment are typically based on a limited number of centralized monitoring stations, spaced apart from several meters to several kilometers, leading to both blind spots in the pollution coverage map and latency in detecting local pollution events.⁽⁴³⁾ Air quality monitoring systems based on AI deploy a decentralised network of sensors over cities, thereby generating high-

resolution pollution maps with fine spatiotemporal granularity.⁽⁴⁴⁾ Machine learning methods are developed to integrate sensor readings with meteorological variables (temperature, wind speed, relative humidity, and atmospheric pressure) to predict pollutant levels at different horizons: immediate (1-6 hours), short-term (24-72 hours), long-term, seasonal, and annual.^(45,46) The deep learning technique has been successfully applied in air quality forecasting. DeepRSM) The two emission perturbations and the responses of air quality predictions, such as this model, can be a very accurate predictor for both temporal variation and space-time pattern on a daily timescale, which can faithfully emulate complex CMAQ models. DeepRSM targets precursor pollutants (NO_x, SO₂, and ammonia) to secondary pollutants (ozone and PM_{2.5}) by using deep convolutional models to forecast real-time air quality responses under policy choices.⁽⁴⁷⁾

The published outputs of deep learning algorithms, when applied to air quality forecasting in large cities, demonstrate a better comparison with traditional statistical methods. The Beijing air quality forecast based on CNN-LSTM models has an average absolute error of 43 % and a root mean square error of 53 %, compared to the SARIMA (Seasonal Autoregressive Integrated Moving Average) model, which increases the R² value by 8,45 %.⁽⁴⁸⁾ CNN-BiLSTM Modelling for Mumbai, India considers 13 pollutants and seven meteorological factors at this level to estimate air quality index and achieves R²: 0,91; MAE (0,45); RMSE (0,60).⁽⁴⁹⁾ PM_{2.5} and the found parameters 'g' were discovered while an optimized feature LSU model was utilized in the ASmart City Air System. This work. 5, PM₁₀, NO₂, along with weather factors including humidity and wind speed, as the major predictors to predict pollution levels.⁽⁵⁰⁾ These models achieve optimal R² for estimating multiple pollutants in large cities, suggesting that AI can predict several pollutants simultaneously by forecasting estimates for various types of contaminants. This is expected to assist overall air quality planning.⁽⁵¹⁾

Analyses of Water and Characterization of Contamination

A DS-internet of things (IoT)-based water quality monitoring system can easily overcome traditional methods by providing real-time and continuous results for multiple parameters.⁽⁵²⁾ Numerous sensor arrays are used to monitor pH, dissolved oxygen (DO), turbidity, conductivity, and other chemical pollutants in water treatment plants, factories, and municipal water supplies.⁽⁵³⁾ PLC SCADA Cloud X: A gateway between IoT and cloud II. Existing techniques are increasingly focused on developing smart, Innovative Water Systems to address issues related to growing urbanization, digital dynamics, and climate change.^(47,48,49,50,51,52) It is capable of providing a minimum error margin of 0,1 and 0,2 in measurements for different parameters, which permits the prompt detection of variations in water quality and contamination events.⁽⁵⁵⁾ Machine learning of water quality data facilitates the detection of anomalies, such as identifying unusual patterns that may indicate pollution, sensor malfunctions, or process faults.⁽⁵⁶⁾ ANFIS could also produce superior results in modeling the water quality prediction (R² = 0,999, RMSE = 0,0274, MAE = 0,0162).⁽⁵⁷⁾ This breakthrough level of performance represents a fundamentally different capability for traditional statistics methods, as practical predictive maintenance can be performed and contamination dealt with proactively.⁽⁵⁸⁾ AI intelligent water sensing systems can lower the sampling period to around 60 %, based on strategically placed sensors calibrated by machine learning (ML) models.⁽⁵⁹⁾ The combination of IoT sensor networks and integration of satellite data (Landsat 8) has made it possible to map water quality in large areas where extensive field sampling was previously needed.⁽⁶⁰⁾ Sophisticated fusion techniques that combine different data sources may provide continuous ranging information for water quality considerations in watershed-scale management.

Smart City Air Pollution Sensing and Abatement

Advanced city deployments. The other two novel and evolutionary city-level deployments

utilize AI-automated air pollution monitoring, integrated into the city structure, to create a detailed picture that was previously unavailable using traditional monitoring approaches, providing both a stationary and dynamic view of pollution in space and time.⁽⁶²⁾ By measuring the quality of air in real-time, urban planning measures can be activated. Traffic is optimized during pollution episodes to reduce congestion and pollutants. Air quality controls public transport schedules and designates clean air areas, places where vehicle access is limited due to persistent poor air quality.

AI-enabled intelligent urban air quality monitoring techniques might predict pollutant concentrations on a neighborhood scale, recognize pollution hotspots, and provide a basis for targeted actions.⁽⁶⁴⁾ In the Greater Chennai area of India, AI-driven air quality monitoring systems are expected to lead to the planting of over 200 000 trees by 2023, as part of a larger plan to reduce PM_{2.5} pollution by 2026.⁽⁶⁵⁾ Variational autoencoders and hybrid AI models, such as those embedded with machine learning and edge computing (e.g., adaptive SVMs controlled by one-rank cuckoo search optimization), have been utilized to enhance the accuracy of low-cost sensors.⁽⁶⁶⁾ The ORCS-ASVM method utilizes real-time data for SO₂, NO₂, and PM_{2.5}.⁵ Monitoring, gathered through Raspberry Pi edge nodes, which enables improvements in prediction accuracy and reductions in computational needs.⁽⁶⁷⁾ This on-device ML-based method will pave the way for reliable air monitoring at scale in resource-constrained urban environments.⁽⁶⁸⁾

Forest Monitoring and Deforestation Alerts

AI-driven satellite imagery for monitoring forest cover improves deforestation detection and evaluation of forest health.⁽⁶⁹⁾ The AI-based satellite image analysis processes utilize multispectral and hyperspectral images taken from the Sentinel-2, Landsat 8, and other Earth observation satellites to predict changes in forest cover, albeit near real-time.⁽⁷⁰⁾ High-speed algorithms can be used to decode deforestation areas for swift organization of interventions and law enforcement.⁽⁷¹⁾ Deep learning models trained on large-scale satellite images learn to distinguish between forest cover and degradation patterns, as well as identify illegal logging and natural disturbances.⁽⁷²⁾ Forest and non-forest classes of satellite pixels are well-discriminated by Random Forests, Support Vector Machines, and Convolutional Neural Networks.⁽⁷³⁾ Time series analysis enables the explicit detection of changes in crown density (degradation) and trends in degradation, as this gradual ecosystem transition precedes complete deforestation.⁽⁷⁴⁾ The combination of optical and radar satellite data with AI-based enhancement enables time-dense monitoring of forests, compensating for artifacts caused by poor cloud accessibility in optical images.⁽⁷⁵⁾

Radar satellites can see through clouds, enabling continuous observations that supplement voids left by optical data. To the extent that these events are shrouded in cloud cover for extended periods, particularly in tropical regions, this is relevant.⁽⁷⁶⁾ This fusion approach has been used to track small-scale disturbances (e.g., illegal logging) that regrow rapidly, as they do not produce temporal aliases (i.e., the recovery of vegetation will not mask deforestation signals).⁽⁷⁷⁾ AI predictive models determine which areas are most likely to be deforested by 1911—the year that historical content ends—factoring in historical trends, land-use changes, population density, and infrastructure development.⁽⁷⁸⁾ Such predictive maps would allow for a cost-effective and pragmatic implementation, where monitoring and enforcement efforts are concentrated in high-risk areas (to facilitate efficient protection of highly vulnerable zones with limited resources).⁽⁷⁹⁾

Agro-food and Marine Ecosystem, Ocean Pollution Observing

AI-driven e-marine systems completely change the way ocean observing is done by utilizing autonomous platforms, intelligent sensors, and on-site data analysis.⁽⁸⁰⁾ The improved presence of autonomous underwater and glider vehicles with environmental sensors thus offers continuous monitoring of water column temperature, salinity, pH, and oxygen, as well as species distributions.⁽⁸¹⁾ Sophisticated imaging technologies (e.g., high-resolution cameras and sonars) are used to produce highly detailed visual imagery, which is then interpreted by machine learning algorithms to discern the species in question, monitor movements among potentially migratory communities, and identify any behavioral deviations.⁽⁸²⁾ Acoustic monitoring, aided by machine learning techniques, analyzes underwater sounds to identify and track the behavior of marine mammals, as well as to study their communication.⁽⁸³⁾ These functions are handy for managing whale populations or examining the migration routes of whales, which also have a significant influence on protecting the maritime environment.⁽⁸⁴⁾ Based on ocean temperature, water salinity, pH balance, and species distribution, among other factors, predictive analytics combined with marine ecosystem data are used to forecast possible changes in the aquatic environment.⁽⁸⁵⁾ Rapid logistical support for interventions, such as coral bleaching events or harmful algal blooms, and ecosystem stress alerts can also be essential.⁽⁸⁶⁾ The small spatial patterns of the environment that are invisible to the human eye can be detected by AI algorithms to forecast species migration and preserve resources.⁽⁸⁷⁾

It has been demonstrated that artificial intelligence (AI)-based systems can be practically used to detect pollution in the sea, such as oil spills and plastic garbage,⁽⁸⁸⁾ as well as pollutants in marine environments using satellite images and distributed sensor networks—satellite-AI for oil spill detection. Satellite AI exhibits high precision in sensing oil fingerprints, slicks, and damage of a spill.⁽⁸⁹⁾ HAB prediction is an environmental forecasting method that combines information to predict the location and magnitude of harmful algal blooms (HABs) for public health protection.⁽⁹⁰⁾

Measuring Greenhouse Gases and Tracing Emissions to Climate

The AI-based monitoring system for GHG facilitates emissions monitoring and reduces errors by pooling real-time information from various sources.⁽⁹¹⁾ Machine learning algorithms and neural networks analyze satellite imaging, IoT sensors, and meteorological models to detect emission hotspots and monitor their spatiotemporal patterns.⁽⁹²⁾ The GHG monitoring methods using random forest, support vector machine (SVM), convolutional neural networks (CNNs), and long short-term memory (LSTM) are developed for a significant improvement on latency from 24 hours to 1 hour in reporting the data; spatial resolution of 30 metres to 10 metres, and accuracy from 80 % to 95 %.⁽⁹³⁾ AI systems detect and estimate emission sources that are not explicitly present in the training data, then extrapolate emission projections with an R^2 of 0.89.⁽⁹⁴⁾

These developments will enable more effective regulatory action and policy for reducing climate change.⁽⁹⁵⁾ AI can further assist in the targeted reduction and quantification of emissions, considering their evolution over time, as well as the evaluation of climate policies.⁽⁹⁶⁾

Integration Technologies and System Architecture

IoT Sensor Networks and Edge Computing 3ENSITY16 define the resources of sensors as their remaining energy. Various methods are employed to conserve computational power through sleep modes, for example, by utilizing software libraries that benefit from modern compilers or minimizing data.

In real-time environmental monitoring systems, IoT sensor networks are integrated with edge computing to process data locally before transferring it to cloud platforms.⁽⁹⁷⁾ This distributed approach minimizes latency, communication overhead, and computation load on centralized servers—Scanes enables local responses upon detection of an anomaly.⁽⁹⁸⁾

Sensor arrays for CO, NO₂, SO₂, PM_{2.5}, PM₁₀, and O₃ require an integrated preprocessing that includes feature extraction to be used as input for a machine learning model.⁽⁹⁹⁾ The AI method can process and correct sensor drift, environmental noise, and calibration to further adjust measurements for long-term precision.⁽¹⁰⁰⁾

The IoT model combines stationary sensors at a permanent monitoring site with mobile ones carried by vehicles and drones to obtain spatial pollution mapping.⁽¹⁰¹⁾ Applications: Combined Hot-Spot and Mobile Sampling Hybrid sensor networks where prolonged monitoring at hot spots is combined with on-demand mobile sampling of the area of interest.⁽¹⁰²⁾

Satellite Remote Sensing and the GIS Analysis

Environmental Monitoring: Satellites can provide coverage of regions inaccessible based on ground-based observations only.⁽¹⁰³⁾ Multi-spectral satellites, such as Sentinel-2 (14) and Landsat 8 (4), provide information in bands that are suitable for performing land cover classification, computing vegetation indices, and detecting water bodies.⁽¹⁰⁴⁾ The better spectral resolution of hyperspectral satellites enables more precise detection of pollutants, vegetation type, and land surface properties.⁽¹⁰⁵⁾

Satellite images can be combined with other geospatial data in Geographic Information Systems (GIS), enabling spatial analysis and visualization.⁽¹⁰⁶⁾ GIS systems powered by AI enable semi-automated analysis of satellite time series data for detecting deforestation and degradation, as well as recognizing recovery and changes in land cover.⁽¹⁰⁷⁾ Machine learning-based classifiers are utilized for analyzing multi-temporal satellite data to generate fine-scale maps of environmental change and conduct trend analyses.⁽¹⁰⁸⁾

UAS for aerial surveillance and computer vision

High-resolution cameras, thermal sensors, and environmental-monitoring-equipped UAVs⁽¹⁰⁹⁾ provide local, low-altitude, fine-grained surveillance to supplement satellite and land-based monitoring. Deep learning-based computer vision algorithms analyze drone imagery in tasks such as object detection, land cover classification, and environmental assessment.⁽¹¹⁰⁾

Real-time detection of pollution threats, such as built-up garbage, illegal e-waste dumping, and environmental degradation, is performed using a state-of-the-art object detection system, You Only Look Once v8.⁽¹¹¹⁾ The proposed YOLOv8 can also implement drone-based pollutant detection, offering the merits of real-time operation, scalability, and cost-effectiveness.⁽¹¹²⁾

Drones are used to detect temperature differentials (such as those generated by industrial emissions, vehicle exhaust, and other thermal indicators) with the aid of small thermal cameras.⁽¹¹³⁾ This would allow the creation of 3D maps from drone LiDAR information, for instance, to execute change detection or elevation studies for monitoring forests or landslides.⁽¹¹⁴⁾

Performance Metrics and Effectiveness Evaluation

Quality of detection and performance of prediction

The AI-empowered ES sensing systems have demonstrated advantages over traditional

strategies in terms of detection sensitivity and prediction performance.⁽¹¹⁵⁾ The enhancement of pollutant detection accuracy ranges from 22 % to 32 % for each pollutant, achieving a 5-fold increase with 94 % accuracy. In contrast, the non-traditional approach, the proposed UVPU method, even slightly surpasses this result with an accuracy of 72 %.⁽¹¹⁶⁾ 59 % (480 %), PM10 Detection accuracy 91 % (vs.68 %, with standard methods), NO2 detection accuracy 88 % (vs.65 %), and SO2 Detection accuracy 85 % (8062 %).⁽¹¹⁷⁾

The prediction horizon in AI systems extends far beyond hours ahead to predict up to seasonal scales,⁽¹¹⁸⁾ such as live pollution warning systems. Live pollution alerts provide the opportunity for real-time management of acute pollution episodes, a protective measure for at-risk populations, and input into public health interventions.⁽¹¹⁹⁾

The deep learning models significantly outperform traditional statistical approaches and other simpler machine learning algorithms. ANFIS achieves a high $R^2 = 0,999$, with errors in the order of (RMSE = 0,0274 $\mu\text{g m}^{-3}$, MAE = 0,0162), demonstrating excellent predictive performance, as reported in ⁽¹²⁰⁾. CNN-LSTM models can achieve $R^2 = 0,91$ with RMSE: 8,216 $\mu\text{g}/\text{m}^3$ and significantly better performance compared to Random Forest ($R^2=0,78$, RMSE=15,2) and Long Short-Term Memory (LSTM) models ($R^2=0,79$, RMSE=15,8).⁽¹²¹⁾

Efficiency and Quality in Operation

A water-depurated reuse system can ensure that water resources are used efficiently, while also demonstrating good operational cost efficiency.

AI-driven monitoring systems are reported to reduce operational expenses by 60 % due to less laborious field sampling requirements.⁽¹²²⁾ At the same time, increasing the maximum sampling frequencies would require manual tasks,, as noted by Long et al. Human-centric Computing and Information Sciences (2019) 9:24 Page 11 of 12 directing the human analyst more to value-added analysis and response.⁽¹²³⁾ Costs for travel to the site or personnel deployment are also reduced due to remote control and other devices.⁽¹²⁴⁾

Speed-up by factors of 24\$-\$832 in computing time (from one day of offline to about one hour for an online case process) provides real-time assistance for decision-making and quick reactions toward environmental events.⁽¹²⁵⁾ This squeezing of timescales redistributes ecological governance away from responsive, event-based modes of constraint towards proactive, prognosis-led types of intervention.⁽¹²⁶⁾

Decreases in the spatial resolution of an order of magnitude (from 30 to 10 m) allow for the mapping of local sources of pollution and environmental heterogeneity that were previously missed.⁽¹²⁷⁾ A 5000 % increase in deployed coverage (from 100 % to 500 %) also permits the observation of previously hidden regions of the world and the performance of systematic global environmental observation.⁽¹²⁸⁾

Table 4. AI applications in various environmental sectors: Techniques, Impacts and Challenges					
Application Area	AI Techniques		Impact/Benefits		Representative Studies
Greenhouse Gas (GHG) Monitoring	CNN + LSTM hybrid, Random Forest, SVM		Reduced reporting latency (24hâ†’1h), 95 % accuracy	Data integration, scalability, validation	Shahana et al.; Kumar et al.

Deforestation Tracking	V i s i o n Transformers, CNNs, Deep Learning	95 % deforestation detection accuracy, real-time alerts	Cloud data cover, volume, computational requirements	G o o g l e Guacamaya; Ramachandran et al.
Blockchain + AI for Environmental Data	Smart contracts, distributed ledger + ML	Immutable records, carbon credit transparency, fraud prevention	E n e r g y consumption (PoW), interoperability, governance	PAIP Platform; Bhatt et al.
Explainable AI (XAI) in Environmental Science	SHAP, LIME, Layer-wise Relevance Propagation	Model interpretability, stakeholder trust, regulatory compliance	Computational overhead, explanation complexity	Yenkikar et al.; Huang et al.
Noise Pollution Monitoring	Acoustic signal processing, ML classification	Real-time alerts, 95 % reduction in false alarms	Sensor calibration, environmental noise interference	Krishnaraj; Soft dB AI
AI-Powered Waste Management	Computer vision, robotics, CNN-based sorting	80 % faster sorting, 59 % labor cost reduction, >95 % accuracy	Initial investment costs, system adaptation	Everest Labs, Glacier, AMP
Wildlife Conservation (Camera Traps)	Object detection (YOLO, Faster R-CNN), CNNs	Automated species identification, 98 %+ accuracy	Data volume, manual processing bottleneck	Wildlife Insights; Velasco-Montero
Climate Change Prediction	Neural networks, ensemble methods, RNNs	Enhanced prediction accuracy, early warning systems	Model uncertainty, data quality, long-term predictions	Gaur et al.; Cowsls et al.
Edge Computing for Environmental Monitoring	Fog computing, local AI processing	Low latency (<1ms), reduced bandwidth, scalable	Device maintenance in remote areas, limited processing power	Baharudin et al.; Lin et al.
Multi-Modal Environmental Monitoring	Graph Networks, multi-sensor fusion	Comprehensive environmental assessment, holistic monitoring	Data heterogeneity, sensor compatibility	EGAN Framework

Field Success and Use Cases in the Real World

Image Greater Chennai’s AI-powered air quality monitoring led to the planting of 200 000 trees and a goal of reducing PM2,5 in 2026, indicating the real efficiency of AI-based environmental intervention.⁽¹²⁹⁾ AI-based pollution monitoring and production control systems in Shanghai have already contributed to substantial improvements in air quality by targeting industrial emission sources more effectively.⁽¹³⁰⁾

The UK’s largest private water company applied the Hydraulic Network Risk Tools (accelerator models that forecast potential water outages through ML algorithms and maintenance predictions to proactively prevent risk). It recovered £7 million of quantity lost due to disturbance.⁽¹³¹⁾ EcoRisk Visualizer configuration reduces pollution from sewage pumping stations by 50 % and the costs of related cleanup and fines by over 20 % through predictive, data-driven insights.⁽¹³²⁾ RiverAware is an instance of a machine learning method that enables cities to measure the health of rivers by acquiring data from past years, with a focus on effective allocation and prioritization of resources for protection.⁽¹³³⁾

Challenges and Limitations

Issues of Reliability and Standardization for Data Quality

The performance of an AI system is also affected by data quality issues related to its environment.⁽¹³⁴⁾ Over time, sensor drift and calibration issues may arise during extended operational periods, resulting in a loss of measurement accuracy.⁽¹³⁵⁾ In scenarios where the observational dataset is absent, possibly due to equipment failure or sensor failures, the monitoring records may contain information gaps that are inapplicable to continuous sequences required by temporal-based models.⁽¹³⁶⁾ Anomalies and outliers in sensor data, which can be induced by the sensors or result from real events in the environment,⁽¹³⁷⁾ require careful handling.

Data harmonization is complex because different types of sensors, measurement processes, and quality standards are associated with other geographical areas, as well as with institutions/organizations.^(138,139) There is also an imbalanced class issue, as some pollution episodes can be well observed, while others are rarely measured. The use of SMOTE to handle data imbalance improves performance, but introduces synthetic data artifacts that should be treated with caution.⁽¹⁴⁰⁾

Model Interpretability and Explainability

On the other hand, deep learning-based models often exhibit better predictive power but tend to be ‘black boxes,’ resulting in a lack of interpretability for each prediction.⁽¹⁴¹⁾ Transparent and interpretable monitoring results for environmental stakeholders, policymakers, and the affected public, facilitated by AI, should be communicated to the public like traditional reporting to build trust and acceptance.⁽¹⁴²⁾ Partial model interpretation: Feature importance and attention mechanisms have also been widely applied to interpret the model partially, which is likely only part of these models’ decision-making.⁽¹⁴³⁾

Computing uncertainty estimates in AI predictions remains an underdeveloped field, as the majority of systems present results in points without associated confidence intervals or error bars, which are essential for risk-aware decision-making.⁽¹⁴⁴⁾ Probabilistic deep learning models may address this problem, but they are often computationally expensive and complicated to implement.⁽¹⁴⁵⁾

Computational load, energy efficiency

Training deep learning models requires substantial computational power, such as powerful GPUs (Graphics Processing Units) and TPUs (Tensor Processing Units), making it unaffordable for resource-constrained organizations and developing nations.⁽¹⁴⁶⁾ The inference latency of the model may not meet the real-time requirements for some applications, particularly when processing high-dimensional sensor data streams.⁽¹⁴⁷⁾

The massive energy consumption of training large deep learning models has raised ecological concerns, leading to a paradox where “green” eco-sensing systems expend carbon, possibly exceeding their ecological benefits.⁽¹⁴⁸⁾ Energy-efficient and low-computation research directions, such as the Green AI approach, become more appealing for sustainable transfer.⁽¹⁴⁹⁾

Algorithmic Bias and Equity Considerations

Models trained in a location with air pollution sources or meteorological conditions that differ from those at the deployment site can deliver suboptimal performance.⁽¹⁵⁰⁾ Such geographical skew in training data penalizes low- and middle-income countries where the performance of AI systems is often lower.⁽¹⁵¹⁾ This geospatial inequity exacerbates existing disparities in environmental monitoring, where affluent areas typically have more robust monitoring

capabilities and usually overlook hazardous exposures to vulnerable groups in low- and middle-income countries.⁽¹⁵²⁾

Temporal bias occurs when the training set is imbalanced across seasons or weather conditions, resulting in minimal model generalization for the underrepresented timescale.⁽¹⁵³⁾ The fairness and representativeness of the model are also important factors that need to be thought about to avoid biases and other possible detrimental effects (as the power of multiple stakeholders' estimations contributes different stakeholder perspectives, including those of all affected groups, should shape AI systems development and deployment.⁽¹⁵⁴⁾

Privacy and Management of Data

Concerns about privacy, surveillance, and information harvesting have been raised with the real-time deployment of large-scale environmental sensors.⁽¹⁵⁵⁾ The non-consensual collection of sensor-based data from private properties has emerged as a significant ethical concern, prompting the need for the evolution of policy and legal frameworks.⁽¹⁵⁶⁾ A satisfactory level of data security should be provided to ensure a strong encryption and access control mechanism that prevents unauthorized access to information.⁽¹⁵⁷⁾

In many jurisdictions, there are weak provisions regarding the ownership of data, rights to access it, and its beneficial use.⁽¹⁵⁸⁾ Carefully planned policy interventions will be required to ensure an equitable sharing of data from AI-capable high-income countries to resource-poor developing nations.⁽¹⁵⁹⁾

Emerging Trends and Future Directions

Federated learning and distributed AI systems

Federated learning is a distributed model training enabling collaborative learning among multiple institutions and maintaining the privacy of data and local control.⁽¹⁶⁰⁾ Cross-border environmental monitoring frameworks, for example, can jointly create shared models without requiring the pooling of sensitive industrial or ecological data in a central location.^(161,162,163) It also facilitates the preservation of privacy and knowledge sharing across geographically separated populations.^(162,164,165)

In the context of federated learning, it reduces the communication bandwidth and computational burden for device owners who participate, while preserving data privacy by sharing parameters in an encrypted form.^(163,166,167,168)

Transfer Learning and Domain Adaptation

The issue of transfer learning has to do with when we want to apply a model trained in one domain (or source) to the processing of data collected from another domain or target (16cabeza2008learn, bengio2012deep).

Transfer learning refers to the ability to acquire knowledge in one environmental context (e.g., environmental or geographic) and apply it to achieve better performance in a similar, yet different, context.^(164,169,170,171) Models trained to predict air quality in one city can be transferred and re-tuned for use in other cities, without the need for re-training from scratch using massive amounts of new data.⁽¹⁶⁵⁾ Multi-task learning enables the simultaneous prediction of multiple interrelated environmental variables and the teaching of a representation of them, which contributes to the quality of the predictions.^(166,172,173)

Hybrid Physics-Informed Neural Networks

PINNs can introduce physical laws and conservation principles into neural networks, thereby constraining predictions to conform with fundamental physics.^(167,174,175,176) This hybrid framework represents a trade-off between the flexibility of machine learning and humanities-constrained predictions, providing more interpretable and physically realizable predictions.⁽¹⁶⁸⁾ Models of ecological systems can be constructed by incorporating the chemistry of the atmosphere, fluid dynamics, and transport equations alongside their predictions.⁽¹⁶⁹⁾

Systems of Decision-Making and Real-Time Control

Here, AI-enabled systems are increasingly transitioning from passive monitoring to active decision-making and control, utilizing not only data analysis but also the ability to respond automatically when pollution events are detected.⁽¹⁷⁰⁾ For instance, reinforcement learning, a mainstream approach for autonomous sensor deployment, is employed to optimize sensing tasks and achieve maximum information gain and pollution-detection capability for deployed sensors.^(171,177,178) Real-time AI-enabled AQCSs integrating predictive models and automatic control (e.g., traffic flow, industrial emissions, or water treatment).^(172,179,180)

Climate Change Integration and Scenario Analysis

Machine learning models of the environment and its degradation can incorporate climate change projections, examining ecological consequences under varying degrees of climate forcing and policy action.^(173,181,182,183) AI-based scenario analysis can help evaluate the efficacy of mitigation measures for evidence-informed policy decisions.

CONCLUSIONS

AI has changed the monitoring “space” in environmental and pollution control through autonomous data collection, intelligent analysis, and decision-support prediction. New AI products show incredibly efficient improvement in performance (95 % detection accuracy out of 50 patterns vs. 80 %, a x24 speed-up, a -60 cost reduction, and a x5 increase in coverage. These improvements enable a shift from reactive response to incidents to proactive and prediction-based environmental management, aligning with the aims of the SDGs.

To enable the successful deployment of AI systems, it is essential to address the challenges related to data quality, model interpretability, computational efficiency, algorithmic fairness, and governance models. Other recent technologies (e.g., federated learning, physics-informed neural networks, and autonomous control systems) have the potential for additional gains in capability.

Furthermore, biofuels such as bioethanol and biodiesel serve as eco-friendly alternatives to conventional fuels; however, their production still poses health risks to factory workers due to the flammable nature of the raw materials and the chemical reactions involved. A study explains that biofuel plants release high levels of isoprene, which reacts with atmospheric ozone and can lead to asthma, allergies, and lung disorders among workers, even with safety measures in place.

Recommendations to move AI for environmental monitoring forward include establishing data collection protocols and quality standards to enable models trained in one region to be transferred to another, a preference towards interpretable methods of AI that can also quantify uncertainty, to foster social acceptance and trust stakeholder distributional support the development of Green A.I., minimizing the computational carbon footprint. The ENVIllogical at E4SD was based on the deep conviction that the large-scale environmental hotspots of our

century - i.e., climate change, the unlimited exploitation of biodiversity, and the release of infinite pollution - are imposing upon us technological challenges beyond human analytical grasp and institutional reaction. Artificial intelligence provides vital tools for comprehending environmental patterns at the largest and fastest times and spatial scales globally, offering green swards in a usable way through swath coverage.

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Chapter 18

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Big data analytics in energy systems and sustainability

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ABSTRACT

The chapter examines the revolutionary impact of big data analytics in the modern energy system with a special focus on sustainability. It begins by outlining the background to big data as applied to energy happens as a result of smart meters, the Internet of Things (IoT) sensors, renewable energy systems such as phasor measurement units (PMU) and systems of supervisory control and data acquisition (SCADA). A separate emphasis is placed on the information of consumers and prosumers, as well as mobility tendencies which grow more crucial in relation to the full energy planning. Using these frameworks as a base, the chapter examines the operational aspects of using big data in incorporating renewable energy, design of smart grids, implementation at a micro- scale in a microgrid, energy storage, and demand optimization. It also explains how EV and mobility data is remodeling energy demand curves and necessary infrastructure. The sustainability component is considered by showing how big data can ease the process of reducing emissions, promoting the vitality of operations, and meeting global objectives of decarbonization. The emergent quantum computing paradigms, artificial intelligence, machine learning, and advanced computational methodologies are reviewed in terms of being the catalysts of the process of accurate forecasting, anomaly detection, and system control in real-time. In addition, the chapter lays the foundations of interrelations between big data and the concept of smart cities and sustainable urban planning, with special attention paid to cross-sectional benefits of such approaches in the realms of energy, transportation and infrastructural activities. Case studies and concept frames demonstrate how data-driven intuitions can make energy networks smarter and more resolute. Finally, the chapter contends that big data analytics is not so much a technical tool, but a strategic driver to sustainability and innovation during the course of an energy transition.

Keywords: Big Data Analytics; Sustainable Energy Systems; Smart Grids; Renewable Energy Integration; Energy Storage Management; Demand-Side Management; Electric Vehicles; Smart Cities.

INTRODUCTION

Due to the accelerating digitalization of energy industry, the significance of Big Data has become significant indeed. In contrast to energy systems where a relatively simplistic equilibrium between production and consumption was the rule in the past, modern systems are dominated by tremendous integration of vast numbers of sensors, measurement devices, and flows of

data. Not only does Big Data improve energy production and distribution efficiency but it also helps to include renewable resources in the grid, regulate electric cars, and plan smart cities which not only promotes ecological sustainability but makes it more economical. Besides, the implementation of Big Data technologies goes beyond household singing to include integrated energy markets. Jia et al. describe new methods of feature extraction in integrated energy equipment machine based on the Big data technology, which has facilitated real-time monitoring of data and grid diagnostics.⁽¹⁾ Their work illustrates the way in which such methodologies may serve as the basis of creating models of intelligent, secure electricity utilization and provides the necessary information about the future decision-making in the complex energy structures. Liu et. al. contribution adds more value to this discussion by examining the applications and systems connected to the energy internet showing the way in which the Big Data can enhance the effectiveness of the energy system at work.⁽¹⁾ Their results shed light on the possibility of using data-based solutions to streamline the work of the energy systems. Moreover, the ratio of security and privacy of the Big Data related to energy systems is also a problem of critical significance. Mai et al. address these issues and highlight the pressing importance of joint security applications of Big Data in power systems as the world in the sector is becoming more digital. Their findings support the use of multi-source complements of security solutions that aim to enhance data safety and analytical effectiveness.⁽²⁾ Such setting highlights the focus on both, direction of relying on the Big 3 Data opportunities and building up of strong data protection structures. The energy storage technologies have significant role to play in facilitating the effective integration of the intermittent renewable sources like the wind and solar. Recent advances in Liquid-Air Energy Storage (LAES) systems are pointing at the possibility to tap into the regasification cold energy to increase system efficiency which is essential to grid peaking and renewable energy storage.⁽³⁾ Nevertheless, internal cold-energy losses remain discrimination issues, and it is important to indicate that this stroke should be combined with other effective energy technologies in order to increase the overall performance of storage. In a particular study Su et al.⁽⁴⁾ examined how energy storage should be set up in the use of hydro-wind-PV in particular geographic locations and concluded that resource utilization efficiency, and specifically ease of cascade hydropower settings, could greatly improve with account of optimal storage configurations. The approach of integrating both places great importance on strategic role of planning in management and storage performance of energy resources so that full use of renewable energy potential could be capitalized. AI has shown significant benefits in the optimization of energy consumption, particularly when it comes to the work of small and medium-sized businesses, which typically have to grapple with increased energy prices and tight environmental policies. The studies have shown that the benefits associated with predictive analytics and real-time automation, as types of AI-driven technologies, grant significant benefits in terms of energy management.⁽⁵⁾ Additionally, the realization of machine learning into the quantum computing paradigm has the potential to transform the process of data on energy analytics. In quantum computing, the speed differences are especially high in the Noisy Intermediate-Scale Quantum (NISQ), where quantum properties of superposition and entanglement are exploited.⁽⁶⁾ A shift to hybrid classical-quantum machine learning algorithms would make it possible to process complex, multi-dimensional data sets that are common in energy analytics, and thus more easily and expeditiously address the energy management challenges.⁽⁷⁾ Information and Communication Technology (ICT) dependency is one of the essential features of smart cities when it comes to increased service delivery and governance. Smart-city models embrace heterogeneous technologies such as Internet of Things, cloud computing and cyber-physical systems to support the creation of sustainable urban environments.⁽⁸⁾ Recently, (gadolinium) doping of carbon nanotubes (CNTs) and graphene oxide (GO) has also been investigated with claims of enhanced structural stability, photoconductivity, and paramagnetic behavior, which are desirable in energy storage, sensing and nano-electronic applications.^(9,10,11,12,13,14,15) This

kind of technological integration maximizes the effect of managing resources and increasing its efficiency in the way the citizens interact and influence governance practices.⁽¹⁶⁾ What is more, the idea of Smart Living arises as a central force behind the creation of the smart-city. The idea of Smart Living becomes a feature of a conventional housing spectrum, and this means a transition to classical human satisfaction settings in accordance with Maslows philosophy of the hierarchy of needs.⁽¹⁷⁾ This is a strategy that does not just make the urban lifestyle focused on the physical aspects but takes into consideration the social and psychological aspects hence offering the holistic living experience that will be flexible and be adapted to the challenges of urbanization that is on a continuous cycle. Digitalization of the energy sector has brought a factor of exponential increase in Big Data, which is fueled by sensors, renewable generation assets, and consumer-level devices. This data transformation creates potentials on optimization of production, distribution, and end-use efficiency.^(18,19) Digitalization and nanotechnology develop quickly, bringing material and energy sciences to a critical edge of convergence data-driven systems and high-tech engineering of materials. Carbon nanotubes and graphene oxide have been in the center of this change, where they have been doped, functionalized and altered in their structures to improve electronic, thermal and photoconductivity.^(20,21,22) Here, the following chapter examines the principles of Big Data in energy, the use of the technology in sustainable energy, and how AI, machine learning, and quantum computing might play a role in developing future smart cities. Combining experimental studies of CNTs, GO, and MXenes with digital solutions to the IoT, cloud computing, and AI, the discussion will focus on comprehensive treatment of sustainable development and the energy transition.

Fundamentals of Big Data in Energy

Information collected by a plethora of sensors, devices, and control systems grounds the cornerstone of Big DATA energy systems. The systematic collection, storage, and analysis of this data facilitate the optimization of energy production, the reduction of losses, and the provision of sustainable management practices. Introduction of big data, in the energy industry, significantly altered several aspects of energy management, consumption assessment, predictive modelling and optimization of the system (table 1).

Table 1. Fundamentals of Big Data in Energy		
Subsection	Description	Key References
Smart Meters and IoT Sensors	Smart meters and IoT-based devices enable high-resolution, real-time monitoring of electricity consumption, grid stability, and energy demand. These data streams feed predictive analytics for efficiency and forecasting.	Khang, Abdullayev et al. ^(23,24)
Renewable Energy Plants (Wind, Solar, Hydro)	Data from wind turbines, solar panels, and hydro plants are integrated for performance optimization, variability prediction, and load balancing. Big data enhances renewable forecasting models.	Abaszade et al. ⁽²⁵⁾ ; Abaszade et al. ⁽²⁶⁾
Transmission and Distribution Grid Data (PMUs, SCADA)	Phasor Measurement Units (PMUs) and SCADA systems generate massive synchronized datasets for real-time monitoring, fault detection, and system control in transmission networks.	Guo et al.
Consumer, Prosumer, and Mobility Data	Data from consumers, prosumers, and electric mobility systems support demand-side management, EV charging optimization, and energy trading. Such datasets also facilitate smart city energy planning.	Khanmammadova et al. ⁽²⁷⁾ ; Khang, Hajimahmud, Ali, et al. ⁽²⁸⁾

Table 1 is a summary of the major contributors of big data in the energy sector. Grid and energy stability can be provided with relatively accurate and real-time data by smart meters and Internet of Things (IoT) sensors. Forecasting and optimisation of business using renewable energy sources (wind, solar and hydro) make use of the data collected by finders of such statutes. Phasor measurement units (PMUs) and supervisory control and data acquisition (SCADA) systems in transmission and distribution systems produce large amounts of co-ordinated information, thus supporting fault diagnosis and system operation. At the same time, insight based on consumers, prosumers, and electric mobility platforms makes the demand-side management, energy trade and smart city planning possible.

Changing the energy systems is an essential transformation that will effectively be driven by the possibility of the high analytical capacities that big data gives, which leads to enhanced efficiency and sustainability in the sector. One of the salient uses of big data is its ability to examine user behavior in terms of how much energy is consumed. As an example, Ma et al. examined links between habitual behavior and home energy consumption, with the postulation to adopt a predictive-maintenance solution based on big data to improve the energy governance of smart-homes.⁽²⁹⁾ This practice can allow inherent insights which would enable a more efficient use of energy according to personal habits. Also, Liao et al. emphasized the role of big-data analytics in the empowerment of electricity-consumption warn-up systems, which in turn promotes user engagement and their understanding of consumption habits.⁽³³⁾ In Audience Russians Noncarbon materials have been highlighted as being sustainable and environmentally friendly and capable of holding energy and true dioxins and eco-tele chemical (ESO) system development in parallel with these advances, natural-source carbon materials such as walnut shells and the fibers of hemp have been emphasized.^(30,31) In addition, composite systems (NiFe₂O₄/ reduced graphene oxide nanomaterials and MXene structure) are also under development due to high surface area, conductivity and stability in supercapacitors.⁽³²⁾ Such inventions highlight the current introduction of nanostructured materials in the renewable-energy solutions, such as supercapacitor, batteries, and fuel cells. Altogether, this research indicates the extensive influence of big-data analytics on the cognition and anticipation of user behavior in energy use, thus allowing to optimize energy consumption, as well as, to foster sustainability, and encourage classes of behavioral manifestations. Overall, it can be seen that the use of big data in the energy industry is complicated, yet it impacts user behavior-analysis, integrated-energy-systems optimization and improvement of data-security. Innovations created through big data not only optimize energy usage and ensure sustainability, but also solve fundamental issues in management and securities of all information, a necessity with regards to the future of energy systems. Big-data analytics can be central to the increased resource-management efficiency, without which sustainable growth is impossible. Sembiring et al. endorse the use of sophisticated technologies such as big-data analytics (BDA) to enhance efficiency and effectiveness of natural--resource management. The authors claim that introducing real-time monitoring and predictive analytics to optimize resource use and, at the same time, minimize the impact on the environment helps to promote sustainable practices.⁽³⁴⁾ This technological innovation and the environmental goal overlap find a reflection in a research conducted by Shi, wherein the author documents that utilization of BDA has an important role to play in terms of sustainable performance deliverables. Shi observes that the utilization of BDA in organizations has had positive effects in all three economic, social and environmental levels hence sustaining sustainability in the overall operation of the organizations.⁽³⁵⁾ Moreover, an increasing number of spheres of professional activity, e.g., healthcare and energy, increasingly recruit BDA, which testifies to its versatility and deep influence. Indicatively, a study focusing on efficiency of the emergency departments in Saudi Arabian hospitals discovered that the combination of BDA and Lean did not only improve operational results significantly but also that it enhanced the

efficiency of these areas.⁽³⁴⁾ The implication of this finding is the possibility of big data improving organizational performance as well as the optimal use of the available resources, a key element of sustainability. Liao et al. once again underline the argument of transformative power of BDA in the energy analysis to facilitate the user-behavior and enhance the energy-consumption behaviors in the context of ongoing consumerism and energy generation, placing how BDA can give a reflection of what and how people use more energy and, moreover, create possible solutions to promote further consumption and address the challenges of energy-efficiency and its sustainability.⁽³³⁾

Smart meters and IoT sensors

Her smart meters and Internet of Things (IoT) sensors enable real-time visits to energy consumption and loads on the grid. All these technologies make the more subtle understanding of prosumer (producer-consumer) behavior possible, demonstrate the effectiveness of implementing dynamic tariff mechanisms, and help to increase the overall energy efficiency. An illustrative case is that smart meters generate large data volumes that can be used to simulate user behaviors; meanwhile, sensor systems based on IoT can observe energy use instantly, which further enhances the precision of demand forecasting and managing consumption.⁽³⁵⁾ These devices joined in smart grid designs give high-resolution data that can be utilized in predictive control plans.

Renewable energy plants (wind, solar, hydro)

There are wind and solar plants as well as hydro plants that come up with large volumes of data with regards to operation and environment. Analytical work of Big Data on these datasets makes it possible to obtain forecasts based on meteorological parameters, offset variability that occurs in nature, and ensure that these have a consistent supply to electric grids. Big Data analytics enable optimization of the plant performance through predictive modelling of the intermittency of renewable generation and optimization of energy efficiency as data collected based on hydrological flows, wind velocity, and solar irradiance are processed into real-time optimization.⁽³⁶⁾

Transmission and distribution grid data (PMUs, SCADA)

Phasor Measurement Units (PMUs) and SCADA have the benefit of having a high degree of accuracy in terms of monitoring both a transmission as well as distribution networks. The large volumes of data obtained out of these technologies helps operators control the electric power flows (voltage, frequency, and power), as well as predict the threats of faults in advance.

Consumer, prosumer, and mobility data

Information gathered on consumers and prosumers- who are consumers and producers of energy at the same time- forms a game changer in enhancing flexibility and interactivity in the energy markets. Other elements in this Big Data ecosystem are electric vehicles and other mobile energy resources. The charge pattern of these sources needs to be checked, and this is beneficial in maintaining grid stability. Big Data on the consumer level make it easy to predict the demand, schedule the charging of the electric vehicle, and trade energy among the prosumers.^(37,38)

Applications in Sustainable Energy Systems

The role of sustainable energy system is increasingly recognized as key facilitator of climate change prevention and long-term ecological balance. More recent research has investigated various aspects of renewable energy technology, how they are combined, and the functions of

digital innovation towards efficiency and sustainability (table 2).

Table 2. Applications in Sustainable Energy Systems		
Subsection	Description	Key References
Renewable Energy Integration	Big data enhances forecasting and integration of wind, solar, and hydro resources by reducing intermittency challenges and improving load balancing.	Abaszade, et al. ⁽³⁹⁾ ; Abaszade et al. ⁽⁴⁰⁾
Smart Grids and Microgrids	Real-time data enables decentralized energy management, fault detection, and resilience in smart and microgrid systems.	Khang et al. ⁽⁴¹⁾
Energy Storage Management	Data analytics optimizes charge-discharge cycles of batteries and supercapacitors, extending lifespan and efficiency.	Singh et al. ⁽⁴²⁾ ; Boychuk et al. ⁽³²⁾
Energy Efficiency and Demand-Side Management	Big data supports energy-saving strategies, demand forecasting, and adaptive control to improve efficiency.	Khang et al. ⁽²³⁾
Electric Vehicles and Mobility	Mobility data analysis improves EV charging infrastructure, fleet management, and integration with renewable energy.	Khanmammadova et al. ⁽⁴³⁾ ; Khang et al. ⁽³⁸⁾

Table 2 outlines the key uses of big data in sustainable energy system. Within the field of renewable-energy incorporation, data analytics helps to forecast accurately and balance the power generation. Smart grids and microgrids enhance resilience and fault tolerance through real-time management. Within energy storage systems, big data contributes to the optimization of battery and super-capacitor operation. At the same time, consumer behavior-driven strategies of energy-efficiency and demand-side management are distinctive. The analysis of data in the sphere of electric cars and movement is an operating foundation of the creation of the infrastructure of charging and its coordination with the grid. The idea of the energy transition does not only imply the integration of renewable energy technologies, but includes broad policy and economic structure changes, which policies and economic structures need to address sustainability. A multiparty bibliometric analysis has suggested that there is a critical united acceptance of the necessity of proactive measures to combat adverse environmental effects caused by the standard of energy sources.⁽⁴³⁾ This move is basic as it forms the basis upon which the future energy systems will be based with prior elements devoted towards ecological care but still remaining economically viable. Furthermore, the online economy is turning out to be a powerful force behind itself in the development of the renewable energy, which is a revolution bent on vibrating to improve sustainability in the energy framework. Liu et al. provided a description of the effects of the digital economy on the renewable energy sector in different national stories and observed that digital technologies would become a critical part of redesigning energy systems and achieving the sustainable development agenda.⁽⁶⁾ Multi-purpose functionality has also been sought after with functionalized thin films and coatings, coupled with nanomaterials, in the context of hydrophobicity, antiviral functionality, and tribology, which have since been applied to tribological interfaces, aerospace and robotic systems.^(43,44,45,46,47) Their applications are especially vital in the latest use of the modern-day anti-carbon technologies of the antenna system, unmanned aerial vehicles (UAVs), and green mobility, all of which coincide with decarbonisation plans worldwide.^(43,44,45) The utilization of these technologies may enable the transformation of renewable energy sources, lead to better management, processing, and integrating of these resources and enable smarter and efficient utilization of the energy. Finally, it is relevant that improvements in forecasting methods, especially hybrid machine-learning techniques, are attracted in their role in real-

time energy control in microgrids. These methodologies also facilitate the accuracy of wind-power predictions in order to support reliability and efficiency of the wind-energy generation which in the end can assist in the management and optimisation of the available renewable energy.⁽⁴⁸⁾ The convergence of predictive technologies and energy-management platforms is reflective of a more general move toward advance fruitfulness of deep analytics in the push to sustainability energy strategy. Overall, policy converges with the digital economy, energy-storage innovation, and advanced predictive analytics in the form of a holistic approach to energy-system developing and maintaining. All these factors serve to foster the resiliency and performance of renewable energy technologies and deal with the urgent issues connecting to the process of climate change.

Renewable Energy Integration

The predictability of renewable energy sources, which will decrease the risks of integrating the latter sources into the electrical grid, is mediated by using Big Data analytics. Precision weather modelling, forecasts of solar radiation as well as speed of the wind is essential in improving stability of energy production. Renewable grid integration also enhances the reduction of intermittency by utilizing methodology based on data-driven forecasting.⁽³⁹⁾

Smart Grids and Microgrids

Smart grids are also fair in balancing the supply and demand using real time exchange of data. Microgrids can be enabled by Big Data as autonomous or semi-autonomous energy units, and it enhances energy resilience. The success of resilient, decentralized grids is based on exchange of data in real-time.⁽²⁴⁾

Energy Storage Management Energy Storage Management

Using the technologies of Big Data in the management of energy storage systems aids in optimization of discharging and charging cycles, which in turn extends the lifelines of the batteries. In addition, such methodology is critical to the stability of grids. The recent findings indicate that data analytics are capable of streamlining charge-discharge relationships both of batteries and supercapacitors.⁽⁴²⁾

Energy Efficiency and Demand-Side Management

Energy-efficiency programs are undertaken through the analysis of consumer behavior. Big Data supported by demand-side management (DSM) allows to reduce peak loads and preserve energy.

Electric Vehicles and Mobility

To control the influence of electric vehicle on the grid, Big Data obtains real-time information. This method forms a core foundation in maximizing the charging infrastructure and implementing vehicle-to-grid (V2G) technologies. EV charging maximization depends on the mobility data analytics.⁽⁴³⁾

Sustainability Impacts of Big Data Analytics

Big data analytics boosts sustainability in the energy industry by cutting down the level of carbon emission, supporting the wider use of renewable sources of energy, diminishing losses attributed to transmission and distribution, and also encouraging fairness in access to the energy. As well, data-based solutions can approve social and economic results, thus helping create a more sustainable future. Sustainability effects of big data analytics (BDA) is a serious junction of technology and environmental responsibility (figure 1).

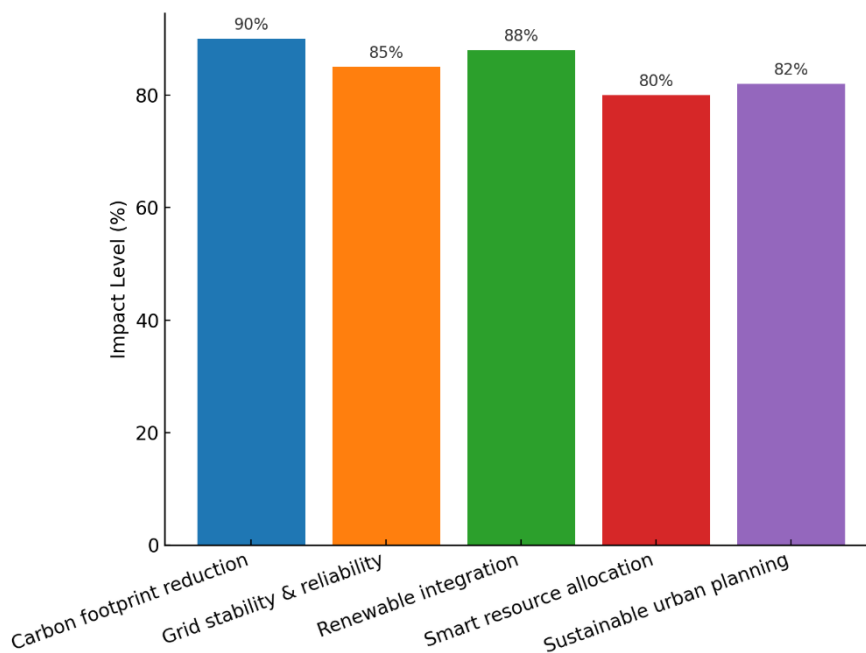


Figure 1. Sustainability Impacts of Big Data Analytics

Figure 1 shows the sustainability implications of the big-data analytics (BDA) in energy systems. It shows that, overall, carbon-footprint reduction, renewable integration, and grid stability are the key areas where contribution is the most significant. BDA also supports strategy of optimal use of resources and sustainable planning of cities and towns, without which it is not possible to say about environmentally friendly energy management. In general, the figure highlights that data-driven strategies enhance environmental and operational aspects of energy infrastructures.

With BDA being more and more commonly used by industries, queues of sustainable practice in various industries and sectors become apparent, which is why this evolution of technology has a lot of positive and negative aspects. Besides, the consequences of BDA are far-reaching to the corporate governance and environmental, social, and governance (ESG) performance. Li et al.⁽⁴⁹⁾ argue that the usage of big-data technologies can help companies to redistribute resources more efficiently, thus, improving their overall ESG performance. These authors claim that beneficial changes in the organizational structures and optimization of capabilities through the application of digital technologies can help firms to initiate sustainable practices. Such aspects of decarbonization as precise emissions tracking, integration of renewable and clever distribution of resources are supported by BDA.^(30,31,32) Renewable-energy systems are not only to be integrated with innovative materials but also with powerful computational and data-oriented models. Smart grids, BDA and advanced analytics make renewable intermittency, grid balancing, and demand-side management an achievable masterpiece.^(35,36,50) Mechatronics double smart materials to improve characterization because of assisting the creation of multi-functional energy appliances that are increasingly efficient.⁽³⁶⁾ Simultaneously, AI due to advances towards IoT are changing manufacturing, healthcare and sustainable infrastructure and make data-centric design indispensable to energy and materials research.⁽⁵¹⁾ However, the authors identify a gap in existing empirical evidence in relation to how BDA has holistic effects in relation to sustainable performance and thus indicate that further inquiry would be necessary

to understand the scope of influence of BDA. Overall, the effects of the integration of BDA on sustainability within multiple areas are significant with regard to the increase of the rate of resource-management efficiency, organizational performance, and proactive environmental strategies. The possibility of using BDA as a way of implementing real time data analysis and decision making makes it a key tool in attaining the sustainability goals in all sectors.

AI, Machine Learning, and Quantum Computing for Energy Analytics

Machine Learning (ML) and Artificial Intelligence (AI) play a decisive role in the energy data processing and analysis. The AI models are used to perform predictive analytics, fault diagnostics, and grid optimization, Einstein models are used to model and optimize intricate energy systems at the same time with quantum computing providing additional opportunities (figure 2).

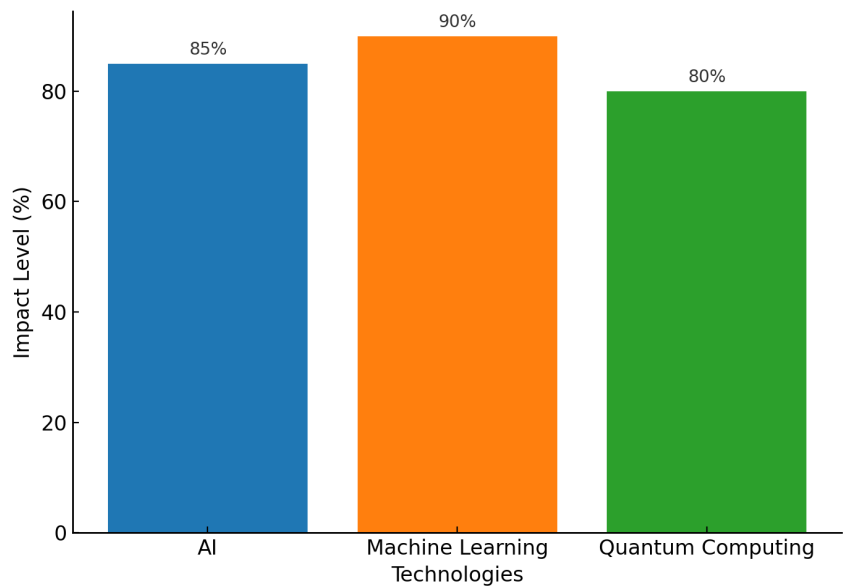


Figure 2. Impact levels of AI, Machine Learning, and Quantum Computing in energy analytics

Figure 2 demonstrates the levels of comparative effects of the artificial intelligence, machine learning, and quantum computing in energy analytics. The most powerful effect is the machine learning, as it is more efficient to predict, optimize, and detect anomalies. Another important contribution is made by artificial intelligence which aids in predictive maintenance and in decision-making. Although quantum computing is not yet demonstrating such high impact, it has an exceptionally high potential in future, with its usage in high-speed simulations and modeling of complicated systems of energy. All these technologies, together with each other, supplement each other, and thus intensifying efficiencies, reliability and sustainability in the modern energy systems.

The synthesis of AI, ML, and quantum computing (QC) is becoming one of the disruptive forces in the field of energy analytics. The proposed triad identifies viable answers to the urgent issue of energy efficiency, cost cutting, and sustainability that many businesses, particularly those that are small and medium enterprises (SMEs), face today. The Internet of Things (IoT), cloud computing, and edge computing contribute to the development of energy analytics and

cannot be met without AI and quantum computing. Such technologies allow real-time making of decisions and low latency data processing which is fundamental to the successful application of the energy-management strategies. Linking sensors, devices, and data to internet services and networks facilitates the process of jet-setting to collect and analyze or analyze data which in turn can be utilized in a wiser decision on energy utilization and develop pervasive environmental awareness.⁽⁵²⁾ Moreover, quantum computing provides possible benefits in optimization of energy systems by the means of sophisticated algorithms, e.g., Bayesian optimization. Examples using quantum measurement zeroing Conventional searches of energy models can be improved with quantum measurement-based methods, which may resolve the complications of energy gradient computations.⁽⁵³⁾ Predictive maintenance, anomaly detectors, and the accelerated optimization of energy systems are made possible by AI, ML, and QC models.^(39,44) They therefore lead to more effective optimization approaches, which will be crucial because the industries are shifting to more and more complex energy systems that quantum computational capacity help shape. Overall, AI, ML, and QC convergence is a strong energy analytics structure capable of solving the energy consumption-related challenges and ensuring sustainability. Through the use of AI to power predictive analytics, quantum computing to process information quickly, and the combination of IoT and cloud services that boost operational efficiencies, companies can make important leaps in their energy approaches.

Smart Cities and Sustainable Urban Planning

Within the framework of smart cities, Big Data takes the form of facilitating optimized consumption trends in energy, transportation systems, lighting and waste management systems. In addition, energy-systems and urban infrastructure synergetic integration facilitates the pursuit of pure environmental quality, which further increases livability (table 3).

Table 3. Smart Cities and Sustainable Urban Planning		
Subsection	Description	References
IoT and Big Data for Smart Cities	IoT-based sensors and big data platforms collect urban data (traffic, energy, water, waste), enabling efficient resource management and citizen-centered services.	Khang et al. ⁽³⁵⁾
Integration of Renewable Energy in Urban Areas	Smart grids in cities integrate solar panels, EV charging stations, and microgrids to support sustainability goals.	Abaszade et al. ⁽³⁶⁾ ; Khanmammadova et al. ⁽⁴⁵⁾
Green Mobility and Transportation	Big data analytics supports EV infrastructure, traffic optimization, and hybrid mobility systems for decarbonization.	Khanmammadova et al. ⁽⁴³⁾ ; Khang et al. ⁽²⁸⁾
Urban Sustainability and Smart Infrastructure	Data-driven planning improves building efficiency, environmental monitoring, and resource allocation for eco-friendly urban design.	Khanmammadova et al. ⁽³⁷⁾ ; Khang et al. ⁽³⁸⁾

Table 3 provides a summary of the critical nature of big-data analytics and the Internet-of-things (IoT) technologies into the realization of smart cities and sustainable city planning. The IoT sensor networks help achieve an effective management of resources, and the smart grids allow the inclusion of renewable energy sources in the inner-city surroundings. At the same time, the development of electric cars and hybrid mobility courses evolves on a greater scale with the help of big-data analytics, thus strengthening the green transportation systems. In urban infrastructure planning, data analytics are used to develop an environmentally friendly and smartly-design urban environment.

The strategy complies with the United Nations Sustainable Development Goals (SDGs). A

holistic approach to city planning and management embodied in the vision of smart cities is one that is centered on sustainability by employing technology. The rapid urbanization is giving the issue of providing efficient services in cities with minimum harm to the environment. The adoption of the principles of smart-city offers a painstaking outline of responding to such predicaments to encourage economic health, social peace, and environmental sustainability. Collective activity of different stakeholders of urban governance is a crucial step in reaching the goals linked with smart cities. It is possible that the combination of innovative technologies and collective government can significantly improve the living standard in cities.⁽⁵⁴⁾ The cohesiveness of different views and skills of different stakeholders, including the government, private industry, and populations, means that smart -city projects will be inclusive and tailored to address the unique set of issues facing urban communities.⁽⁵⁵⁾ The role of human-resource development in smart-city is also highly significant, and in the urban reality, talent multidisciplinary and capable of operating within the intricate technological environments must also be adopted. Technology-savvy and cross-functional workforces are necessary to take up emerging governance demands that is linked to smart-city infrastructure.⁽⁵⁶⁾ Smart urban infrastructure is nurtured by the synergistic combination of big data and IoT, artificial intelligence (AI) as well as green mobility.^(35,36) Further, quantum computing and AI are applied to materials science to generate structural evolution predictors, defect-engineered, and system-optimization models, thus clearing the divide between theory and practice.⁽⁵⁷⁾ These relay networks of advanced materials and intelligent technologies make a new paradigm of big data and nanomaterials collaboratively bringing about sustainable solutions in energy, health, robotic, and smart-city systems. By placing great emphasis on the training and development of digitally literate workforce, the cities are placed in a position to use the potential of digital changes to its full charity. Overall, a complex, integrative method to smart cities realization entails the combinatorics of high-tech solutions, effective city governance, synergistic interaction, and high- ability human resources. The harmonious approach to these aspects will help urban planners guide cities to sustainable destinies where the needs of the inhabitants will be addressed and the environment remains a guardian.^(58,59)

CONCLUSIONS

It has been shown in this chapter that Big Data is more than the core of the development of the sustainable transformation of modern energy systems. New opportunities have been created by the market proliferation of extremely large data flows of sensors, renewable plants, and consumer behavior, which can be optimized in new ways. The higher monitoring and behavioral insights are supported by smart meters and IoT gadgets. Weather-weather predictive analytics and environmental analytics enable the inclusion of renewable energy into power system design with increased confidence. PMUs and SCADAR data help to enhance transmission and distribution stability. Prosumer and mobility information deepens the flexibility and dynamism of the market. The area of application spans across smart grids, levels and behind the scenes in microgrids and storage which are also enjoying the advantages of real-time analytics. Demand-side management is more efficient, because it lowers peak demands and allows responsive pricing. The electric vehicles become both consumers and storage devices, introducing balance to the grid with V2G technologies. The sustainability effect is clearly seen in the decreased emissions, decreased losses and fair access to energy. AI extends the opportunities of predictive and prescriptive energy control. System diagnostics and anomaly detection is optimized by machine learning mechanisms. Quantum computing will bring radical change in computationally intensive optimization and forecast problems. On the city level, Big Data helps to make smart cities and sustainable planning more solid. The mutualization of digital and ecological ambitions is an illustration of the revolutionary power of data. The way forward in research would be to

combine AI and quantum technologies to obtain scalable energy analytics. Amazingly, Big Data is not a tool alone but a strategic pillar toward a creation of a greener, smarter energy future.

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Chapter 19

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Cybersecurity in AI-enabled Infrastructures

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ABSTRACT

Artificial Intelligence (AI) is now an aspect of advancing future infrastructures because it promises to be more efficient, flexible, and automatized. Tech infrastructures are generally more prone to cyber attacks because AI-enabled infrastructures, including smart grid, smart cities, and smart transportation, are interconnected. Entrenched in the underpinnings of such infrastructures is an amalgamation of IoT, big data and cloud computing, which unleash increased potential attacks and potentials. The critical services can be affected by cybersecurity by endangering their reliability with adversarial attacks, data poisoning, and a denial-of-service. It also uses the AI defense that allows identifying the anomaly, predictive analytics, and automated systems to respond to the incident. The aspects of the AI construct which have been discussed as its radar aspects include the complexities in its facet of transparency and argumentative to manipulative data, yet it poses new problems. Among such examples of case studies that still became a target of sophisticated attacks include energy network, health care and urban infrastructure. To solve out these concerns, researchers are considering the possibility of integrating blockchain and quantum computing technologies into the future with digital twins. These new technologies are associated with the added security and stability. However, AI will not become stagnant because it is not only a possible threat but also an effective means of fighting cybersecurity. Innovation and defence initiatives of a firm are the future of safe infrastructures. Finally, in designing adaptive, resilient and sustainable infrastructure systems, AI informed, adaptive and transparent security frameworks will be adopted.

Keywords: Artificial Intelligence; Cybersecurity; Smart Infrastructures; IoT; Big Data; Cloud Computing; Blockchain; Digital Twins; Quantum Computing.

INTRODUCTION

This has turned AI into one of the most powerful success trends in the major infrastructures. It has infiltrated smart city networks, energy and transportation, and health care networks, and has been more efficient and resilient and responsive. Thanks to the seeming convergence of more and more infrastructures and AI, they, too, are apparently prone to cyberattacks. The Top Percent of the Foundation of the attack surface percentages were 90 percent with 100 percent point of high rate of data transfer and real time decision making. The shift in the threat of the enemy indicates the level of urgency of the need to develop efficient cybersecurity measures. Compared to animeghom, then on the side of the draining actuality, the cyber threats, also,

command a wake-up call in the memory of the real material space wherein the societies of such formations were earlier formed. This, in turn, has opportunities and problems of its own because it presents AI into the realm of cybersecurity. On the one hand, AI could identify elaborate fires, intervene within the minimum duration feasible and could be utilized to counter new assaults. On one hand, AI models can be black boxed and hacked, abused and maliciously and maladaptively hacked. The doubling capacity of AI i.e. the thing exists and must bear some degree of responsibility to the harmonization between the safeguard and the innovation. Thus, even this characteristic of the data safety in the AI-led systems has become an object of the controversial list, as to the guarantee of the sustainability and the non-dangerousness of the technological processes. Medical scene has not been the last one to join the wave of implementing the trend to adapt to the utilization of the artificial intelligence to position jobs on the auto shutters and provide more reliable outcomes to the patients. The introduction of the AI into clinical practice proved successful as the hospitals received an opportunity to familiarize themselves with the vision and the plan within the context of air intelligence development.⁽¹⁾ This has not only been achieved by harmonizing the enabling technology technological latency, but also professional health care service providers training the skill-base to be in the forefront of the AI endeavors.⁽¹⁾ It has become an ethical perspective on revolutionizing engineering and materials sciences as well as digital infrastructures because the idea of artificial intelligence (AI) has turned out to be an ethical perspective. It enabled its application not only in smart cities but in health and energy production and production through its predictability and efficiency. The additional available concentrated walls around the surrounding sphere of infrastructures are, nevertheless, contributing incrementally gradually parallel to the contribution of the increase of the smartness intensity of the infrastructure life.^(2,3) It is quite understandable that the threats and the opportunities posed by AI make it create such emotion as the need to install even more security equipment. The predictive modeling and the visualization of the high-performance are compared on the examples of the nanomaterials, i.e. the graphene oxide and the carbon nanotubes.^(4,5,6,7) Since structural resiliency or material research is a research study, digital resiliency adopts (AI) infrastructures. Introduction makes AI a more distinguishing technology, and more that is needed in the realization of the infrastructure and security generation of the future. Support in AI integration simplifies the working process and here in this respect the rule rule in terms of concentrated time-frames governance and quality control can be executed according to will, the outcome of which is a reorganization of a entire healthcare delivery construct. The strength of AI also extends as far as the lifecycle management of the infrastructure, yet it was civilization engineering underpinnings which broke it. The fixes presented by the adoption of AI technologies intensify the intensive infrastructures, as they strengthen their heavy degree of schedule, cost inertia, and price monitoring during the cycles holidaying the construction.⁽⁸⁾ The other AI service unmistakably linked to the construction two sector is the structural health monitoring (SHM) that offers an opportunity to rely on retroversion to any defect and the forecasting of the upkeep that enables expanding of the durability to both its structural property and its stability. So too can the latter perhaps aid in adequately supporting the objective of building efficient cities, yet delivers smart cities thanks to integrated AI and infrastructural building. There is also cloud and edge AI that offers even more scale and responsiveness that will theoretically take advantage in health tracking and patient outcome in the future.⁽⁹⁾ The issues of implementation on AI with the old systems, however, are there. The subsequent issues are outlined by Singh in the sense of how the existing structures will transform into the implementations of the real time communication into the AI. He not only disinfects the necessity to achieve the improvements of the outdated systems but also to mitigate the risks and working enactment of operating AI and merits of application AI in the coming decade.⁽¹⁰⁾ It implies also that the business risks in the cloud-based facility will zero on the venture-basis that will be actively personalized on the broader scale, and that the division of the herein goals at the safety status in general i.e. the

possibilities of resources expansion with the help of the AI assistance can, in the objective sense, be multiple.⁽¹⁰⁾ The susceptibilities of the Critical National Infrastructures (CNIS) system of the energy, the waters system, and the transport system among others are some of the issues. The electronics which form its infrastructures and which these authors are already starting specifying as core to the current day society and which can and even may be the subject of emerging growth in cybersecurity-related anxieties are not only reinforced by generative AI tech but are also capable of being protected by so-called Critical Infrastructure Protection (CIP).⁽¹¹⁾ The threats can be alleviated as the development of Large Language Models (LLM) progresses, and their results can be assessed regarding the standards, which have been released as part of the analysis by Yigit et al. These complexes upon each other are so interdependent that there will be no need to sever the connections of a strong AI security in order to prevent the possible attacks under the assumption that they are working with the arrangement in place that networks do, in fact, exist. Another cybersecurity players also offer another form of electronic insurgency. But when it comes to high-performing the performances of the pieces as it is imagined by its creators, the realization of AI, or at least of the processes that are, somehow, still in its infancy, e.g., Generative Adversarial Networks (GANs), is not only encouraging an aura of demonization of the authenticities; it also is not merely trafficking in the propaganda of spreading information into the scene, which contains, it must be noted, some of the most important Web 2.0 machinery.⁽¹²⁾ The reputational retribution is perhaps too bad under these circumstances of massive opportunity of multimedia material, the strangulation of genuineness in upshot communications and because of the same reason the importance of a confidential being of a procedure of a forensic of the media and substantiation cannot be cursed. The primary benefit of applying AI as an aspect of road cybersecurity is that it may be activated to prepare bulk of past information and locate faint and recognizable patterns aside within them that can be related to the conduct of the pathogen, especially phishing-capability or malicious behaviors. This will be possible since the intruders will always be motivated to evolve and the AI that represents itself must also possess the ability to respond and PD the attacks at their initial levels.⁽¹³⁾ Beyond this, there is explainable AI finding with SHAP and LIME enabling a more objective evaluation of how AI frameworks of cybersecurity capacity allocate and react to danger that would otherwise define a strictness to credit cybersecurity capacity across or even concern itself with. The fallacy of generalizability and prejudice is the first error in the case and the second disadvantage of introducing calls to apply the models of the machine learning (ML) and Deep Learning (DL) in healthcare. The fact they are handled in some of these disadvantages is unethical in nature. The healthcare facilities will need to set up programmers policy-complex to which sticking with technological infrastructure conformity, cost, and such biases into unifying the devices into the, as yet, heterogenous pattern in health care environment conditioned medical examination and treatment practices will add even further layers of distorting to the procedure of diagnosing and treating instruments in patients.⁽¹⁴⁾ The latter is at least a disadvantageous fact, where the ingestion of AI has to balance data feeds in real-time and show breakdowns as a risk to patient safety in the situation of ineffectiveness. Second, the cyber-harmonize pug also threatens the anti-cyber capabilities of our national infrastructures (CNIs), however, data on the digital properties, especially the radiation of modern technology to the employability of AI technologies, harmonizes the labor, is that cyber infrastructures are enduring sinister enemies in the digital realm. Even the fact that there is a threat that actually exists that those AI systems made holes in the infrastructure, and therefore even exceptionally important services, power, water service and communications infrastructure, is also threatened. In the context of safe usage of the machine and learning systems in the critical infrastructure, there must be sufficient preventative mechanisms in the inclusive nature of the periphery of machine learning processes.⁽¹⁵⁾ In addition to that, the conditions under which the effectiveness

of AI based strategies may be debated as a subset of the paradigm of the critical infrastructural protection (CIP) frameworks are interjoined with the presence of even more stringent terms of assessment that would involve the physical challenge and the cybersecurity challenge.⁽¹¹⁾ These systems need susceptibilities and regular exercising to identify and rectify these points in order to become stronger to rectify any sort of assaults. VAD design has filled another vacuum in the health sector by introduction of new technology in the facilitation of better patient outcomes in other ways. One of these insists that decadence between more convenient and modernized VADs is already a trend and is compulsory in the majority of the cases of the occurrences of the heart diseases in the diseased. Suchsyntactic makeup of their equipment and the contemporary surgery can radically shift the propensity of prospects of survival of their heart failure patients as shown by both the studies and Edhen the explanation as to why the new studies appear noteworthy as to such significance in the sphere studies of the cardiac assist technology.⁽¹⁶⁾ The machine machining and precision would also be regarded as part of the technological revolution in the manufacturing improvement. They have been recorded in literature as such machining systems were highly exact and the overall production line more efficient. The ability to continue to exist in the highly altering global environment is already a can-do and a bread-and-rose of production smarter and the smarter drones.

Fundamentals of AI-enabled Infrastructures

Communication systems and transport systems and even energy distribution systems are types of nature that constitute part of the AI-enabled infrastructures. The Internet of Things (IoT), big-data based analytics, cloud computing, and edge computing are also the basis of such infrastructures. The positive implications AI can bring can be seen lowering downtimes due to real time data analysis, preventing complex maintenance systems since the outcome will be automatically decided, and operating many subsystems simultaneously. One of those is smart grids that structure the energy demand and supply it on a dynamic basis within the principles of AI. Similarly, transport can also be optimized using AI-related solutions as they can minimize traffic and decrease congestion (table 1).

Table 1. Fundamentals of AI-enabled Infrastructures		
Aspect	Description	AI Role
Core Technologies	Includes IoT, Big Data, Cloud Computing, and Edge Computing as foundational elements	Provides data-driven analysis and automation for infrastructure management
Key Applications	Smart grids, intelligent transport, healthcare systems, and smart cities	Optimizes performance, safety, and adaptive control in critical services
Data Requirements	Massive, high-quality, real-time data streams for AI training and decision-making	Processes large-scale datasets to enable accurate forecasting and mo

The characteristics of such systems are characterized by unceasing data and information exchange and communication between two or more connected devices whose relationships rely on each other. It thus leads to unnecessary formulation of data, which is likely to be investigated in the most skilled and in the safest way. Such dependence on AI does not merely introduce opportunities to resilience but also fresh grounds of weakness, as well. The need to have AI algorithm transparency and trust arise. The good must have justifiable reasons to be overcome by the evils of AI powered infrastructures. These are then based on either a sound security and good governance mixture and good technology development mix. AI has moved even further and has revolutionized in other spheres as well and been more of the manifestations of the abject effects to the contemporary infrastructures and structures. To be accustomed to the

existence and content of high levels of AI usage, one must get used to the component of the multi-layered usage of AI on the sphere of health care, floor design, and agricultural energy stability. Furthermore, the value of the crossroad of AI and sustainability lies not merely in the opportunity but also in threats, in the first place, in terms of the governance of the climatic change. Regarding the necessity to create AI-based systems that are more energy efficient, i.e., the inclination to introduce such systems into the sphere of cryptocurrency, is already also already having negative implications at the environmental level as a side effect of implementing energy-consuming systems.⁽¹⁷⁾ Code technology s (IoT, Big Data, Cloud, and Edge computing) are used by AI-enabled infrastructures. These systems encode real time information into action information in order to make a decision concerning the energy, health and transportation. According to the existing analysis of field-specific counterparts known as graphene oxide and CNTs, predictive models can be employed to smarten material activity, and could act as a reference to AI aided material optimization.^(18,19) An aeronautical artificial intelligence will only augment efficiency but it will also add complexity and avalanche interoperability to scalability. Smart grids and transportation Infrastructure These constitute the kind of infrastructures that do not just appear to be over-reliant on AI forecasting models, but are also undergo significant consumers of AI forecasting models.⁽²⁰⁾ Fundamentals consider both the opportunities and the risk of the introduction of AI to the essential things initially. In the defined scenario, an artificial intelligence data center knitting, greener energy, and carbon neutrality will present an opportunity of climate-neutral operation re-introducing the digital infrastructures scene with a new veil of sustainability moving forward. Besides, AI has already entered the agricultural sector as well and discontinued the tradition of employing IFST by making recourse to Internet of things (IoT) technologies. The latter may be characterized as a logical extension of AI implementation by the sphere of smart agriculture, it is precision agriculture that may be asserted to have such Facebook benefits as actual tracking of crops and actual decision making based on raw data.⁽²¹⁾ This radicalization is not always what makes the resources deployment simpler, yet the sustainability and feasibility of the agriculture industry, as one of the prevalent uses of AI to stream and refine the efficiencies of my-to-may and seasonal farming management, serve on it. The paradox of the use of AI in the lower-middle-income countries (LMICs) possesses its own concerns. To get deeper insights into the situation, challenges, and mediating factors of AI acceptance in the healthcare (when deployed to diabetes interventions), a study presuppose that the experimental assessment of the immediate environment and existing structures would be carried out on a mass scale.⁽²²⁾ Such variables shall be identified and not only be utilized to replicate AI applications according to modern care delivery models in these areas but also account to priorities in the care of health. On balance, it is possible to say that it is a sophisticated argument in which different sectors in which AI-based infrastructures are discussed, and it assumes the availability of other efficiencies, sustainability, and structural beneficial effects. There will never be a feeling that AI is out of place since AI is still being scaled and is still being stretched to its limits to encompass the areas of the professions as well as taken to any other setting thus there is need to emphasize on the interface between the classical engineering and AI safety structures e.g. Google DeepMind Frontier Safety Framework. Those models might be used to deliver safety operationally credentials of wider thresholds by the critical parameters to the AI systems that would ultimately settle trustworthiness and reliance by the AI usages.⁽²³⁾

Fundamentals of AI-enabled Infrastructures

In addition to a pragmatic factor, AI-planned infrastructures need to be initiated time-gradedly upon a multitude of mindful domains. Electronic intelligence and digital archduers together with 5G communication make them more flexible and efficient. AI can be used to make water management, waste systems, and environmental observation models in the smart

cities. Hospitals have also practiced the use of AI to diagnose and manage certain disease and optimization of some resources. Robots The industry of 4.0 robots has the form of an AI industry. These are quality infrastructures built on the source of the distributed computing environments and performance and complexity is optimized (table 2). Blockchain, 5G communication is defined as the long-range and prevent blocks AI in the digital twin. The breakthroughs are introducing new advances in tracking and prediction systems and performance systems. The healthcare industry is one of the sectors through which the AI-driven data analysis can be implemented; specifically, the patient management facility Penetrak.⁽²⁴⁾ According to Industry 4.0, one has to streamline the process of manufacturing with the use of IoT and AI.⁽²⁵⁾ Nonetheless, to be within the avenue of discussion, the publications that analyze nanomaterials and other technologies report also that predictive modeling is also implemented in large scale, e.g., a predictable reality in the infrastructure of the future, yet predictor in that case, is the precise and multi-vagant entity.^(26,27,28,29,30) 2 Unsurprisingly, AI is not a free phenomenon, but exists as systems that have acquired digital transformation.

Table 2. Fundamentals of AI-enabled Infrastructures		
Aspect	Description	AI Role
Technological Foundation	Built on IoT, Big Data, Edge Computing, Cloud, and 5G networks.	Provides intelligence, automation, and predictive capabilities.
Applications	Smart cities, healthcare, energy, transportation, and Industry 4.0.	Optimizes urban services, energy flow, traffic, and healthcare management.
Data Role	Continuous, large-scale, real-time data is critical for AI decision-making.	Transforms raw data into actionable insights for forecasting and control.
Industrial Integration	Robotics, automation, and predictive maintenance in industrial systems.	Supports real-time monitoring, adaptive robotics, and quality control.
Challenges	Interoperability issues, legacy system integration, and scalability problems.	Facilitates flexible solutions while reducing system vulnerabilities.
Security Imperatives	Cybersecurity must be embedded to ensure trust, privacy, and system resilience.	Enables anomaly detection, secure decision-making, and risk mitigation.
Opportunities	Efficiency, sustainability, innovation, and adaptive infrastructures.	Drives digital transformation and next-generation resilient infrastructures.

The design should include the imposition of the protection and regime to all the layers. The data in AI quality presupposes that even the wrong input or even the corrupted one can destroy the whole machine. Cybersecurity as phenomenon cannot be viewed as an add-on, or as something complementary to the whole. At this point, the societies will be able to high risk as well as guarantee efficiency and security of emerging and operational infrastructures. The reality of interdependence between the stages of technological, economic and security levels is represented in the long-term vision. Incorporated into the systems infrastructure as a form of artificial intelligence (AI) is installed have properties like the users of major paradigm shifts and optimization of the quality of work, and is innovative on most domains. Nevertheless, in this situation, the fortuitous appearance of AI is going to require the corresponding illumination as well not only in the context of the security of the frameworks but also of informing the theory of information exploration and adherence of the system to the already existing systems. Physically meaningful AI safety is in the objects where physical infrastructure, be it civil engineering or mechanical engineering, needs to be taken into account. Specifically, by declaring such idea to propose the very concept of defining the safety brackets and buffers, Farahmand and Neu draw conclusions about the importance of the probabilistic strategies that at one point will

be integrated into the portfolio of AI safety systems.⁽¹⁵⁾ Otherwise, yet another architectural choice made in the information modelling undertaken on the precinct of the nature of AI application figures among other factors in making sure the utilization of AI-based infrastructure are helpful and scalable. Myeka explains how the AI-based database systems will outwit the virtual database systems not only to correct the aspect of quality performance but also to effectively improve the process of developing data into the systems.⁽³¹⁾ The above techniques (partitioning and specialized indexing methods) is crucial in dealing with the massive data that the AI systems demand. With such practices all considered, the infrastructures will be designed to the extent that they are not only capable of addressing the contemporary demand of AI needs, but thematic of some more advanced technologies that can be developed in the long run, given time availability.⁽³¹⁾ It would apply equally to the healthcare sphere in particular, wherein people would have an opportunity to benefit even more due to the coverage of AI in the specified combination of explainable artificial intelligence (XAI) and cloud processing when the latter runs on an edge computing platform. Those assumptions serve to withstand the learning that with the addition of XAI, we will be able to ensure that the medical personages will be capable of inferring the output that will be created by AI and be more certain that they can. Both the companies that also happen to be audaciously viewed, and that are hypothesis-shifted in that matter of the topic of the risk mitigation models, can effortlessly introduce the AI technologies without usability of altering the nature of the business, at large, including the business-critical component in particular.⁽³²⁾ A statistic advantage of AI-based infrastructures is also in cloud computing, which Wang explains by the management techniques of the resource. Using AI assists resource selection according to utilization of all potential park of consumed energy and least amount of the carbon they provide its function as it is brought up against the concept of sustainability.⁽³³⁾ Concisely, the AI-regulated infrastructures implement these principles to reflexivity its aspect of the safety, smarter modeling and thorough incorporation of the systems that can comprise it along with the effective use of the resources within the clouds. All these are essential because AI technologies should not only be successfully operationalized but also tied to the sustainability, efficiency, and the objective of safety.

Cybersecurity Threats in AI-enabled Infrastructures

The cybersecurity threat becomes a rather complex and interstice issue in AI-oriented constructions. Classic advanced attacks such as malware, phishing, and denial of service attacks can also be advanced and now be mounted with complex attacks against AI systems. Adversarial examples- they are motivated manipulations through artificial intelligence models where data is altered to influence change by causing slight deviations or alterations that predict miscarriage of justice. It can create a threat to the training process of the model because the model will learn vulnerable regions that it can apply later in life. They are attractive targets including critical infrastructural portions of power systems, transportation, healthcare and others (table 3). The nanomaterials-based literature study also marks such kind of problem stability among such kinds of situations as the predictive model validity.^(33,34,35,36) These cyber security dangers, thus, coexist in multi-layers with both the digital and physical consequences.

Attack of such systems can be highly disabling and even damaging. Such ripple effects are intensified by the fact that various infrastructures are interlinked in manner that a collapse in one system can be transmitted into another system. Complex criminals exploit the trivial authentication or just insecure software or just insecure IOT toys. More to the point, state-sponsored cyber operation habitually employed infrastructures as its method of strategic interference.

Table 3. Cybersecurity Threats in AI-enabled Infrastructures

Threat Type	Description	Impact on Infrastructures
Adversarial Attacks	Manipulation of AI models by introducing small, imperceptible data changes.	Causes misclassification, wrong predictions, and unsafe decisions.
Data Poisoning	Corrupting training data to embed hidden vulnerabilities into AI systems.	Undermines AI reliability and enables backdoor access to critical systems.
Denial-of-Service (DoS/DDoS)	Overwhelming infrastructure services with excessive traffic to cause disruption.	Interrupts essential services such as energy, transport, and communication.
Malware and Ransomware	Malicious software designed to steal, encrypt, or damage infrastructure data.	Leads to financial losses, data breaches, and operational downtime.
Phishing and Social Engineering	Deceptive techniques used to trick users into revealing sensitive information.	Compromises user identities, system credentials, and trustworthiness.
IoT Device Exploitation	Exploiting weakly secured IoT devices as entry points into infrastructure systems.	Creates cascading failures across interconnected infrastructure networks.
Insider Threats	Malicious actions from authorized personnel or compromised insider accounts.	Breaches internal security, leading to sabotage or data exfiltration.

These requirements need to monitor them on a regular basis, to prepare on the working side, and reshape the cooperation across the divisions. The evolution of cyber threats has been proliferator with the result of offering infrastructures-specific resilience (facilitated by AI). The manifestation of multidimensional cybersecurity risks in the form of intermittent, dynamic and rapidly increasing integration of artificial intelligence (AI) and into all spheres of activity, namely areas of operation critical infrastructure and those under threat, is growing. AI can fuel more efficient processes, and may also be a source of ill intent that deserves its own consideration to cybersecurity policy. In addition, the industries such as healthcare are in some way susceptible to the degree that the information there is sensitive. This is because Zakhmi⁽³⁷⁾ constructed Zero Trust Architectures (ZTA) as the obligative security apparatus during these hazards of high-stake immediate localities. The phrase will always verify never trust comes very well in the area where patient work and integrity put the risk very high. Application in ZTA may be applicable in curbing AI targetcyber threats, since there is found gaps in the connectedness between the theoretical instructions and the practice-based applications. In the paradigm of the supply chain management, the incorporation of AI will point to potential areas of optimization yet will also bring phishing of the cybersecurity. Cybersecurity hazards, which Samuels brings out, reveal that there exists the necessity to mitigate them since the organizations move to the Industry 4.0 and beyond.⁽³⁸⁾ The abatement of the above-discussed barriers, along with AI analytics integration in the supply chains, can be applied to the formation of regulatory landscapes and the establishment of a sustainability and cybersecurity culture. All this and more is a sign of desperate need of prompt overall solutions that will not only inconvenience the development of AI but will curb the unparalleled flood of cybersecurity threats being unleashed in separate f nails. It is significant to establish a synergistic policy, which is regulatory and technical modifications, and culture one adjustments in order to avail the creation of sturdy infrastructures, which can resist the changing climate of cyberthreats.

AI for Cybersecurity Defense

AI has become a powerful tool in raising security levels of infrastructures than infrastructural and information sharing. The issue of locating anomalies with the help of machine learning models can arise because the proportions of data are significant, and locating datasets can occur in real-time. Deep learning can discriminate more expert example patterns of an attack that

might be missed with a more traditional approach. Predictive analytics are also useful in those situations where an organization anticipates threats before they happen to the organization so that it prepares beforehand by anticipating threats. The threat intelligence log captured by the AI is not merely automated but it also presents the fewest elements of reaction to human error and response time. Simultaneously, the development of new graphene sensing and predictive nanomaterials to offer insights on the development of sturdier infrastructures might be presented.^(39,40,41,42) Defense tactics based on favorable dangers can be mitigated by the reinforcement learning. These models must however be conditioned to train under good samples to make them effective (table 4).

Table 4. AI for Cybersecurity Defense		
Defense Strategy	AI Approach	Benefits
Anomaly Detection	Machine learning models analyze traffic patterns to detect irregular behaviors.	Early detection of cyberattacks before damage occurs.
Predictive Analytics	AI forecasts potential threats by analyzing historical and real-time data.	Proactive risk management and improved resilience of infrastructures.
Automated Incident Response	Automated systems respond instantly to security breaches with minimal input.	Faster response times and minimized human error in handling threats.
Reinforcement Learning Defense	Reinforcement learning adapts defenses dynamically against evolving attacks.	Continuously evolving defense strategies tailored to new attack vectors.
Threat Intelligence Systems	AI-driven platforms aggregate and analyze global threat data for defense.	Improved preparedness with real-time global threat awareness.
Identity and Access Management	Biometric systems and AI algorithms manage secure authentication processes.	Enhanced protection of sensitive systems and reduction of unauthorized access.
Fraud and Intrusion Detection	Deep learning models identify anomalies in user behavior and transactions.	Greater accuracy in detecting fraud, hacking, and insider threats.

The AI may also help to authenticate identities, stopping of an intrusion and fraud. The artificial intelligence devices of smart infrastructures have the capacity to capture this information when suspicious energy flow, traffic records, or communication connections occur. These applications show that AI can be applied to serve as a computing defense against attacks related to cyber terrorism. AI, however, should not be carelessly applied in the defense with regards to transparency accountability, and maintenance of ethics. Over the past several years, an AI and its associated sub dependencies, such as Machine Learning (ML) and Deep learning (DL), have changed the fence of cybersecurity. These technologies contribute to the traditional cybersecurity that enables building more efficient, more responsive systems, and adapting the environment that varies with cyber threats. With AI, as the new facet of cybersecurity, the general trend in how organizations identify, react and eradicate different types of cyber menaces has greatly transformed and therefore becomes critical in the issue of modern cybersecurity practices. Besides that, AI methods can be employed in many more aspects of cybersecurity, including intrusion detection, spam detection, botnet, and malware. According to Mohamed, these AI techniques can significantly enhance the performance of the threat detectors not only in relation to the traditional systems, but also eliminate the vulnerability of the legality of older defense systems, in which the cyber-attacks were fully advanced.⁽⁴³⁾ But with restrictions, complexities etc that such models contribute to, one cannot deny them. They also foster the level of accuracy at the detriment of interpretability in the majority of cases, and make AI systems more difficult to apply and utilize in such fields as cybersecurity.⁽⁴⁴⁾ In a manner akin to

a machine to this shift in adversity degree, fresh approaches, including reinforcement learning (RL) have been developed. Rahmati explains the ways RL can be deployed in improving real-time threat abuse by a lowering agent of false positives deployed to trusted infrastructure adhering to adversarial robust architecture as compared to the traditional one.⁽⁴⁵⁾ This enhanced automation of smart cybersecurity can be combined with the highlight of applications capable of safeguarding new-born threats without human intervention almost. Additionally, AI has the capacity to increase cybersecurity rather radically, but straddling that, the device is also some way compromising in the sense that the device can be used by the ill-intentioned user to commit cybercrime. El-Eremy⁽⁴⁶⁾ which provides a single glimpse of how the generative AI would operate in zero-day attacks and, consequently, any 2-sided applications of AI in relation to cybersecurity, are as multifaceted a way of implementing AI as possible. AI-assist cybersecurity is, however, a refreshing addition to the practice of responding to attack, thereby boosting it to the practice of detection and resolution in the wake of multifaceted cyber-crimes. Another aspect, although with the positive image, is to be wary of the moral aspect and potential imperfection of the application of the AI technologies to the realm.

Vulnerabilities of AI in Infrastructures

Amidst some of these advantages, there is also insecurity which the enemies of these infrastructures would also exploit although there are some aspects of positivity which are provided. All of the flaws absent AI models may be introduced when they are trained using the data tied to the stage of data poisoning. It plays a conrotatory role in decision making where decision-making handing skewness is concerned where misjudgment is propagated. Many AI jobs are black boxes, and by that very fact can be difficult to audit and justify their outputs. That can be explained by the fact that there is no transparency which casts doubt on the accountability in making sensitive decisions with regard to security. The attackers will also be able to have the security systems hacked via an algorithmic bias. These offer us their solutions as 0 trust architecture and it must be accomplished swiftly. Research in materials is also not much less close to resolving this problem related to predictive models reliability and validation.^(47,48) Collusion with AI also presents a serious danger in that excessive dependence with AI can result in human laxity. Even the currently testable AI-based systems frequently cannot reveal any capabilities to resist zero-day attacks and new vectors. It is still to apply the law and ethical applications of AI to infrastructures. Explainable AI, extensive testing and a higher level of regulations can shape such weaknesses. AI weaknesses in infrastructures are trans-dimensional and inter-disciplinary in the sense that they cut across many lines (such as for example healthcare, critical national infrastructures, and the small and medium-sized enterprises (SMEs). The security, functional and ethical issue increases the danger that the technology AI can erode it and that they will need a bit of planning in strategic management. Also, SME, especially among low-income areas, poses a high risk to a digital divide. Significant earthquake of these business entities is very poor in finances, resources, and technological capabilities to make use of AI technologies. Such difference could permit justifying the differences in other domains such as tourism where AI could be employed as a competitive advantage provider. This form will necessitate slightly exceptional government assistance and infrastructure and even the possibility to parity distribution AI tools and to drive those vacuity areas to the extreme ends.⁽⁴⁹⁾ The reason is that the population dependence on AI is excessive, and this also imposes greater threats to the comparative freedom of discretion of the decisions of the humans. At the apex AI is highly sensitive to bulk data volumes, (this makes AI models reliant on data quality) entire systems can be bad (table 5), by pipelines of available data.

The development of infrastructure to facilitate the digital capacity plays a crucial role in making sure that small business does not fall behinds in the AI technology economy. The fact

of being an internal organizational weakness and involvement in employment practices also largely contributes to the AI vulnerability.

Table 5. Vulnerabilities of AI in Infrastructures		
Vulnerability	Description	Impact on Infrastructures
Data Poisoning	Injection of malicious or corrupted data into AI training sets.	Leads to unreliable AI systems vulnerable to exploitation.
Adversarial Examples	Small, imperceptible modifications to input data cause wrong predictions.	Causes misclassification and unsafe infrastructure decisions.
Black-box Models	Opaque models with limited explain ability hinder auditing and trust.	Decreases transparency and reduces trust in AI-enabled systems.
Algorithmic Bias	Biased training data leading to unfair or incorrect decisions.	Undermines fairness, accuracy, and inclusivity in infrastructure management.
Data Integrity Issues	Errors or corruption in data pipelines compromise system reliability.	Weakens system resilience and increases likelihood of cascading failures.
Overreliance on AI	Dependence on AI reduces human oversight and situational awareness.	Increases risk of undetected errors or manipulation in critical systems.
Zero-day Vulnerabilities	Exploitable flaws in software or systems unknown to developers.	Exposes infrastructures to high-impact attacks with no immediate patch.
Insufficient Regulations	Lack of standardized frameworks for accountability, ethics, and governance.	Hinders widespread adoption of secure AI practices in critical infrastructures.

Moreover, internal threats, i. e. misinformation, and AI-based ethical dilemmas also exist, which require an attentive assessment of the organizational communication practices. It may appear that the tic approach, i.e. the synthesis of mindsets of communication experts can illuminate the structural errors, which are the unavoidable consequences of the introduction of AI technologies.⁽³⁾ This two-facet security issue, the expressly outward threats, and the covert internal-to-organization challenges render this question, why should the organizations declare the ethical problematic situation of AI implementation, knowing that it will be able to preserve the integrity of functioning. Finally, discussing a weak AI vulnerability in infrastructures is a matter that should be discussed in a multidisciplinary fashion. Such a plan should take into account technical means of possessing cybersecurity, strategic thinking regarding the equal use of AI technologies, and morality put into the center to consider internal and external issues that may arise because of implementing AI.

Emerging Technologies and Future Directions

The future of the new technologies of integrating the AI-enabled cybersecurity infrastructures into the future is bright. Data transactions are provided with strong and univalent security pointlessness of the blockchain. The digital twins are applicable to real-time simulation and monitoring of infrastructures, and in the resilience of cyber threats. Quantum computing has projected it to be mind-altering not only in the encryption level but also in the-decryption level. Such technologies comprise multi-layers defense and infusion or combination of AI. To form a secure power distribution, information blockchain and the use of AI will also take place in a smart grid. The output of individual treatment (table 6) data could be provided using digital twins which could be used to simulate patient data plotted under the healthcare system. The extra aspect of the use of the 5G communication is another factor complicating the interconnection of the infrastructures and requires extra protection. The level of this scope is that there is a need to do more studies on the solution to how the technology can be innovated without

compromising ethical and legal requirement. The current gap lies in the fact that cybersecurity is a problem that the world is currently confronting that demands an inter-disciplinary approach to rising to the challenges. The emerging technologies will be implemented in infrastructures that will be more open, flexible and strong. Lastly, AI-driven infrastructures must be created to counter the evolving threats. They are also required to build intelligent and vulnerable infrastructures with AI. The technologies to be covered later on are altering various fields of the industries that impact the arena of healthcare, manufacturing, and energy and production regulation of the agriculture sector. On this appeal to increased efficiency, to correctness and duration of the product are determined the strides of innovation in the future. Smart grids improve their energy management system in artificial intelligence and edge computing aspects as well. Similarly, the realization of nanomaterials today has come to include the element of innovation towards versified long term sustainability and versatility.^(50,51,52,53,54,55)

Application of deep learning algorithms in processing and analysis of massive bodies of operational data has been very useful and has garnered success in providing the accurate loads forecasting and settlement on issuing the energy assets. Such predictive analytics service will be essential in sidestepping and optimizing the performance of the energy distribution networks that will be heart of the road as the dynamics in the demand swings based on the raising number of renewable energy.⁽²⁰⁾ With big data and machine learning, the process of agriculture in the farming sector of agriculture is transforming. The recent tendencies in the PM ag technology lie in adhering to the overproduction of the presented resources and ongoing adjustment to the altering environments. These technologies were found to be able not only to contribute to the effectiveness of farming source operations but also work harder to secure the food security as farmers can now react suffice to the customer demand and environmental conditions.^(56,57,58,59) In sum, the tendency toward the creation of the surge-forming technologies in the mentioned domains can be formulated as the field of the converging intelligent systems and the improved analysis of the data and creative designing that will eventually become the input of the advances of the efficiency,^(60,61,62,63) sustainability, and the health outcomes.

Table 6. Emerging Technologies and Future Directions		
Technology/ Approach	Description	Impact on Infrastructures
Blockchain	Decentralized and tamper-resistant technology ensuring data integrity and secure transactions.	Enhances trust, prevents tampering, and supports secure data sharing.
Digital Twins	Virtual replicas of infrastructures for real-time monitoring, simulation, and resilience.	Improves proactive maintenance and disaster management in smart systems.
Quantum Computing	Advanced computing that can break classical encryption but also create stronger security.	Provides new cryptographic methods to secure AI-enabled infrastructures.
5G and Beyond	High-speed, low-latency communication enabling massive IoT and real-time AI applications.	Expands connectivity but requires robust safeguards against cyber risks.
Edge AI	Deploying AI models directly on edge devices for faster processing and reduced risks.	Reduces dependency on centralized servers and improves privacy/security.
Explainable AI (XAI)	AI systems designed for transparency, interpretability, and accountability.	Strengthens user trust and adoption of AI in critical infrastructure security.
Cross-disciplinary Collaboration	Joint efforts between governments, academia, and industry for sustainable cybersecurity.	Ensures holistic resilience and shared responsibility in cybersecurity.

This is a favorable omen in that because research is not likely to be silent in providing such guidance the trends are bound to discover the fate of automatized industries.^(64,65,66,67)

CONCLUSIONS

Artificial intelligence has infiltrated both services of disruptive technologies, and a security risk in contemporary infrastructures. Its use in smart grids, transportation and urban control has also resulted in massive efficiency and automation. Nevertheless, the developments equally are revealing other cyber-attacks to cause devastations to infrastructures. The vulnerability of the interconnected systems can be signaled by cybersecurity attacks like hostile demonstrations reportedly through adversarial attacks, data poisoning, and denial-of-service. Defensive aspects of AI also include the cases where the latter is implemented to identify anomaly, real-time monitoring, and predictive analytics. Despite these advantages, AIs in themselves are liable to being manipulated and not being transparent. To address these pitfalls multidisciplinary solutions which require the use of technology, regulation as well as ethical standards are needed. New developments are made in the field of quantum computing and the blockchain that stand chances of more certain cyber security structures. Artificial Intelligence (AI)-driven digital twins, have offered the capability to observe and warn in time against developing threats. However, cyber-attacks are multidimensional in their essence, and they require ongoing advancement of adaptation and innovation. The industry and academia should work together with the government to put strong infrastructures. It will need to reach a middle ground where they can both have AI/intelligible. It is crucial that both have the potential to weaponize AI, rooted in the stability of the future and based on the scaling policies, which are essential to sustainability in the long run. The high potential is to work towards creation of smart infrastructures more resistant to cyber-attacks. With it, AIs cybersecurity will help it become the critical corpse solution to active, adaptable, and future-proofed structures.

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Chapter 20

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Global Regulatory Frameworks and Sustainable Policy Approaches

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ABSTRACT

This article examines global regulatory frameworks and sustainable policy approaches, emphasizing the central role of regulation in addressing persistent market failures linked to long-term environmental, social, and technological risks. It analyzes how international treaties, soft-law instruments, and supervisory standards cascade into national and sectoral regulations, shaping sustainability outcomes across jurisdictions. The study compares major policy instruments—including command-and-control regulation, market-based mechanisms, disclosure-based policies, fiscal tools, and experimentalist governance—assessing their effectiveness, equity implications, and implementation constraints. Particular attention is given to sector-specific frameworks in climate and environmental governance, energy and industry transformation, sustainable finance and corporate disclosure, digital and artificial intelligence systems, and health and food systems. The article further explores regional regulatory approaches in the European Union, the United States, China, South Asia, Africa, Latin America, and the ASEAN-Pacific region, highlighting how state capacity, industrial strategy, and political economy influence policy design and enforcement. The analysis underscores that regulatory success depends less on aspirational targets than on institutional coherence, robust measurement, reporting and verification systems, enforcement capacity, and standard interoperability. Finally, the article outlines future scenarios toward 2035, arguing for adaptive, data-driven, and justice-oriented regulatory frameworks capable of managing emerging risks—particularly those associated with the growing environmental footprint of artificial intelligence—while ensuring durable and inclusive sustainability transitions.

Keywords: Global regulation; Sustainable policy; Climate governance; Regulatory instruments; Artificial intelligence impacts; Just transition

INTRODUCTION

Why Regulation Shapes Sustainability Outcomes

Markets are strong capital allocation mechanisms, but long-term social and environmental risks are chronically mispriced by the market. An example is climate change: harms that are decades old, which cut across boundaries and are full of profound uncertainty, which traditional discounting and incomplete information cannot readily represent.^(1,2) The degradation of biodiversity is also under-priced since most ecosystem services are not priced until they fail, and invasive species and habitat destruction will be the diffuse costs that cannot be internalized by the individuals acting privately.⁽³⁾ These failures are augmented by new digital externalities: AI and data-centers increase the energy and water demands growing with their size and not reported in forms helpful to decision-making, so under-incentivising efficiency and decarbonization of grids.⁽⁴⁾ In those markets in which markets respond, such as consumer

pressure, investor activism, or voluntary standards, it has been found that the response is often incomplete or slow without clear signals of policy.⁽⁵⁾

There is regulation to rectify such failures: first, it charges or limits externalities through carbon taxes, emission trading, performance requirements, endangered-species safeguards, and product-stewardship requirements.⁽⁶⁾ Second, it establishes guardrails to avoid high-probability harms (e.g., methane leaks, deforestation) and to deal with low-probability, high-impact risks (e.g., cascading ecosystem or power-system failures).^(2,3) Third, it increases the rate of innovation diffusion through the reduction of the costs of adoption (auctions, tax credits), harmonization of infrastructures (grid codes, data and reporting standards) and provision of certainty which stimulates private investment.^(7,8) Lastly, it would facilitate a fair transition through cost-sharing and benefits by worker, region, and supply chain, including through reskilling benefits, specific rebates, and community benefits, to make decarbonization a politically and socially sustainable transition.⁽⁹⁾

This chapter charts the world-system of sustainability regulation and demonstrates the way the international treaties, soft-law norms, and supervisory expectations trickle down into national and local regulations.^(2,3) We evaluate the effectiveness of policy tools, including command-and-control, market-based, disclose, fiscal policies, and experimentalist, and compare them in terms of their effectiveness.^(5,10) Then we examine regional differences in the European Union, United States, China, India/South Asia, Africa, Latin America and ASEAN/Pacific based on the influence of state capacity, industrial strategy and political coalitions on instrument choice.^(8,11) The whole time, we pre-implementation realities implementation realities measurement, reporting, and verification (MRV); enforcement capacity; interoperability of standards; distributional design since results are dependent less on aspirational goals and more on institutional implementation.^(5,7) We conclude with future directions to 2035 that are neither fast nor swift enough to drive but are balancing with the emerging risks of AI energy footprint, or the nature-related financial risks.^(2,4)

Road map: section 3 elucidates some important concepts and governance prisms (polycentricity, precaution vs. innovation, policy feedbacks). Section 4 scans over the treaty layer and the institution layer. Part 5 explores sector schemes: climate, energy-industry, finance and disclosure, digital/AI, and food-health; making the choice of instruments to be quantifiable. Section 6 makes a comparison of instruments and provides a design matrix. Section 7 is case comparisons on a regional level. Section 8 deals with cross-border coordination, trade and standards interoperability. In Section 9, 10, and 11, there is information on justice, implementation, and adaptive regulation and continuous improvement metrics. The case studies are succinct and contrasting in section 12. Section 13 illustrates scenarios up to 2035. Sections 14 to 17 are topped off with practical recommendations, glossary, discussion prompts and resource guide.

Key Concepts & Analytical Lenses

Policy objective of sustainability is a combination of the environmental integrity, social equity and long term economic resilience. Environmental integrity poses the question of whether policy pathways should not exceed planetary limits and keep ecosystems across generations intact; social equity based on distributional outcomes and procedural fairness; long-term economic resilience based on structural change and adaptive capacity to shocks.⁽¹²⁾ These three dimensions are complementary, yet tend to conflict in the short term, that is why sustainability policy is not only about what targets to achieve and what tools to use, but about how to design governance.⁽¹³⁾

This design space can be mapped with the help of regulatory typologies. Command-and-control standards impose definite limits or technological imperatives and cannot be dispensed with in case harms are acute, measurable, and demand certainty (e.g. ban on ozone-depleting substances). Internalized by market-based instruments, such as carbon pricing, tradable permits, and differentiated charges, market-based policies are effective in that they reduce externalities, but they are not costly since they require coverage, price paths, and complementary actions alleviating frictions between political economy.⁽¹⁰⁾ Sustainability reporting (via disclosure-based regulation e.g. under emerging global baselines) is tried to discipline markets by information; in effect, only works best when comparable and audited disclosures are decision-useful and investors can act on them.⁽¹⁴⁾ Co- /self-regulation and meta-regulation move focus of organizational systems, such as risk management, governance, and learning loops, which are subject to the supervision of the masses; their potential is flexibility, the danger is performative compliance without enforcement.⁽¹⁵⁾ Experimentalist governance focuses on iterative goal-setting, benchmarking and revising across jurisdictions; it can speed up the learning in a state of uncertainty with accountability being preserved.⁽¹⁶⁾ Lastly, polycentric governance acknowledges various decision centers including local, national, transnational that operate through norms and mutual adaptation instead of hierarchy; it is more consistent with commons problems of heterogeneous contexts.⁽¹³⁾

The binding tissue between instruments and levels is known as policy coherence. On a horizontal front, energy, industry, agriculture, finance, labor and environment ministries need to coordinate their efforts to ensure no whiplash (e.g., industrial competitiveness plans eroding emissions caps); on the vertical front, local-national-global connections have to coordinate to ensure there is no leakage and duplication.⁽¹²⁾ Even though the term coherence does not imply uniformity, plausible national strategies tend to combine tools and arrange them, such as pilots, scaled standards, pricing, or coordinate with trade and innovation policy.⁽¹⁰⁾

Other criticism prisms enhance design decisions. Just transition lens foregrounds shares regional, sectoral, and worker distributional effects and has social dialogue and support policies (retraining, income support, place-based development) to climate and industrial strategies.⁽¹⁶⁾ The precaution innovation lens describes decisions in the face of uncertainty: take action now to insure against irreversible damages but permits trial and error and spread of alternatives that are cleaner.^(17,18) The feedbacks of policies and lock-in remind us that the present-day regulations condition the future coalitions, e.g. carbon pricing to finance visible benefits will be more popular, and infrastructure decisions may compromise the high-emissions paths.⁽¹⁰⁾ Path dependence means that there is a need to utilize reform windows to re-route investment cycles and standards at the time of technological change or crisis.⁽¹⁶⁾ The role of incumbents, new entrants, and organized labor, along with the role of the durable change to unite the plausible commitments with the transitional support and the open burden-sharing, is emphasized by the political economy of reform.⁽¹²⁾

Global Treaties & Institutions: The Rule-Setting Layer

MEAs offer anchor norms, targets and reporting structures which domestically based regulating bodies convert into national law. The UNFCCC and Paris Agreement provide long-term temperature objectives, nationally determined contributions (NDCs), transparency levels, and a five-year ambition cycle, which thoroughly incorporates domestic policy changes^(12,16) in climate. The Kunming -Montreal Global Biodiversity Framework (GBF) is a document that outlines four goals and 23 targets of the Convention on Biological Diversity, now incorporates a continuously evolving system of monitoring to assess progress - an instance of target-and-

review governance, which now requires integration at the domestic level, primarily in land-use, finance, agriculture, and trade.^(12,19)

Montreal Protocol on Substances that Deplete the Ozone Layer is one of the brightest examples of an adaptive treaty-making: non-compliance regime, technology switching schedule supported by finances, and binding control schedules. It applies this reasoning to HFCs in its Kigali Amendment; recent studies highlight the importance of lacing the fridge transition with an appliance efficiency standard to get the greatest climate gains- a lesson in how sectoral policies can be made consistent with the objective of treaties.⁽²⁰⁾ The Basel Convention on hazardous-waste governance has increased restrictions on the transboundary flows of plastic wastes; national governments are now implementing prior informed consent and quality standards, and tracking, which can be seen as examples of how treaty amendments can transform the global value chains when combined with domestic capacity.⁽¹⁸⁾

The interfaces of trade and investment become the precursors of sustainability. WTO regulations determine the policy space on carbon pricing, border adjustments, subsidies and product standards. With the spread of climate measures, the system is fumbling towards interoperability by design (common methodologies, due process, and transparency) to ensure a minimum number of frictions are not created at the cost of not pursuing decarbonization ambition, indicating that there is a need to improve the alignment between trade disciplines and climate/biodiversity ambitions.^(10,12) Sustainability chapters are now incorporated in preferential trade agreements, and in some cases value-chain commitments; these need to be monitored, enforceable, and followed up domestically in addition to having a hortatory text.⁽¹⁶⁾

The social gaps in the sustainability governance are bridged by the labor and human rights. The principles that have triggered the national due-diligence regimes and reporting requirements are ILO just transition guidance and UN Guiding Principles on Business and Human Rights (UNGPs). However, it has been revealed that many companies are still talk-oriented and the disclosure in them is only thin, which indicates that enforceable obligations, supervisory ability, and enforceable backstop of liability are essential.⁽¹⁵⁾ Integrating labor rights within climate-industrial policy (e.g. conditional subsidies, workforce transition alliances) makes it more legit and faster to adopt.⁽¹⁶⁾

Standard setting institutions transform general norms into technical specifications. The measurement, management, and assurance of energy, environmental, and circular-economy sectors, as well as of finance, rely on ISO/IEC standards, and the International standards board (ISSB) has published IFRS S1 and S2, a global standard of investor-centered sustainability disclosure all spillovers to risk management of corporates and capital allocation.⁽¹⁴⁾ Disclosure regimes are based on comparability, assurance, and integration into financial supervision, otherwise they are likely to remain as box-ticking exercises.^(14,15)

The soft law and compliance work simultaneously. Most of the treaty obligations are based on national transposition, peer review, transparency and mutual recognition as opposed to supranational enforcement. Hard sanctions can be replaced by sunset-plus-review clauses, learning-based stocktakes, watchdog transparency (registries, standardized reports), and making coalitions reform ready.^(12,16) Polycentricity is relevant in this respect: cities, regions, and transnational networks tend to become more rapid than the national governments, which produces demonstration effects and closes the ratchet.⁽¹³⁾ In situations with uncertain but potentially disastrous risks, precautionary design, in combination with innovation sandboxes and periodic reviews of evidence, is useful in helping treaties and standards navigate between

stagnation and blindly rushing ahead.^(17,18) Overall, the rule-setting layer is effective when it is MEA-coherent, aligns disclosure, standards, and incentives, and it institutionalizes the process of learning and tightening by policy.^(10,12)

Sector/Domain Frameworks: Where Rules Meet Real Economies

Climate & Environment

Policy goals: internalize environmental externalities, bend absolute emissions and biodiversity loss curves, and build climate resilience while safeguarding livelihoods. This means achieving timely, measurable reductions in greenhouse gases (GHGs), halting ecosystem degradation, and minimizing pollution across product life cycles.⁽¹²⁾

Core instruments

Emissions governance: the main tools of price-based motivators are cap-and-trade and carbon taxes. Cap-and-trade provides certainty of quantities, and allowances in the trade, taxes provide a stable marginal abatement incentive and recycling possibilities of revenue. Things are becoming more blurred with hybrid designs (price floors/ceilings in ETS; emissions-indexed tax credits). The use of offsets has to be limited to high-integrity credits that have conservative baselines, strong permanence, leakage protection, and a transparent project level.^(10,21) MRV systems need to be digital-first: standardized protocol and 3rd-party verification and asset level data to facilitate audits and enforcement.

Natural capital: the rules of biodiversity net-gain (BNG) mandate ecological improvement of developments; no-deforestation supply-chain requirements associate compliance on imports with geolocation and geolocation; and watershed governance (watershed governance) combines permits, quality trading, and source-water protection compacts to align upstream land use with downstream water quality results.⁽²²⁾ Waste & circularity. Extended Producer Responsibility (EPR) causes producers to be economically and operationally liable to dispose of their goods at their end-of-life; eco-design establishes durability, reparability and quantity of recycled content criteria; right-to-repair policies allow access to parts, manuals, and diagnostics with no harm and a security risk and data protection.^(23,24)

Implementation challenges. Abatement is undermined by too low price signals, limited coverage or enforcing these signals. The offset programs can be prone to excessive over-crediting in the absence of conservative baselines and independent verification.⁽²¹⁾ Without ecological skills and expertise, data, and compliance capacity, local authorities in charge of watersheds and BNG may come to a halt.⁽²²⁾ The instruments of circularity demand product data (materials, chemicals of concern) that is interoperable and coordination among thousands of SMEs.

Equity considerations: carbon pricing may be retrogressive when the revenues are not recycled; equity-by-design implies that it has targeted subsidies of the form of rebates, rural mobility options, and low-income building retrofits. BNG must avoid green gentrification where funding is done on community stewardship and respecting tenure rights. The informal waste pickers should be incorporated in EPR programs through producer responsibility organizations based on the living-income contracts and safety standards. Metrics. Emissions: GHGs by absolute and intensity; price of allowance; tax coverage. Nature: hectares of habitat increase, richness of species, importation of deforestation. Circularity: rates of collection / recycling of each material, rate of repair, lifetime of the product, phase out of hazardous substances. Equity: proportion of the carbon-pricing revenues to the vulnerable groups; the scores of community participation.^(10,23)

Energy & Industry

Policy goals: rapidly decarbonize power, electrify demand, scale firm low-carbon fuels, and transform materials industries (steel, cement, chemicals) while maintaining reliability and affordability.

Core instruments

Clean power deployment: technology-neutral or targeted auctions that have strong pre-qualification, performance insurance and bankable offtake use less money and less delivery risk, Renewable Portfolio Standards (RPS)/Contracts-for-Difference use more scale, grid codes and interconnection queue reform use more deliverability and minimize curtailment and flexibility markets (storage, demand response) use variable renewables.

Industrial decarbonization: performance targets (e.g., tCO₂ per ton of steel / cement) are ratcheted down with long lead-time visibility; hydrogen support targets upstream production standards and demand-side contracts; CCUS authorizes pore-space access, liability, and MRV and leaves support of hard-to-abate processes to governments.⁽²⁵⁾ Carbon leakage tools. Embedded-carbon costs to imports are equated by the border adjustment mechanisms, and a decarbonisation transition plans with time constraints ensure competitiveness, without disregarding price signals or contingent assistance on decarbonisation paths.⁽²⁶⁾

Implementation challenges: under-bidding at auction, congestion in the supply chain may lead to non-delivery; backlog in the queue and sluggish network build-out strands the projects. The requirements of industrial standards (credible product-level MRV (e.g., low-carbon cement clinker ratios), harmonized definitions) are to prevent the problem of green protectionism.⁽²⁵⁾ The CBAM-type measures entail a high quality of embedded-carbon data and a sound customs administration.⁽²⁶⁾

Equity considerations: design auctions that come with community benefits agreement and local hiring; safeguard the low-income consumers through special purpose bill credits. In the case of industry, pair standards together with just-transition compacts, reskilling, regional investment fund, and SME supplier enablement.

Metrics: levelized cost of electricity (delivered), price in an auction, average interconnection time; industrial emissions per unit of output; cost of hydrogen and its usage rates; CCUS capture rates and permanent storage; carbon-intensity differentials between domestic and imported good.^(25,26)

Finance & Corporate Disclosure

Policy goals: align capital markets with sustainable outcomes by improving decision-useful transparency, curbing greenwash, and pricing climate- and nature-related risks in supervision.

Core instruments

Reporting baselines: the ISSB's IFRS S1/S2 create a global floor for investor-focused sustainability and climate disclosures (governance, strategy, risk management, metrics/targets). Jurisdictions adopting double materiality expand scope to outward impacts alongside financial materiality. Taxonomies & labels. Decision-useful classifications (with "do no significant harm" and minimum safeguards) guide product labeling, disclosures, and public procurement; transition categories can crowd-in high-emitting sectors with science-based pathways.

Prudential/supervisory tools: climate scenario analysis and stress testing assess credit-

market vulnerabilities; stewardship codes formalize investor engagement escalation (Flood-tests and exploratory exercises are maturing toward capital frameworks).⁽²⁷⁾ Implementation challenges. Interoperability across standards (global baseline vs regional requirements), data gaps (Scope 3, private firms), and assurance capacity. Taxonomy usability for SMEs and banks is often low without simplified criteria and digital tags. Stress tests can become “model theater” if not linked to risk appetite, underwriting standards, and disclosure feedback loops.⁽²⁷⁾

Equity considerations: avoid excluding MSMEs and emerging-market issuers by providing proportionality, simplified templates, and technical assistance; ensure transition finance reaches carbon-intensive regions to prevent stranded communities.

Metrics: disclosure coverage/assurance rates, taxonomy-aligned revenue/CapEx shares, portfolio-level financed emissions, scenario-consistent capital allocation, escalation outcomes in stewardship.^(27,28)

Digital, Data & AI

Policy goals: unlock trustworthy sustainability data flows; manage AI’s environmental footprint and systemic risks; and harden cyber-physical infrastructure as part of resilience.

Core instruments

Data & cross-border flows: establish sustainability “data rooms” with shared schemas; mandate interoperable emissions/energy data at asset and product level (digital product passports); ensure privacy/security via risk-based data protection. AI safety & sustainability. Require model-risk management, transparency on training data/limitations, and energy-use disclosures (training and inference). Encourage compute-efficient methods and siting powered by low-carbon grids.^(4,29)

Cyber-resilience: critical-infrastructure standards (zero-trust, SBOMs, incident reporting), third-party risk rules for cloud and OT systems, and minimum encryption/authentication across supply chains. Implementation challenges. Sparse and non-comparable AI energy data and confidentiality claims limit accountability.⁽²⁹⁾ Product-level emissions data face fragmentation and IP concerns. Cyber rules can overburden SMEs without shared services and templates.

Equity considerations: prevent data monopolies by mandating access to public-interest datasets; ensure AI energy-cost pass-throughs do not disproportionately burden low-income users; include SME-friendly cyber compliance toolkits.

Metrics: share of assets/products with machine-readable emissions data; model energy per parameter/training run; percentage of critical entities meeting resilience benchmarks; incident response times.^(4,29)

Health, Food & Biosafety

Policy goals: contain antimicrobial resistance (AMR), manage biosafety/biosecurity risks, and steer food systems toward nutrition, safety, and climate resilience.

Core instruments

AMR controls: integrated One-Health plans: prescription stewardship, surveillance, water/sanitation investments, and market-entry rewards for novel antimicrobials; procurement that favors access-oriented licensing. Biosafety standards. Risk-tiered lab and field protocols, gene-

drive governance, and incident reporting with independent oversight.

Food-system sustainability: sustainable input standards (fertilizer efficiency, pesticide risk), nutrition labeling, food-loss reduction mandates, and climate-resilient agriculture (soil health, water efficiency) paired with farmer extension. Implementation challenges. Financing gaps for AMR innovation and surveillance; fragmented food standards; limited biosafety capacity in low-resource settings.

Equity considerations: ensure equitable access to diagnostics and antibiotics, support smallholders through climate-smart extension and credit, and protect indigenous/community food systems. Metrics. Infection and resistance prevalence; antibiotic consumption intensity; food-loss rates; nutrition outcomes; farm-level emissions and water productivity.

Governance Models & Policy Instruments

Command-and-control: harms are acute and irreversible or they are priced in a poor way and therefore the harms they cause are clear and the guardrails are clearly indicated by bans, limits and performance standards. They suit best where performance can be measured, where tightening can be done in stages, and where flexibility in design is required (e.g. output-based allocations changing to absolute caps). There is the risk of technology lock-in where standards identify solutions directly, not results; overcome this by drafting outcome-based regulations and by ensuring that there are many ways of compliance.

Market-based: externalities are monetized by carbon pricing (taxes or ETS), tradable permits (renewable portfolio obligations, vehicle fuel-economy credits), differentiated tariffs, and congestion pricing and can promote cost-optimal abatement. This has been demonstrated by emerging results demonstrating that carbon pricing has provided quantifiable cuts when properly instituted even at small amounts and has complemented, rather than substituted, complementary policies to generate innovation, infrastructure, and equity.⁽¹⁰⁾ Border adjustments have the benefit of safeguarding policy ambition against leakage, but entail effective embedded-carbon accounting and an effective domestic regime.

Information & disclosure: information asymmetries are minimized through corporate reporting, product labels, asset-level transparency, as well as open data. The ISSB standards (IFRS S1/S2) create a worldwide investor-centered standard; those jurisdictions which impose double materiality mandate disclosure of effects on both people and the planet in addition to financial materiality.⁽²⁸⁾ The lack of assurance of disclosure, comparability, and post-disclosure supervision is prone to transparency theater. Disclose assurance, enforcement, and supervision of capital markets.

Financial & fiscal: first-of-a-kind projects are de-risked with subsidies, tax credits, green public procurement, concessional/blended finance, and just transition funds and diffusion is hastened. Protect against windfalls through the competitive allocation (auctions), additionality tests and payout based on milestones. Observe the standards of low-carbon materials in order to establish the demand pull in the hard-to-abate sectors.

Collaborative/experimentalist: mobilized coalitions to deal with uncertainty through regulatory sandboxes, adaptive licensing, challenge prizes, and mission-oriented programs. Publish learning of pilots, make use of sunset and review clauses and scale what works. The use of experimentalist governance is bright in the situations when technologies and risks change rapidly (e.g., AI energy-use disclosures and model- risk controls).^(4,29)

Institutional design: whole-of-government taskforces, cross-ministry action, arm-length implementation by independent regulators, stakeholder councils (labor, SMEs, communities) all help in reducing the friction in implementation.

Invest state capacity: digital permitting, MRV infrastructure, and local-government technical support.

Regional Approaches Comparative Perspectives

European Union

Strategic narrative: the European Green Deal aims to hard-wire climate-neutrality and circularity into the single market. The EU leans on economy-wide standards, product policy, and carbon markets to drive systemic change.

Flagship instruments: EU ETS (and ETS2 for buildings/road transport), Effort-Sharing Regulation, product eco-design and energy labeling, circular economy package (EPR for packaging/e-waste; right-to-repair trajectories), corporate sustainability due diligence and reporting, and the Carbon Border Adjustment Mechanism (CBAM) for leakage control.⁽²⁶⁾

Strengths/weaknesses: strengths include rule-making capacity, market integration, and increasingly interoperable disclosures. Weaknesses are uneven national capacity, slow grid expansion, and compliance complexity for SMEs.

Spillovers: EU product and reporting rules are de-facto global standards for exporters; CBAM pushes trading partners toward better emissions accounting.⁽²⁶⁾

United States

Strategic narrative: incentive-heavy industrial policy plus regulatory backstops. Federal tax credits and loans catalyze private investment, while EPA authority and state leadership handle standards and procurement.

Flagship instruments: long-duration tax credits for clean power, storage, hydrogen, CCS; EPA performance standards; state RPS/clean energy standards; federal and state procurement of low-carbon materials; transmission siting reforms.

Strengths/weaknesses: deep capital markets, innovation ecosystems, and demand-pull from procurement are strengths. Weaknesses include litigation risk, interconnection backlogs, and policy whiplash across administrations.

Spillovers: global clean-tech cost reductions and supply-chain diversification; competitive pressure on allied industrial policies.

China

Strategic narrative: dual-carbon goals guide a state-led transition, integrating ETS evolution with powerful industrial policy in clean tech manufacturing and grids.

Flagship instruments: national ETS expanding beyond power to heavy industry; large-scale renewables plus ultra-high-voltage transmission; local performance targets; data governance tightening with emerging sustainability data initiatives.

Strengths/weaknesses: strengths: speed/scale of manufacturing, grid build-out, and pilot-to-national policy diffusion. Weaknesses: data transparency, varied provincial enforcement, and coal reliance in power balancing.

Spillovers: cost leadership in solar, batteries, and EVs; global standard-setting in supply chains.

India & South Asia

Strategic narrative: energy-security-led transition, with rapid renewables growth, grid expansion, and an adaptation-forward agenda.

Flagship instruments: competitive auctions for solar/wind; green open-access and transmission corridors; renewable purchase obligations; green hydrogen and storage tenders; climate-resilient agriculture missions and sustainability finance frameworks.

Strengths/weaknesses: scale and auction experience are strengths; DISCOM finances, land/permits, and grid congestion remain bottlenecks.

Spillovers: regional power-pooling and standards for low-cost renewables in emerging markets.

Africa

Strategic narrative: universal energy access, resilience, and green industrialization anchored in mineral value chains and nature-based solutions.

Flagship instruments: IPP frameworks and renewable auctions, mini-grid regulations, clean-cooking standards, and land-use policies to protect high-value ecosystems. Nature- and climate-risk stress testing for banks is emerging (to price ecosystem loss and climate shocks).

Strengths/weaknesses: young markets with high marginal benefits from electrification; constraints include finance cost, utility creditworthiness, and transmission deficits.

Spillovers: innovation in distributed energy regulation; leadership on nature-risk financial supervision.

Latin America

Strategic narrative: protect natural capital, decarbonize grids already rich in renewables, and leverage critical minerals for a just industrial strategy.

Flagship instruments: deforestation controls linked to supply-chain due diligence; EPR and deposit-return systems; carbon-pricing pilots; green bonds and taxonomies.

Strengths/weaknesses: abundant renewables and biodiversity offsets potential; governance and enforcement gaps in frontier regions persist.

Spillovers: global supply-chain tightening for deforestation-risk commodities; growth in sustainable aviation fuel feedstocks and mineral processing.

ASEAN & Pacific

Strategic narrative: balance development and decarbonization with regional power trade,

common taxonomies, and climate adaptation for islands.

Flagship instruments: cross-border power trade frameworks; national and regional taxonomies to guide finance; coastal adaptation standards and disaster-risk financing; early AI-energy disclosure pilots as data-center hubs grow.

Strengths/weaknesses: dynamic manufacturing base and openness to standards cooperation; vulnerability to storms/sea-level rise and limited fiscal space.

Spillovers: interoperable taxonomies and digital product passports can reduce compliance friction for exporters.

Cross-Border Coordination, Trade & Standards Interoperability

Sustainability policy is now transnational just like supply chains, capital movements and data flows. Regulatory interoperability is a strategic capability, therefore. Three modes prevail, namely equivalence (admission of other rules that provide similar consequences), mutual recognition (admission of other conformity tests), and common baselines (co-established minimum standards). Equivalence and recognition can reduce duplicate testing, accelerate approvals, and reduce barriers to trade clean-tech, but they need reliable evaluation mechanisms and continuous peer review to prevent the risks of the race to the bottom.⁽³⁰⁾ In the areas of low political trust, it may be simpler to maintain common baselines, including aligned product safety or sustainability disclosure minima.⁽³⁰⁾

Trade policy: the best-known example is the Carbon Border Adjustment Mechanism by the EU (CBAM) which is intended to impose price on embedded emissions of imports and counteract leakage as the free allowances of the EU ETS are lowered.^(26,31) CBAM will be able to strengthen incentives to decarbonize overseas and facilitate domestic climate ambition, however, it will impose distributional and administrative issues on developing-country exporters and small importers. The coverage, default values, indirect emissions, and foreign carbon prices crediting are design-related characteristics that make or break CBAM to promote or trigger conflicts.^(26,31)

Information & reporting interoperability: corporate sustainability reporting is also moving towards investor centric baselines, which have knock-on consequences on supply chains. With the alignment of the disclosure frameworks embraced by markets, assurance scopes and audit trails should be interoperable to ensure that the cost of compliance remains manageable.^(32,33) Digital product passports (DPPs) that transport structured information (materials, repairability, emissions) throughout the life cycle of a product are maturing product-level traceability which can unlock the use of circular business models in the event that identifiers, data schemas, and access rights are coordinated across jurisdictions.^(34,35)

Finance channels: money is also important in interoperability. In blended-finance platforms, which are based on multilateral development banks (MDBs), the mobilization of private capital occurs through the standardization of taxonomies, risk-sharing terms and verification rules across deals.^(33,36) Partnerships and country platforms in the style of Just Energy Transition are effective when the disclosure, MRV, and eligibility requirements are compatible with the international standard to make concessional, commercial, and sovereign sources co-invest without individual due diligence.^(33,36)

Justice, Inclusion & the Just Transition

Sustainable transition should provide answers to three distributive questions: who pays, benefits, and decision-makers. Relative prices, asset values, and employment opportunities are unevenly distributed in areas, industries, and even population groups due to industrial decarbonization. The burdens are, without intent, generally transferred to low-income earners, carbon-intensive regions, and workers with less easily portable skills and the gains are reaped by capital-intensive industries and workers with more high-skill labor.^(9,37)

Distributional analysis: strong ex-ante analysis must measure impacts on households energy and stranded-asset risks, on workforce and it should disaggregate by gender and age and place to bring up inequities in the background.^(9,37) The policy mix is then informed with credible evidence, such as the combination of price in carbon with gradual recycling of revenues and special support of industrial transition.

Design features: three levers dominate. First, households at risk are insulated by specific rebates and lifeline tariffs, and the decarbonization signalling to high-consumption users is maintained.⁽⁹⁾ Second, sequencing plant retirement plans with reskilling and job-placement funds based on actual employer demand and supplemented by wage insurance or mobility support should be made available to women and young people who are burdened by care or have a credential penalty.⁽³⁷⁾ Third, legitimacy is anchored by community ownership and benefit-sharing the form of royalty streams, local equity interests, or community trusts, and redistributes the upside.⁽⁹⁾

Procedural justice: the early, ongoing and empowered forms of participation enhance sustainability: social consultation of unions and employer associations; local planning commissions with direct access to real budgets; and grievance systems that lead to conflict resolution before it develops.⁽³⁷⁾

International fairness: CBAM need to be accompanied by transition assistance, including concessional finance, access to technology, and capacity building, to ensure the costs are not passed on to the producers and consumers in the developing countries.^(26,31) The country platforms which could be a mix of the public and the private capital can be used to fund the transitions of coal-to-clean, grid investments and social protections with eligibility, MRV, and safeguards consistent with international standards.^(33,36) The logic behind it is straightforward: matching domestic equity (in countries) and global equity (between countries) in such a way as to ensure that climate ambition grows not disintegrates.^(9,37)

Implementation, Enforcement & Political Economy

Capability building: aspirational regulations require institutions that are resource endowed. There are three investments that can be done soon. First, individuals: the specialist regulatory personnel (economists, engineers) and professionalized inspectorates minimize backlog and enhance the quality of the rules. Second, MRVs systems: monitoring, reporting and verification at the facility, product and social levels should be modular in order to allow sectors to connect to a shared data backbone.^(30,33) Third, digitalization: e-permitting, machine-readable disclosures, and API-based data exchanges can enhance compliance, reduce administrative discretion, and open up risk-based supervision to analytics.^(34,35)

Enforcement toolkit: switch to a risk-based oversight as compared to the blanket inspection that directs resources to areas where the harms are most significant and compliance risks are the greatest. Alternate penalties with restorative enforcement e.g. enforceable undertakings which

remediate harm (e.g. habitat restoration, worker remediation) but do not eliminate incentives to self-report. Third party verification built into MRV (publicity through rotation of auditors, independence protection and public sums) scales are not privatized in the public interest.⁽³⁰⁾ In the case of cross-border value chains, certificates should be available in searchable, time-bound and auditable conformance registries by accepting accepted verifiers across jurisdiction.^(34,35)

Political economy: reform runs into incumbency. The producers of carbon intensive, legacy producers and individual region blocks have the ability to unite to water down standards or glean rents. Three strategies help. (1) Sequencing: no-regret, no-compensation: initialize at no-regret; phase data quality as quality increases.⁽³⁰⁾ (2) Coalition-building: attract beneficiaries - clean-tech suppliers, finance, labor finding new employment, consumer groups, etc. - around foreseeable rules and investment channels.⁽³³⁾ (3) Credible commitment: lock-in with statutory targets and budgeted transition funds and independent oversight; align trade and procurement and disclosure rules with backsliding (making visible costs to firms and financiers).^(26,31)

Controlling leakage and coordination issues: in the case of a domestic ambition endangering offshoring of emissions, introduce border policies with subsidies to partner nations to implement similar prices, MRV and technology. The acknowledgment of foreign carbon charges and high quality of offset has the ability of transforming trade friction into a convergence ladder.^(26,31) Publicate default values and other methodologies to unwind little importer frictions although protecting against creative compliance.

Subnational role: experimentation of cities and provinces is ideal, such as the building code, distributed energy zoning, industrial symbiosis parks and circular-economy logistics. Experimentation (regulatory sandboxes, pilot waivers) and diffuse learning through playbooks and shared datasets should be licensed by national regulators. Make fiscal payments and purchases based on performance (e.g., verified emissions reductions, job quality indicators), not effort.⁽³³⁾ Templates and grid codes can be aligned throughout a region, which reduces transaction costs on developers and SMEs of projects.^(34,35)

The through-line is doable: construct data-rich, risk-responsive institutions; implement fairly but visibly; connect domestic regulations to cross-border regimes to allow capital, technology, and accountability to scale. When done properly, implementation is not a cost burden but an investment vehicle coming to make sustainability regulations bankable projects and sustainable political alliances.^(30,33)

Measuring Impact & Adaptive Regulation

A good sustainability policy begins with a theory of change connecting inputs (funding, staffing, data infrastructure) to actions (rulemaking, permitting, enforcement), outputs (licenses issued, disclosures filed, kilometers of grid upgraded), outcomes (reduced emissions intensity, increased resilience), and, finally, impacts (avoided climate damages, increased biodiversity, social inclusion). Visualizing this chain at the beginning of the chain presupposes assumption, aligns agencies, and trade-offs are legible.⁽³⁸⁾

There should be a limited number of KPIs and indicators that are similar and relevant to decisions. On climate, pegged to intensity of emissions (e.g., tCO₂e/MWh; tCO₂e/ton of steel) and absolute emissions paths. To be resilient, avoidance of track downtime, time taken to restore services, and asset level risk scores, which are a combination of hazard, exposure, and vulnerability. Nature measures are capable of matching area metrics (hectares of conservation,

no-deforestation compliance) with biodiversity outcome measures (species abundance, habitat connectivity). Social indicators are to be tracked in terms of affordability, quality of jobs, and involvement (e.g. share of community-owned projects), with equity integrated as opposed to being added. The choice of KPIs that can be calculated using high-frequency operational data will minimize such lags between signal and policy adjustment.⁽³⁹⁾

Regulation can be evolved by adaptive cycles: write sunset clauses, which activate reviews, periodically audit performance (e.g. after every 2436 months), and test new technologies, business models or MRV techniques with regulatory sandboxes before going to scale or codifying them.⁽⁴⁰⁾ Pivot prescription to outcome-based controls (e.g. performance standards) where possible so as to incentivize innovation whilst maintaining safeguards.⁽³⁸⁾

Adaptation is built on a strong learning infrastructure: data collaboratives to exchange information on an asset-level (grids, buildings, supply chains), open APIs to standardize submissions (emissions, product passports, grid interconnection status), and independent evaluation to prevent self-assessment bias and regulatory capture. In the rapidly relevant fields, AI and digital infrastructure, transparent energy and water KPIs are the most important to align the innovation with climate objectives.⁽⁴⁾

CASE OF STUDY

Power Sector Auctions in Emerging Economies

Context: as FITs gave way to competitive procurement, many emerging economies adopted technology-specific auctions to accelerate renewables while lowering costs.

Instrument mix: reverse auctions with pay-as-bid or uniform pricing, pre-qualification (land, permits, grid-connection evidence), bid bonds, and realization penalties. Complementary policies include standardized PPAs, grid code updates, and local content rules tied to industrial strategy.^(41,42)

Results so far: auctions reliably delivered steep tariff declines and volume at pace where pipeline quality, PPA bankability, and grid readiness were credible. Where interconnection lagged or curtailment risk was high, realized capacity fell below awards; underbidding and concentration risks emerged when pre-qualification was weak or lot sizes were oversized.⁽⁴¹⁾ Targeted design—e.g., zonal caps, ceiling prices, and milestone-based securities—mitigated failures while preserving competition.⁽⁴²⁾

Equity impacts: tariff reductions improved affordability, but local content rules produced mixed outcomes unless paired with skills and supplier enablement. Community benefit schemes and land safeguards helped reduce siting conflicts.

Lessons: auctions are powerful if embedded in a policy mix: bankable PPAs, timely grid expansion, and realistic penalties. Periodic design reviews prevent lock-in and address market concentration.^(41,42)

Corporate Climate Disclosure & Investor Stewardship

Context: the post-2020 surge in climate reporting norms (e.g., TCFD-aligned frameworks and their successors) reshaped how firms quantify transition and physical risks, while investor stewardship moved from awareness to escalation.^(43,44)

Instrument mix: baseline reporting on governance, strategy, risk management, and metrics/

targets; transition plans with near-term capex and scope-coverage milestones; stewardship codes and coalition engagements; escalation ladders (vote against, file resolutions, reallocate capital).

Results so far: evidence shows private engagements can improve ESG practices and reduce downside risk; climate proposals have become more targeted and data-driven.^(43,44) Yet greenwashing risks persist where metrics are unaudited, targets exclude Scope 3, or scenario use is cosmetic.

Equity impacts: better disclosure supports workforce transition planning and supplier enablement, but costs can burden SMEs without proportionality and interoperability. Lessons. Mandatory decision-useful disclosure plus credible stewardship drives progress; add assurance, scope-inclusive targets, and escalation protocols to deter greenwashing and align capital with real-economy decarbonization.⁽⁴⁴⁾

Circular Economy via EPR (Packaging/E-waste)

Context: EPR shifts end-of-life responsibility and financing from municipalities to producers, spurring design changes and improving collection/recycling for packaging and e-waste.^(6,45)

Instrument mix: producer Responsibility Organizations (PROs), modulated fees (eco-modulation by recyclability/toxicity), take-back obligations, eco-design standards (repairability, recycled content), and litter-prevention schemes. Integration with informal waste sectors via registration, safe-work standards, and price floors builds inclusivity.⁽⁶⁾

Results so far: where fee signals are strong and enforcement credible, EPR improved collection rates and nudged design-for-recycling. Weak data and fragmented standards, however, limited comparability and cross-border trade in secondary materials.⁽⁴⁵⁾

Equity impacts: formalizing informal collectors raises incomes and safety, but requires transition support and access to PRO payments. Fee design must avoid regressive pass-through to consumers.

Lessons: pair EPR with eco-design rules, common data standards, and market development for recycled outputs; use adaptive reviews to refine fee modulation and prevent perverse incentives.^(6,45)

Future Outlook to 2035: Scenarios & Strategic Inflection Points

Convergence: by the early 2030s, major jurisdictions align on disclosure baselines, digital product passports, and carbon accounting; auction and transmission planning co-evolve; EPR interoperability lowers costs; AI governance internalizes energy/water impacts. Finance scales through blended vehicles and transition-finance taxonomies; policy risk premia fall. Diffusion of green tech accelerates, shaving emissions intensity across power, industry, and mobility.^(4,38)

Patchwork: progress is mixed: regional clubs advance standards but create compliance complexity. Auction design improves but grid bottlenecks persist; disclosure quality rises unevenly; investor stewardship pushes laggards case-by-case. EPR advances in some markets; leakage and waste trade remain problematic. Adaptive regulation becomes essential to manage divergence.^(41,45)

Backlash: political reversals stall carbon policies; reporting is diluted; data standards fragment; AI-driven energy demand collides with decarbonization pathways, raising emissions and public costs. Investment slows as policy uncertainty widens risk premia.⁽⁴⁾

Watch items: critical minerals supply and recycling economics; AI × climate interactions (demand management vs rebound); adaptation finance for infrastructure hardening; supply-chain resilience in grids and clean-tech manufacturing.⁽⁴⁵⁾

Build interoperability: (reporting, product passports, EPR data) to cut friction. Invest in regulatory capacity MRV systems, grid planning, competition oversight, independent evaluators. Hone just-transition compacts reskilling, place-based investment, affordability shields. Institutionalize adaptive cycles—sunset clauses, scheduled reviews, sandboxes linked to outcome-based rules.⁽⁴⁰⁾ Target KPIs that matter—emissions intensity, resilience performance, biodiversity outcomes, and distributional metrics—to keep policy aimed at real-economy change.⁽³⁹⁾

CONCLUSIONS

For governments: design coherent mixes that combine standards, markets, and information; embed equity-by-design (affordability, worker transition, participation); fund capacity (regulators, grid operators, data systems); and mandate machine-readable reporting with assurance to strengthen accountability.

For business: integrate policy risk into strategy; publish credible transition plans with capex-backed targets across Scopes 1-3; enable suppliers (toolkits, financing, data sharing); and monitor operational energy/water footprints of digital systems—including AI—against science-based thresholds.

For finance: use stewardship escalation ladders (vote, file, re-allocate) and time-bound engagement to close performance gaps; expand transition financing for hard-to-abate sectors; and apply robust taxonomies that prevent greenwashing while rewarding real emissions intensity improvements.

For civil society & academia: scale monitoring (citizen science, watchdog analytics), curate evidence syntheses for policymakers, and co-design participatory processes that legitimize transitions and improve uptake.

Across contexts, the through-line is adaptive regulation: pick KPIs that track what matters, build feedback loops that learn in public, and revise rules on schedule. That's how regulatory frameworks remain legitimate, lower compliance costs over time, and deliver durable sustainability impacts.

Discussion Questions & Applied Assignments

Seminar prompts

When do disclosure-only regimes work, and when do they fail? Consider incentives, comparability, auditability, and enforcement spillovers. What's the fairest way to design a carbon border measure? Discuss equity, exemptions, use of revenues, and compatibility with trade rules. Which policy mix best accelerates industrial decarbonization in your country? Weigh standards, pricing, procurement, finance, and just transition supports.

Applied assignment

Draft a two-page policy memo proposing a regulatory sandbox for a climate-tech or circularity

use case. Specify objectives, eligibility and governance, consumer and environmental safeguards, data/MRV requirements, exit criteria, and success metrics (e.g., cost per ton abated, time-to-permit, SME participation).

Further Reading & Resource Guide

UNFCCC Paris Agreement; Convention on Biological Diversity; OECD Regulatory Policy Outlook; IEA Net Zero Roadmap; World Bank State and Trends of Carbon Pricing; IFRS/ISSB S1-S2; GRI Standards; ILO Guidelines for a Just Transition; Ellen MacArthur Foundation Circular Economy Handbook; PRI Active Ownership 2.0.

Open data: WRI Climate Watch; World Bank World Development Indicators (including environment/climate series).

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Chapter 21

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Harnessing Artificial Intelligence and Big Data for Innovation and Sustainability in the Oil and Gas Industry

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ABSTRACT

The oil and gas industry has a significant political and economic weight in a number of countries around the world. Therefore, the issue of improving management methods in this industry is considered relevant. For this purpose, the article provides a number of basic characteristics of the object. Then, the issues of using scientific innovations that are or can be applied in the management of the oil, petrochemical and gas industries, including the use of various areas of artificial intelligence, are considered. The use of a large amount of data in the management of this industry is inevitable. The article is devoted to the use of artificial intelligence and big data in the oil and gas industry.

Keywords: Oil and Gas Industry; Artificial Intelligence; Management; Big Data.

INTRODUCTION

First, let's briefly describe the main characteristics of the facility. As we know, oil, as well as the petrochemical and gas industries, have a significant political and economic weight in a number of oil and gas producing countries of the world. The oil and gas industry includes the extraction, storage, transportation, processing, sale and resolution of other issues of crude oil. Work in this area begins with geological exploration. After oil or gas is extracted, it is transported to a refinery. Here, after a series of "testing" procedures, the oil is separated into several products that are directly used as raw materials in industry after the first distillation. After this, re-distillation, hydrotreating and deep cleaning are carried out.^(1,2,3) The result is the following: several types of fuels such as petroleum oils, diesel, automotive, jet, aviation, gas turbine, boiler fuel and so on. Natural gas extraction involves extracting gas from the earth's crust using wells, while processing includes the processes of cleaning, transporting, and preparing raw gas for use.

Petrochemical products include the following substances, which mainly belong to three classes: hydrocarbons, sulfur compounds and naphthenic acids.

The main raw materials for the production of petroleum products are hydrocarbons. The simplest of these products are methane, ethane, propane and butane. Ethane, propane and butane are paraffins and are subsequently converted into olefins by chemical processing. Aromatic hydrocarbons include benzene, toluene and xylene.

Methane processing produces methanol, ammonia and methyl chloride compounds. These are used, respectively, to produce antifreeze, ammonia fertilizers, and acids.

Ethylene or ethyl alcohol is extracted from hydrocarbons in large quantities, which is then

used to produce polymers, solvents and chemical fibers.

Other products are obtained as a result of complex chemical reactions. Their derivatives are mainly raw materials or intermediates for fuels, lubricants, and explosives.

In the modern oil industry, crude oil is not used in the form in which it is extracted from the well. This is the raw material that goes directly to the oil refinery.

Transportation is most often carried out by pipeline or tankers. Since oil has a very complex composition, which depends on the conditions of its formation, different types of oil are distinguished. In addition, any of the types is always divided into several fractions, depending on the density characteristics and boiling point.⁽⁴⁾

Fractionation allows you to determine the distillation methods and the amount of products that can be obtained from a particular type of crude oil.

All these processes are carried out in factories in laboratory conditions, which is a rather complicated process, despite the modern level of science and technology, the knowledge that a person has and can apply in practice.

Only then is rectification carried out - the separation of the raw material into gasoline, kerosene, paraffin, lubricating oils, ligroin, fuel oil, gas oil and other components.⁽⁵⁾

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Currently, scientists are investigating alternative sources of hydrocarbons, in particular, gas hydrate emissions in the seas. The main promising areas of chemical oil refining include: expanding the raw material base; maximum use of oil production waste; improving exploration and production technologies; using alternative raw material sources.

Artificial intelligence (AI) is a broad, practical field of science. Although one of the main issues here is the organization of the use of human heuristic knowledge, the acceleration of data collection, transmission, processing, and storage in making operational decisions is also of

great importance.

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The use of artificial intelligence in this type of enterprise allows the following to be achieved: optimization of production processes, management of equipment and devices, market management, risk management, production design, etc.

Currently, the application of Artificial Intelligence in the oil and gas industry is developing rapidly, as the concept of artificial intelligence is gradually integrated into various stages of the industry, such as smart drilling, smart production, smart pipeline, smart processing, etc. With artificial intelligence algorithms, developers have developed a series of practical application technologies in exploration and development. The use of ANN method in the exploration field has already achieved good results in reducing exploration risks and improving the success rate of exploration wells.⁽⁷⁾ In the drilling field, new equipment such as automatic drilling rig and smart drill pipe have improved the drilling level and significantly reduced the cost.⁽⁸⁾ In oil field development, optimization of the development plan based on historical oil field production data is the main application mode of Artificial Intelligence technology.^(9,10,11)

In order to optimize production processes, the company is faced with the need to make many management decisions every day, which affects the economic efficiency of the company. Entrusting such decisions to artificial intelligence can significantly reduce the chance of error and improve quality.

As we have noted, work in the oil industry begins with geological exploration, and then with the extraction of crude oil. Here, using artificial intelligence, attempts should be made to solve the problems of developing “smart wells”, optimizing the geological exploration and production process.

Machine learning⁽⁶⁾ algorithms are used to determine the exact location of individual devices and equipment used in the oil and gas industry and to monitor them. Sensors help detect malfunctions and accidents.

Artificial intelligence is also used to optimize oil and gas extraction processes. The analysis of information used in the process opens up wide opportunities for reducing costs and using green technologies. To achieve this, seismic and geological information received from sensors and various monitoring systems is processed, and the volume of oil or gas produced over a certain period of time is automatically determined. This also plays an important role in forecasting in this area.

For example, neural networks help LUKOIL stabilize production in mature fields.⁽²⁾ Artificial

intelligence algorithms allow for maximum use of reservoir potential and infrastructure capabilities by optimizing equipment performance.

As mentioned, the modern concept of artificial intelligence in the oil and gas industry is mainly associated with machine and deep learning algorithms. This allows them to apply the knowledge gained from training to large data sets. Unlike a control system with manually coded instructions to perform specific tasks, artificial intelligence provides the control system with the opportunity to independently learn to recognize new situations, make predictions and suggest the most optimal solutions to problems. Of course, artificial intelligence cannot solve these problems without the necessary devices and equipment. Of course, devices and equipment do not require small costs.

Computer vision, a specialized area of artificial intelligence, can be used to radically improve the management of these operations. From vast networks of pipelines snaking beneath the ground to towering drilling rigs extracting oil from miles beneath the earth, computer vision offers a new perspective on the industry. Figure 1 depicts the segments of the oil and gas industry.⁽¹⁾

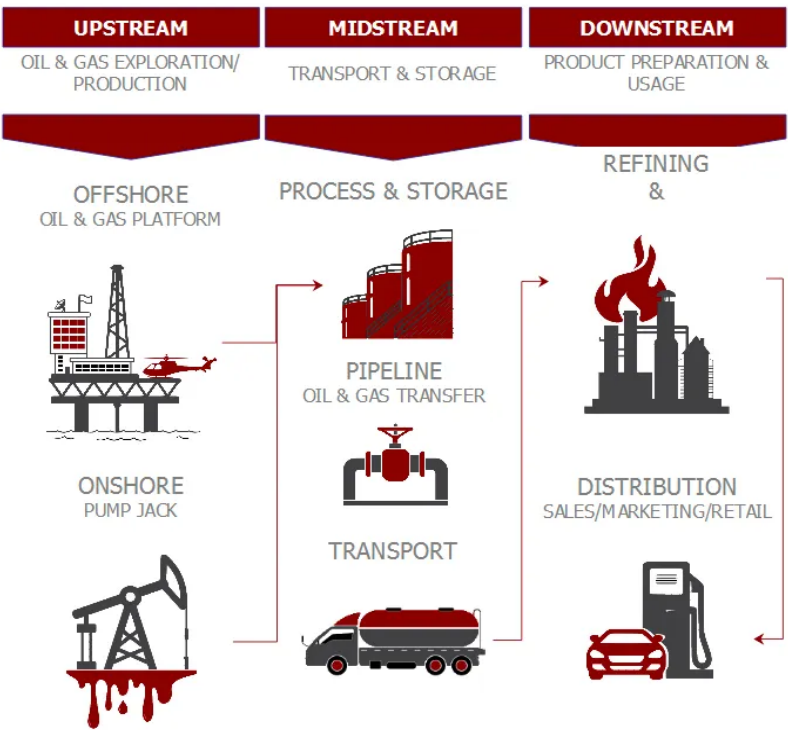


Figure 1. Segments of the oil and gas industry

The oil and gas industry can be divided into three main segments: exploration and production (extraction), transportation and storage, and refining and marketing. The first segment of oil and gas is exploration and production. Geologists and engineers search for oil and gas deposits, then drill them out from under the ground and extract them. Then comes the transportation and storage segment. This segment transports natural gas, mainly through pipelines, and crude oil, mainly through pipelines, tankers, and trucks, to refineries or storage tanks. Finally, refining and

marketing companies convert crude oil and natural gas into useful products such as gasoline, diesel fuel, jet fuel, and various petrochemicals.

Computer vision can be applied to every segment of the oil and gas industry. Almost anywhere a camera can monitor an operation, computer vision can intervene and improve efficiency. Various computer vision tasks such as object detection, image segmentation, and object tracking can be used to extract valuable information from visual data.

Let's look at a few examples of how computer vision can be applied to every segment of the oil and gas industry.

During the drilling process, computer vision can be used to analyze video footage from a camera-equipped well. By identifying the characteristics of the rock formations encountered, AI can help optimize the location and trajectory of the wellbore to maximize production from each oil well.

The main applications of AI in the oil and gas industry include the following:⁽⁴⁾

- In oil exploration, AI algorithms analyze seismic data to predict the presence of oil and gas with high accuracy.
- For example, Shell uses AI to interpret geological data and accelerate the discovery of new resources by 30 %.
- In production optimization, AI predicts equipment wear and prevents accidents. "Digital twins" of oil fields simulate different production scenarios and select the optimal one.
- In logistics and oil refining, AI plans transport routes taking into account weather and demand. Neural networks in oil refineries monitor fuel quality and reduce failure rates.
- In ecology and safety, AI monitors emissions and helps companies comply with ESG standards. Drones with AI analytics quickly detect pipeline leaks.

ESG (Environmental, Social, Governance) standards⁽⁵⁾ are a set of criteria covering environmental, social and governance aspects to assess the sustainability and responsibility of companies. These standards help measure a company's impact on the environment, its treatment of its employees and society, and the transparency of its corporate governance practices.

Drones equipped with cameras and computer vision can be used to autonomously scan miles of pipelines, detecting leaks, cracks and corrosion in pipelines in incredible detail. This can replace risky manual inspections and reduce the costs associated with downtime for repairs.

Oil refineries and petrochemical plants are complex systems with multiple processes that require monitoring. Computer vision can analyze video feeds from cameras in these facilities to identify inefficiencies or potential equipment failures. It also provides for the reception, pre-processing, and transmission of information from transmitters and other devices.

For example, Ultralytics YOLOv8⁽³⁾ supports multiple computer vision tasks and can be used to create innovative solutions in the oil and gas industry.

YOLOv8 is a computer vision model architecture developed by Ultralytics. You can deploy YOLOv8 models on a wide range of devices, including NVIDIA Jetson, NVIDIA GPUs, and macOS

systems, using the open-source Python package Roboflow Inference to run your vision models.

Another example is vapor detection and segmentation using Ultralytics YOLOv8 (figure 2).

YOLOv8 supports the task of sample segmentation in computer vision.

Storage Tank Detection with YOLOv8-ORB (Oriented Bounding Box) - Tanks are used in the oil and gas industry to store crude oil, petroleum products, and other materials. The integrity and proper maintenance of these tanks are essential to prevent leaks, contamination, and other safety hazards.

The YOLOv8-ORB (Oriented Bounding Box) model is specifically designed to detect and localize objects with arbitrary orientations. It is ideal for identifying storage tanks from the air. Once a tank is detected, further processing can be performed to segment the tanks from the background and even identify specific features such as rust spots or structural deformations. Automated detection processes can better support the safety and efficiency of storage operations.

Big data analytics helps in regulating the major oil and gas operations such as exploration, drilling, production and supply in three sectors - upstream, midstream and downstream. Among all the business segments, upstream segment is the most dominant segment due to the increasing use of big data analytics for unconventional shale gas discovery. Moreover, volatile oil prices are increasing the uncertainty in the oil and gas business. Thus, organizations are adopting a data-driven approach to minimize their risks. Next, downstream is expected to be the second-largest segment due to the increasing use of product analytical solutions that help refineries standardize the chemical composition of finished products.⁽¹²⁾

As in other industries, the oil and gas industry must consider six key criteria or six “V” characteristics of Big Data.

1. Volume: at least 150 GB of data should be collected per day.
2. Velocity: the enterprise should be provided with the required increased computing power (virtual or physical) to work with data arrays in real time.
3. Variety: the incoming information has different formats or levels of structure. For example, social media content can be very different even on the same page.
4. Veracity: the data sources can be trusted and the results of their processing are reliable enough to make decisions.
5. Variability: the flow of data is variable, it can even be affected by the time of day or weather conditions. For example, during rush hour, more data comes from taxi drivers.
6. Value: data can have different meanings for the company. For example, transactions with large buyers are considered more important than transactions with small buyers.

Big data software for the oil and gas industry collects and analyzes data from multiple sources, both in real-time and in batch mode, i.e., on a specific calculation schedule (e.g., every 12 hours, every 24 hours, every week). The real-time component allows for response to events (e.g., shutting down equipment during an oil spill, adjusting drilling fluid pressure), while the batch layer is responsible for comprehensive historical analytics (e.g., drilling patterns).⁽¹³⁾

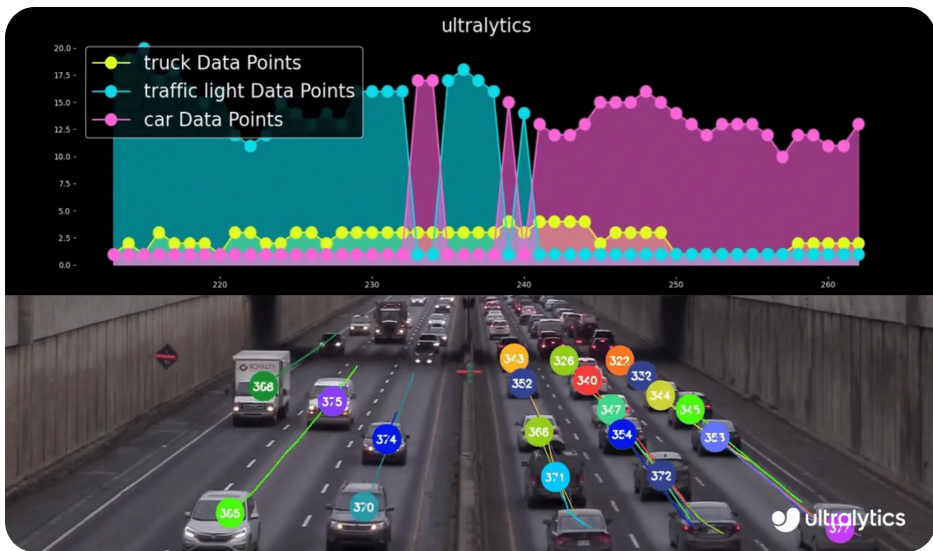
Applications of Big Data in the oil and gas industry fall into various categories:⁽¹⁴⁾

- Exploration management: here, mainly geophysical, seismic and geochemical data sets are used.

- Reservoir engineering: here, data sets such as pressure, temperature and fluid composition are used.
- Drilling management: here, data sets for monitoring and analyzing velocity, pressure and temperature are used.
- Production management: here, sensor and automation data sets are used. In short, the analysis of all the general data is used to manage the various sub-areas, and finally the overall management level is organized.

In general, the potential applications of Big Data in the oil and gas industry are as follows: Exploration Seismic data analysis, Microseismic data exploration, 1D, 2D and 3D geological mapping, Closed Reservoir Management, asset modeling, Reservoir modeling, Enhanced oil recovery, Automated production decline analysis, Engineering Production sharing techniques, forecasting, Well casing damage prediction, Remote smart oilfield management, Pipeline monitoring and repair, Transportation Energy efficiency improvement, Downstream Oil Asset management, Well productivity management, Health and Safety, Safety forecasting, Trade and Market volatility analysis, Sales Crude oil price forecasting, etc.⁽¹⁵⁾

High efficiency is also achieved when YOLOv8 is used for vehicle tracking and monitoring at oil and gas facilities.



Source: ⁽¹⁶⁾

Figure 2. Vapor detection and segmentation using Ultralytics YOLOv8

Artificial intelligence, particularly computer vision and models like YOLOv8, is transforming operations in the oil and gas industry. Computer vision can improve intelligence and maintenance through use cases such as steam detection and vehicle tracking.

Now let's explain the rules for working with Big Data.

Before starting to create a database, it is necessary to determine which technologies will be used to collect, store, process and analyze data.

Collection: it all starts with the collection of information, identification of its sources and

integration of the necessary processing technologies. It is also important that data cleaning specialists who set up filters for further analysis participate in the process.

Storage: since even a few computers are not enough for large volumes of information, companies resort to the services of cloud providers and use distributed computing power. At the same time, new technologies (Data Vault, Data Lake, Data Mart) should be used for storage:

Processing: MapReduce technology is more often used for processing large volumes of data.

Analysis: at this stage, it is necessary to get the most useful and valuable from the entire data warehouse. A number of analytics are used in the process. Analysts help to find hidden patterns and develop solutions to improve the product.

CONCLUSIONS

In the modern world, the most important factor for the collection, storage, processing and analysis of data for decision-making in the oil and gas industry is considered to be the most important. Here, the correct and efficient use of new information technologies is an important requirement. Also, by analyzing big data, ways to collect, process, store, transmit information about the management object in the oil and gas industry and the ability to use this information are obtained.

YOLOv8-OB, which is specially designed to detect and localize objects of arbitrary orientation, should be used.

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A blue-tinted photograph showing a person's profile as they work on a model of a wind turbine. The person is wearing a light blue shirt. The background is slightly blurred, showing other parts of the model and some equipment.

Chapter 22

Advanced Materials, Artificial Intelligence, and Sustainable Technologies for Energy and Environmental Engineering

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Renewable Energy Integration and Smart Grid Management

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ABSTRACT

This chapter seeks to propose the current pattern of rising penetration of renewable energy sources (RES) and evaluates how this trend has restructured the operations in the modern power systems, thus creating a two-sided opportunity and challenge regarding sustainable electricity supply. The optimization of intermittent resources, solar photovoltaic and wind turbines, requires the installation of advanced control, prediction and balancing systems in order to balance the system. Smart grid technologies are considered the new way out and are viewed as the focus of energy flow optimization and the extension of system reliability. Smart grids allow distributed generation amendments to be effectively integrated through two-way communication, real time monitoring, and dynamic management. Storage energy systems and the power electronic equipment play critical roles in balancing the supply and demand process and simultaneously aid in maintaining stability in voltages and frequency. The demand response strategies also aid the adaptation of a system by ensuring that the consumers become active consumers in the energy management processes. The system decentralization caused by the implementation of microgrids, combined with the introduction of electric vehicles, serves to support resiliencies. The speed and scope of integration of renewable energy take decisive impact due to policy frameworks and standards that are in effect at regional and international levels. Such environmental benefits as the reduction of emissions and efficient use of resources should highlight the sustainability potential of the smart grid implementations. Their wider societal value is testified by socio-economic effects, including creation of jobs and access to more energy. However, issues related to cyber-security, assets investment and the need to adjust to regulations remain core issues. Altogether, the chapter provides a systematic review on energy integration and smart grid management with a focus on technology, environment and policy aspects.

Keywords: Renewable Energy; Smart Grids; Energy Storage; Demand Response; Power Electronics; Microgrids; Sustainability; Policy.

INTRODUCTION

Rapid growth of renewable sources has emerged as a central ingredient in strategies across the globe to build sustainable and low-carbon power structures. In contrast with traditional fossil-fuel power generation, renewable energy sources, including solar, wind, and small-scale

hydropower, are inherently intermittent, and require advanced techniques of integration. One transformational framework that has arisen to challenge these areas of concern has been in the form of smart grids. Smart grids support more agile and robust architecture of energy infrastructure sources by allowing real-time monitoring, adaptive control, and effective use of distributed resources. Integrating renewables as a part of smart grids also facilitates environmental sustainability, societal socio-economic growth, energy security. In its turn, this chapter dwells on the core of renewable energy integration conditions, technologies and policy, with a particular emphasis on smart grids management. Bringing renewable sources of energy (RES) on board in the modern power production represents a challenge and a solution to the global change to sustainability. Studies into nanostructured carbon materials such as carbon nanotubes and graphene oxide has established the basis upon which new energy applications may be developed especially in sensing, storage and conversion devices. As an example, Abaszade et al.⁽¹⁾ studied the physical characteristics of gadolinium-modified carbon nanotubes that have distinctive electrical and structural specifications that can be implemented into smart grid sensor networks. Similarly, research by Figarova et al.⁽²⁾ has revealed a negative differential resistance of derivatives of graphene oxide- sulphur, which further shows the importance of the research towards use as sophisticated switching components in renewable energy management systems. These material innovations do not only provide improved capabilities on the device level but also improve the technological foundation that needs to be built to achieve credible opera with the inclusion of RES-grid. The first major issue with RER integration is found in its internal variability that may have a negative impact on grid stability.⁽³⁾ It is stressed by several authors that the effective implementation of renewable energy depends greatly on innovative technologies and methodologies that can accept these fluctuations. As a case of adaptation to fluctuation of supply, one additional purpose of applying proton exchange membrane (PEM) electrolysis with wind energy is an attractive idea to provide efficient storage of the excess renewable energy.⁽⁴⁾ In addition, en pointed technologies in smart grids improve the efficiency of energy dispatch on a demand side, which implies that consumption is more consistent with both generation and can reduce the effects of RER variability.⁽⁵⁾ The other significant area of integration renewable concerns the utilization of energy storage systems (pumped storage systems are examples), capable of stabilizing production and demand.⁽⁶⁾ Also, it has been pointed out that multi-port energy routers (MERs) are an important device required to support the incorporation of different renewable sources and energy storage systems.⁽⁷⁾ Such novel technologies play a role in controlling the unpredictable output of renewables through facilitating more flexible energy distribution facilities.

The infrastructure of smart grids integrates the modern levels of information and communication technologies (ICT) in changing the conventional approaches towards energy distribution and consumption. By facilitating large-scale computational and communication activities, smart grids increase the reliability, efficiency, and sustainability of the services in the domain of electric energy.^(8,9) This advanced architecture allows controlling, monitoring, and maintaining energy in real-time through intelligent devices which are indispensable to enhance the adaptability and responsiveness of the energy systems.^(9,10) To ensure two-way communication inter-utility and consumer, smart grids use advanced metering infrastructure (AMI) to support the functionality of timeofuse charging and improved fault detection.⁽¹¹⁾ The addition of the concept of artificial intelligence (AI) to the smart grid architecture may also lead to further increases in the performance by facilitating improvements in load prediction and optimization of power distribution, among other issues, in order to effectively serve the changing demands of electricity.⁽¹²⁾ Another aspect that AI provides to smart grids is the feature of self-healing, which allows anomalies or failures inevitably present in the system to be identified and

resolved automatically.⁽¹³⁾ The employment of AI on smart grids is another dimension of radical change in the context of contemporary grid management. The AI approaches are critically applicable in the optimization of grid functions, hence leading to the movement of energy saving and user satisfaction.⁽¹²⁾ Additionally, new technologies including hybrid converters are essential to controlling energy flows in smart grids, and especially to renewable sources such as solar photovoltaic (PV) systems. Vinayakumar et al.⁽¹⁴⁾ address the use of DC-DC converters in PV systems that provides higher levels of control over competing energy loads, thereby allowing a better level of stability and reliability of the power distribution, but also diminish the increased total harmonic distortion (THD) in the grid. Parallel to this, the emergence of smart microgrids has become a key emphasis in the process of the overall shift toward the sustainable energy system. Zong et al.⁽¹⁵⁾ investigate systems of collaborative control in such microgrids and highlight that collaboration between many sources can lead to a significant improvement in efficiency and the level of reliability. They conclude that it is important to maximize such control measures with a view to attaining low-carbon targets hence in line with the wider environmental goals. Besides, the international movement in favor of renewable energy has been gaining steam within the last twenty years, not just around the integration of renewable technologies but also the revision of current principles, structures of the economy and social life that favor long-term sustainability.⁽¹⁶⁾ Concept of energy transition requires multidisciplinary framework where different stakeholders are collaboratively encouraged in order to support innovation and green technology. Sustainability in the way of renewable energy application need and requires strengthening of policies and the promotion of a public partnership between the partners.⁽¹⁷⁾ Economics has a great role in this transition. Although the initial contribution of resources in renewable energy tools might seem high the results on transition in coming years would include economic savings due to governmental financial aid and increased energy efficiency.⁽¹⁸⁾ The growing research in the field of renewables boosts energy production as well as promotes environmental stasis, but it implies that the prerequisites of the successful switching to a photovoltaic (PV) framework and the use of renewables are already in place.⁽¹⁹⁾

Fundamentals of Renewable Energy Integration

Table 1. Fundamentals of Renewable Energy Integration	
Aspect	Description
Definition	Integration of renewable energy sources (RES) like solar, wind, hydro, biomass, and geothermal into existing energy systems.
Key Drivers	Decarbonization goals, energy security, sustainable development, cost reduction of RES technologies.
Challenges	Intermittency of RES, grid stability, storage limitations, power quality issues, infrastructure adaptation.
Core Components	Smart grids, energy storage systems (ESS), demand-side management, advanced inverters, forecasting tools.
Technological Enablers	Artificial intelligence (AI), blockchain, Internet of Things (IoT), digital twins, power electronics.
Benefits	Reduced carbon footprint, enhanced energy efficiency, diversified energy mix, long-term cost savings.
Policy & Regulation	Supportive policies, incentives, feed-in tariffs, renewable portfolio standards, international agreements (e.g., Paris Agreement).
Future Trends	Hybrid RES systems, AI-driven grid management, vehicle-to-grid (V2G) integration, hydrogen economy, 100 % renewable-based grids.

Renewable energy integration refers to the development of incorporating clean and sustainable energy sources into the existing and potential power systems, in a way that is dependable, cost efficient, and economical. Trade-offs A transition to distributed renewable-based systems triggered by the replacement of fossil-based centralized generation fosters new technical and operational challenges (table 1).

Because renewable resources are subject to variability and intermittency, and geographically dependent they require more intricate prediction methods, more advanced balancers, and the implementation of flexible grid architecture. The modern integration solutions include digital control, smart metering, demand-response, and big storage solutions that are used as a combination to improve operational efficiency and reliability. In this section, the most critical dimensions of renewable-energy integration are described, outlining the opportunities that are available, as well as the pitfalls that emerge in a power-system environment. Such an implementation of renewable-energy resources (RERs) into the remaining electrical grids is equally challenging and, at the same time, a substantial solution problem as far as sustainable energy development is concerned. The natural changes and fluctuations in the weather, including such renewable energy sources as solar or wind, prompt the necessity of new approaches aimed at enhancing grid resiliency, reliability, and efficiency. The literature left lists a continuum of methods and technologies that help to reduce these issues. More importantly, the peculiarities of grids functioning characteristic of an island reveal the multidimensional interdependence of integrating renewable sources and managing energy.⁽²⁰⁾ These stand-alone systems face the challenges of varying loads and different generation variability that cause them to approach with unique strategies in order to have an efficient operation. To this end, the combination of renewable energy with complementary energy sources, especially power-to-gas (P2G) and carbon-capture technologies, gives an organized roadmap, not only to development towards increasing use of renewable resources, but to lowering carbon emissions on a larger scale.⁽²¹⁾ Finally, a viable evolution towards integration of renewable energy would need a complex process that brings different technological innovations in parallel with careful planning and management strategies towards the system. As countries transition to more sustainable energy paradigm, ensuring grid structures with enhanced resilience and efficiency by integrating some of the latest energy-management tools will be crucial to achieving climate and sustainability goals.⁽²²⁾ Integration of renewable-energy requires a comprehensive knowledge of the nature of resources, and their overall effects on the system. On the material level, Abaszade et al.⁽²³⁾ synthesized and characterized graphene-oxide flakes in transparent thin films, making them offer new prospects in photovoltaic devices and optoelectronic devices that could be integrated into the system concerning the use of renewable energies. Similarly, to define photoconductivity in carbon nanotubes, Mammadov et al.⁽²⁴⁾ examined how nanostructured conductors can be used to optimize grid-connected devices. Such studies resonate with the larger challenge on integrating variability, reliability, and effectiveness in the inclusion of renewable sources into the grid.

Characteristics of Renewable Energy Sources

The types of renewable energy sources known as solar, wind, biomass, small hydropower, geothermal energy and tidal energy also have some unique features that cannot be compared with the conventional fossil fuels. Solar and wind energy is free and yet very intermittent and its productivity varies with the meteorological and seasonal changes. Hydropower has a relatively low GAP, but it is relatively limited in geographical utilization as it was demonstrated in figure 1. Biomass is a source of dispatchable electricity, but still requires an appropriately sustaining feedstock supply. Geothermal and tidal sources are very reliable but require significant initial

investment in capital and are place-dependent constraints. All of these resources are green, carbon neutral, and difficult to replace in global decarbonization efforts. However, they also require creative grid-integration approaches to ensure reliability and continuity of supply and stability of the system. Graphene oxides and carbon nanotubes are structurally and electrically versatile with the ability akin in variety to the variability of renewable energy sources. As an illustration, Abaszade⁽²⁵⁾ explored production of graphene oxide flakes along with their characteristics, a finding that described optical and electrical attributes that can supplement solar harvesting and flexible energy devices. This was later extended by Guliyeva et al.⁽²⁶⁾, who synthesized the nanostructured graphene oxide thus suggesting scalable methods of thin-film energy components. These material investigations give analogies to the intermittency and heterogeneity of renewable energy sources, suggesting a call to more sophisticated approaches to integration.

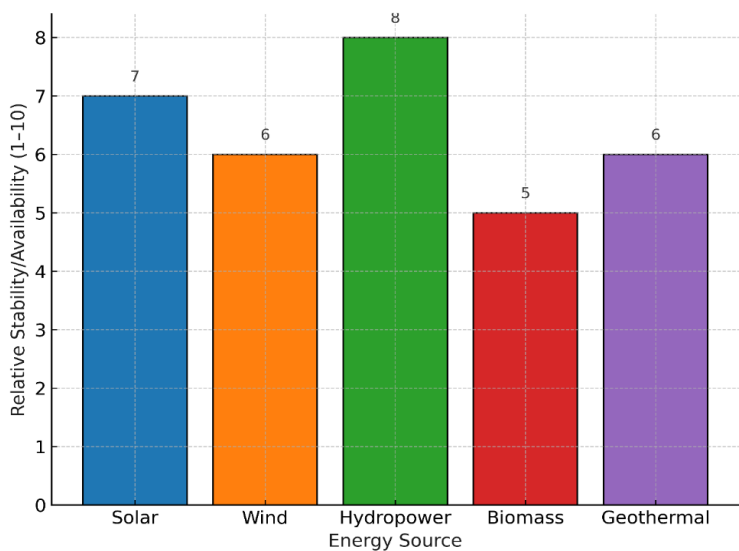


Figure 1. Renewable Energy Sources Bar Chart

It can be seen in figure 1 that solutions based on renewable energy have relative stability and availability. The chart shows that hydropower implies the best stability rates and availability. Solar and wind energy have considerable potential of utilization; nevertheless, their variation nature places them in the medium stability level. Biomass proves to be relatively less stable only because of the limits to feedstock availability and logistic issues. Although geothermal power is inherently sustainable and stable, the energy source is geographically limited to preferred areas.

Impacts on Power Systems

Renewable energy integration has far-reaching impacts on the power system and relates to the grid stability, voltage control, frequency deviation and system security. Such intense penetrations of solar and wind power can create volatility in generation, thus resulting to disparities in supply and demand. Renewable energy systems are decentralized and this feature disrupts traditional models of centralized grid-management. Furthermore, the bi-directional flow of the generated electricity of distributed resources creates new demands of the grid protection and monitoring. However, incorporation of renewable energy also prevents the reliance on fossil fuels, decreases the carbon emissions, and increases energy security.

As such, these effects ought to be addressed by relying on the implementation of smart grid technologies, flexible generation, and energy crop stores. The work on carbon nanostructures already shows how carbon nanostructures show respond to modification at the material scale and, subsequently, to system scale correspondingly, as with the impact of a renewable source on grid operation. Abaszade et al.⁽²⁷⁾ investigated the structure, and electrical characterization of sulfur-doped graphene oxide composites reporting their increased stability and conductivity. In the same way, their graphene oxide/sulfur compounds modeling provided support about current voltage behaviors relevant to the design of components on a grid.⁽²⁸⁾ These results are similar to the problems of renewable energy sources to the grids, which include stability in the voltage and control of frequency.

Smart Grid Architecture

Smart grid architecture is an elaborate design model that will incorporate power system infrastructure and modern information and communication systems. Wireless grids have a bonus to allow both unit and bidirectional flow of electricity and data as observed in table 2, unlike the conventional grid mostly unidirectional.

Table 2. Smart Grid Architecture		
Layer/Component	Description	Key Technologies / Elements
Perception Layer	Collection of real-time data through physical sensors and measurement devices	Smart meters, PMUs (Phasor Measurement Units), IoT sensors
Communication Layer	Reliable and fast transmission of collected data	5G, LTE, PLC (Power Line Communication), ZigBee, Wi-Fi, Optical Fiber
Network Layer	Routing of collected data among control centers and management systems	IP-based networks, SDN (Software Defined Networking), Cloud/Edge Computing
Application Layer	Delivery of energy services for users and management systems	Demand Response, Home Energy Management Systems, Smart EV Charging
Control & Management Layer	Management of energy flow, stability, and security	SCADA, EMS (Energy Management Systems), AI-driven forecasting
Security Layer	Protection of data and infrastructure through cybersecurity measures	Encryption, Blockchain, Intrusion Detection Systems (IDS)
Market & Business Layer	Digital management of energy markets and dynamic pricing models	Dynamic pricing, Peer-to-Peer (P2P) trading, Blockchain-based markets

The main layers of the smart grid are further presented in table 2 where their various functions are listed. The first tier, the Perception Layer, ensures real-time data being obtained through sensors and smart meters. Network and Communication Layer, it requires the Communication and Network Layers to be dependable in order to transmit and route this information. The Application, Control and the Management Layers enable the delivery of energy services and supervision of system stability. The Security Layer will protect cybersecurity, but the Market and Business Layer will be useful when performing the activities of the digital market and formation of dynamic rates with ease of use. The high-level architecture includes

generation units, transmission and distribution networks, control centers and end-user systems which are connected by means of digital platforms. The use of sensors, phasor measurement units (PMUs), and advanced metering infrastructure (AMI) gives the possibility to monitor and modify measurements in real time. In addition, interoperability, cybersecurity and scalability are vital qualities of smart-grid architecture. This regular plan encourages energy resourceful execution of the renewable energy, makes the power dependable and allows the customers to be ones to determine their own energy management styles. In spite of these benefits, there are considerable problems posed by the increased complexity and inter-connectivity of smart grids. The increased number of devices and sensors expands the cyber-attack footprint, thus, requiring the implementation of effective security models.^(8,29) Scholars also point out that combining sophisticated intrusion detection mechanisms is inevitable in securing vulnerable critical smart-grid infrastructure against under attacks including false data injection.⁽³⁰⁾ The smart-grid architecture enables two-way energy and information interactions, combining sensor networks with edge/cloud computing and cyber-physical control; modular scalability and reliability supports the inclusion of renewable energy sources (RES). Flexible electronics and thin-film technologies furnish innovative platforms for smart meters, distribution-level sensors, and adaptive energy-management systems.^(31,32,33) Telecommunication Antennas and aerial platforms improve the reliability of the communication in distributed monitoring systems.^(32,34,35,36,37,38) Mechatronics based material characterization enhances the accuracy of in-situ monitoring.⁽³⁹⁾ Nanoelectronics devices and sensors based on carbon-nanotube provide high-sensitivity sensors that are relevant to the grid.⁽⁴⁰⁾ Additionally, AI, IoT, and Industry 4.0 may be used to expand predictive analytics, anomaly detection, and to conduct topological control in grid architecture.^(41,42,43,44,45) The implementation of new technologies, especially machine-learning algorithm and graph-convolutional networks, are central to the continuous sensitisation and optimization of smart-grid security systems.^(13,46) With the maturation of smart grids, architecture needs to balance between innovation and security to achieve resilience and reliability in terms of smart-energy delivery. Such long-term research and development related to cybersecurity systems and innovative intelligent technologies are, therefore, required to optimize the tasks of smart-grids, as well as to protect against new risks. To conclude, smart-grid architecture is characterized by highly developed computational models, augmented interaction capabilities, and the presence of AI, thus providing the energy infrastructure, which is focused on responsiveness and efficiency. As such networks continue to get more sophisticated, a proactive stand-by protection is becoming variable to the integrity and reliability of such critical infrastructures.

Integration Technologies and Methods

Integration of renewable energy requires modern technologies and methodological frameworks to address the solutions to variability, intermittency and balancing of the system (figure 2). Such frameworks do include grid interconnection plans, demand management plans, power storage system and power electronic appliances. The integration strategies also choose depending on the grid connected or the stand-alone system where each has different operational characteristics. Grid-connected systems enjoy central balancing and integration into the market, and off-grid systems have resiliency and access to energy in remote areas. Both operational paradigms still rely on the thermal management and conversion technologies.^(47,48)

Figure 2 offers comparative study of Grid Connected and Off-Grid configuration on four main dimensions; interconnection to utility grid, demand-side management, energy storage and power electronics. The Grid - Connected architecture exhibits better performance with regards to interconnection fidelity and power- electronics sophistication, a situation due to centralized grid-balancing algorithms and utilization of more sophisticated grid technologies. Oppositely, the Off -Grid regime has an increased reliance on the demand-side management strategies and

energy-storage solutions in order to achieve operational resilience in geographically remote environments. The two configurations consequently highlight the complementary competences that are essentially specific to their respective operational settings.

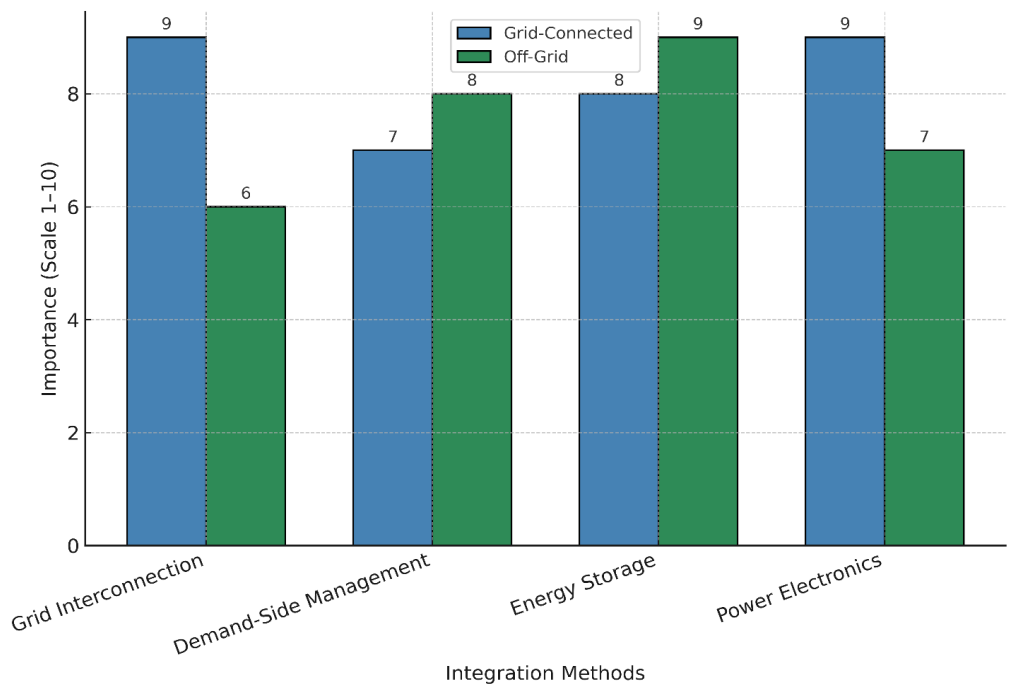


Figure 2. Renewable Energy Integration Bar Chart

Grid-Connected vs Off-Grid Renewable Systems

Grid-tied renewable energy systems feed direct to the last grid, and thus enable excess generation to be shared at scale and ensures that there is a backup generation provided by conventional generation plants. The advantage of such systems is that they have economies of scale and consolidated inventory control. In comparison, off-grid systems are autonomous devices needed in out-of-group areas or in isolated settings; systems usually couple photovoltaic panels, wind turbines or Mike-hydropower goals and battery back-up or generator with auxiliary or backup fuel. Both forms are of strategic significance: grid-connected applications support dynamic decarbonization on a big scale, and off-grid applications promote energy access and resilience. UAV-based surveillance enhances reliability in off -grid microgrids.⁽⁴⁸⁾

Demand Response Mechanisms

Demand response (DR) is a technology-based prerogative in a paradigm of smart grid protocols that adjust consumer electric use to supply limitations or price variations, or grid contingencies. As a result, load redistribution over time ourselves makes grid load become reduced during non-peak periods and enables higher use of renewable generation sources. This strategy is represented by mechanisms like time-of-use tariffs, price discrimination, and Linked load control by implementing smart appliances. DR hence improves flexibility of the system, minimizes cost of running, and creates partnership with the consumer in energy management. Demand response mechanisms also increase grid flexibility as the load changes will be synchronized with the market indicators. The accuracy of load-forecasting and detection

of anomalies are improved with artificial intelligence (AI) and Internet of Things (IoT) analytics.^(43,45) Demand-adjustment mechanisms are required to be automated and made possible with cloud-heavy platforms.^(49,50) At the same time, socio-technical factors related to the cyber-physical environment need to be taken into account.⁽⁴⁴⁾

Role of Energy Storage Systems

Energy storage systems (ESS) are central to renewable integration, as they mitigate intermittency and ensure stable power supply. Technologies include lithium-ion batteries, flow batteries, pumped hydro storage, compressed air, and emerging hydrogen storage solutions. ESS smoothens output from solar and wind farms, supports peak load management, and enables frequency regulation. They also allow renewable energy to be stored during surplus generation and dispatched during high demand. The rapid decline in battery costs has accelerated global adoption of ESS, making them indispensable for smart grids. Energy storage is indispensable for balancing intermittency and providing system flexibility. MXenes are reviewed as promising supercapacitor materials.⁽⁵¹⁾ NiFe₂O₄/rGO composites and bio-derived carbons (from walnut shells and hemp fibers) improve cycle life and stability.^(36,37,52) Gadolinium-doped CNTs demonstrate enhanced thermal stability, essential for robust ESS.^(53,54,55,56) Negative thermal expansion in sulfur-doped GO suggests potential in packaging stability.⁽⁵⁷⁾

Power Electronics in Renewable Integration

The interface, fundamental between renewable energy sources and electric power system, is Power electronics. Direct current-alternating current, direct current-voltage regulation, and direct current-harmonic reductions are easily accomplished in devices the inverters and converters, as well as solid-state transformers. Multipurpose power electronic systems provide more stability in gas grids, better fault ride through capability, and flexible functioning of distributed generation. They are especially needed in the incorporation of the following variable resources: photovoltaic arrays and wind turbines to provide continuity with the main grid. Interference with the grid of renewable energy sources requires power electronics. Rapid switching (SS) and protection (PP) devices are based on photoconductive CNTs structure and negative-differential-resistance (NDR) nano-based substances based on graphene.^(2,58) The nanoelectronics monograph⁽⁴⁰⁾ and the phase analysis of CNTs⁽³⁸⁾ shed light on the innovations about nanoscale that are related to converters and inverters. Long-term performance of power electronic components that work in harsh environments is enhanced with the help of protective coatings.⁽⁵⁹⁾

Smart Grid Management Approaches

The achievement of efficient management of smart grids is inevitable in a bid to streamline the benefits that have been brought about through integration of renewable usage. The smart grids management involves a set of functions, such as high-level monitoring, decentralized work, predictive analysis, and automating the decision-making process (table 3).

Table 3 identifies the key measures that are used to arrive at efficiency, reliability, and flexibility in modern power systems. It places emphasis on the way in which Demand Response is able to synchronize consumer usage with grid requirements, and DER management incorporates distributed generation and storage as a means of localized resilience. Energy Storage Management stabilizes variances in supply/demand, with Advanced Metering Infrastructure (AMI) facilitating real time data exchange. In contrast to Market-Oriented Management where competitive models like blockchain-based energy trading are offered, Grid Automation and Control increases the efficiency of the operation by predictive AI and SCADA.

Table 3. Smart Grid Management Approaches

Approach	Description	Key Features / Tools
Demand Response (DR)	Flexible adjustment of consumer energy usage according to grid demand	Dynamic pricing, real-time load control, smart appliances
Distributed Energy Resources (DER) Management	Integration and control of small-scale energy producers and storage systems	Rooftop solar, microgrids, distributed storage
Energy Storage Management	Optimization of storage systems to ensure grid stability	Batteries, pumped hydro, supercapacitors
Advanced Metering Infrastructure (AMI)	Collection of real-time data and enabling two-way communication	Smart meters, data analytics, IoT
Grid Automation & Control	Maintaining energy flow and quality through automated control	SCADA, AI-based forecasting, automated fault detection
Market-Oriented Management	Dynamic management of the energy market, competition, and price optimization	Blockchain-based trading, P2P energy markets, dynamic tariffs
Cybersecurity Management	Ensuring grid reliability through cybersecurity measures	Encryption, intrusion detection, blockchain security

Lastly, Cybersecurity Management helps keep smart grids out of harm’s way of the digital threats and thus, facilitates the smooth stable operation of smart grids. Smart grid management practices are a mix of diverse policies that tend to enhance energy distribution, consumption and reliability by adopting new high-end technologies. One of the main aspects of these strategies is the demand-side management aimed at the optimal use of consumer energy. This is matched with increasing integration of renewable energy, which is paramount in the conservatory energy regimes. According to Zaman et al.⁽⁵⁾, proper efficiency of these mechanisms relies upon effective measurement mechanisms in the context of a smart grid. To analyses faults, optimize operations and maintain grid stability, real-time topology analysis is necessary. Guo et al.⁽⁶⁰⁾ introduces a new concept that is using graph neural networks to enable privacy-preserving analysis, thus illustrating the significance of establishing a secure and effective analysis of data in the integrated world of smart grid. Their work covers the dynamics that have been added by dynamic topologies and the criticality of having stable working frameworks. To conclude, approaches to smart grid management can be described as based on the use of the newest technologies and combined efforts needed to design more efficient, reliable, and sustainable energy systems. The combination of artificial intelligence, innovative energy solutions, and real-time analytical tools creates a holistic business model that underscores the dynamic needs in today’s energy systems.

Real-Time Monitoring and Control

Application sensors, Supervisory Control and Data Acquisition (SCADA), Phasor Measurement Unit (PMU) and Internet of Things (IoT)-enabled devices can be utilized to provide constant data on the performance of power grids, in part by detecting real-time grid status and events. Control systems use these streams of data to make adjustments in real time with respect to voltage, frequency and load-balancing parameters. Machine-learning (ML) and artificial intelligence (AI) algorithms are becoming more widely utilized to predict variability and maximize control measures. Smart grids rely on a real-time information collection. ZnSe/GO nanocomposites have enhanced electrochemical sensitivity in the detection of heavy-metals, which makes them reliable in the environmental surveillance operation in grid systems.⁽⁵²⁾ The paramagnetic centers of Gd-doped graphene oxide are analyzed with electron-paramagnetic resonance (EPR),

and they have the ability to improve sensor calibration.⁽⁵⁵⁾ Flexible, nanostructured electronic platforms enable reliable in-situ monitoring.⁽³¹⁾ The presence of the unmanned aerial vehicles (UAVs) with industrial antenna systems can contribute significantly to the capability of inspection.^(34,48) The AI systems based on the cloud are used to scale the functionality of predictive control and anomaly detection.⁽⁴⁵⁾

Distributed Generation and Microgrids

Distributed generation (DG) refers to localized renewable based electricity generation, commonly coupled with micro-grids. Microgrids are small-scale individual energy sources, which can either work separately or in parallel with the main grid. They build better resiliency of the systems, minimize losses when transmitting energy, and achieve energy trials. Microgrids have been used as a method of maintaining power supply to vital infrastructure during cases of emergencies to locations like hospitals and military bases. Microgrids derive benefits from thermal management frameworks⁽³⁴⁾ and conversion technologies⁽⁴⁸⁾. MXenes and ferrite/rGO supporting supercapacitors enable high power density to support local balancing.^(36,51) Biochar-derived carbons are a sustainable source of electrode.^(35,37) Surface engineering^(59,61) increases the service life of assets of distributed generation.

Integration of Electric Vehicles

Electric vehicles (EVs) are not only a continuous challenge but also a possible opportunity in the setting of smart grid systems. EV uptake on large scale basis raises the power demand, and through vehicle-to-grid (V2G) EV batteries may serve as distributed storage facilities. This bi-directional feature can make EVs ancillary, facilitate shaving of peaks and increase renewable usage and thus transform their integration into a strategic aspect of sustainable smart grid operations. EVs simultaneously increase demand and offer distributed storage. Comparative analysis of EVs and hybrid electric vehicles (HEVs) point to the differences in the effects on the control strategy and resonance properties.⁽⁶¹⁾ The materials of supercapacitors such as MXenes, carbon nanotubes (CNTs), and porous carbons enable rather fast charging.^(35,37,51,62) Vehicle-to-grid is optimized through Internet-of-Things (IoT) and artificial-intelligence (AI) tools.^(49,63) Data flows in EV charging infrastructure are supplemented with the help of antennas and unmanned aerial vehicles (UAVs).^(59,61)

Sustainability and Policy Perspectives

Beyond technical aspects, renewable energy integration requires supportive policy frameworks and sustainability strategies. Smart grids not only enable technological innovation but also promote environmental protection, regulatory evolution, and socio-economic benefits. The discourse surrounding sustainability and policy perspectives in renewable energy is increasingly critical as nations navigate the dual challenges of energy demands and climate change. The transition from fossil fuels to renewable energy sources is not merely an environmental imperative but also an economic necessity. Energy serves as the foundation for any nation's economy, and transitioning to renewable energy is vital for meeting energy needs while mitigating greenhouse gas (GHG) emissions. Investment in renewable energy infrastructure, technological advancement, and supportive policy incentives are essential to achieve this transition effectively.⁽⁶⁴⁾ The challenges and limitations faced during this transition necessitate effective policy responses that prioritize renewable energy initiatives. By formulating policies that incentivize green technology investments and promote a circular economy, nations can ensure that their transition to renewable energy systems is both effective and sustainable.⁽¹⁷⁾ In conclusion, the discourse around sustainability and policy perspectives in renewable energy encompasses a multi-faceted analysis of environmental, economic, and technological factors. The empirical evidence underscores the imperative for nations to realign their energy policies

and investment strategies towards renewable energy to foster a sustainable future while simultaneously addressing the pressing issue of climate change.

Environmental Benefits of Smart Grids

Smart grids reduce greenhouse gas emissions through two ways: First of all, they allow introducing an increased portion of renewable sources, and second, they prevent the underutilization of energy sources. They help to minimize transmission losses, promote the decentralised production of clean energy, and give support to electrify the transport and industrial sector. The switching to smart grids is also parallel in the reduction of air pollutants and water use related to the power facilities based on fossil fuel, which serves to strengthen the process of climate change reduction and material preservation. The example of circular economy practices reducing the carbon footprint is bio-derived carbon issued using the walnut shell and hemp fiber.^(35,37) The energy management systems made with the assistance of artificial-intelligence and Internet of Things (AI-IoT) decrease losses and increase efficiency.^(41,42) Industrial sustainability is promoted by the wastewater treatment frameworks that integrate bioelectronic IoT systems.⁽⁶³⁾ Inspecting the buildings by drone lowers travel emissions.

Regulatory Frameworks and Standards (Europe, USE, Asia, China, India, Azerbaijan)

Achieving the smooth and swift adoption process of the renewable energy sources (RES) into the electric grid is a primary goal of the modern energy policy. The relevant legislative provisions, grid codes and technical standards are explained regionally and country-by-country.

Europe: in the European Union, a main legal tool to address this growth in renewable energy is the Renewable Energy Directive (RED III). The directive provides a binding proportion 42,50 percent of renewable energy sources (RES) with an additional aspirational figure of 45 percent by 2030 and is working towards harmonizing the approving regulatory formalities, making investments quicker and instituting sector category sub-targets. Moreover, the Electricity Market Design reform adopted 21 May 2024 and implemented since 16 July 2024 will strengthen long-term contractual relationships (including CFDs and PPAs), further support consumer protection, and broader flexibilities, which should help to increase the role of variable renewable sources in the grid. PN transmissions system, manufactures, and consumers are coordinated on the basis of the ENTSO-E network codes and guidelines by clearly defined rules of connection, operation, and balancing.

United States: FERC Order No. 2222 is the principal regulatory tool on the integration of renewable in the United States. It is an order that allows the distributed energy resources like rooftop equipment's, storage devices, and electric cars to participate in the wholesale markets. On the technical level, IEEE 1547-2018 means that there are several of the functional and the performance requirement specifying the interaction of DERs, including the support of voltage and frequencies, interoperability, or fault-ride-throughs. Regarding cybersecurity, the mandated standards of NERC CIP (especially CIP-002 and CIP-013-2) seem to enforce risk management and classification of assets in Bulk Electric System. On a state level, California Rule Decrements In place of distribution tier, DER interconnects need to be implemented at a distribution level, and smart inverter functionality should be deployed with certification to UL1741sa.

China: in China, renewable energy sources still form part of the long-term national development program through grid integration. In vesting its objectives of capping emissions by 2030 and carbon neutrality by 2060, The 14th Five-Year Plan on a Modern Energy System is a package aimed at major grid modernization, rural reliability, and the implementation of clean

energy technologies. Also, GB/T/36547-2024 national standard defines technical requirements to connect the electrochemical energy storage systems to the grid. Such requirements include frequency and inertia response, fault - ride-through (FRT), protection systems, communication protocols, and test methodologies.

India: the two key policy tools guiding the development of the renewable energy in India are the Jawaharlal Nehru National Solar Mission (MNRE) and the National Smart Grid Mission (NSGM). The programmers allow faster introductions of solar technologies and extend smart grid infrastructure. Technically, there is the adoption of the Central Electricity Authority (CEA) Technical Standards, which define the interconnection protocols and communication procedures from idle distributed energy resources, and are building upon regulatory guidance established by the Central Electricity Regulatory Commission (CERC). Also, governmental announcements regarding the Renewable Purchase Obligations (RPOs) and energy-storage obligations map the yearly paths, whereas consumer-rights legislation internalizes flexible demand-management provisions and protects the interests of end-users.

Azerbaijan: in Azerbaijan, the major law-making mechanism that supports the establishment and execution of renewable energy is the Law on the Use of the Renewable Energy Sources in the Generation of Electricity (No. 339-VIQ, 31 2021). This law offers the legal parameters that govern renewable energy projects, with an auction system, and, in the pilot projects, direct bargaining. The country is in the compilation of auction rules and standard template contracts with the aid of the European Bank for Reconstruction and Development (EBRD) which increases the level of openness and draw interest to investments in the renewable energy industry. Simultaneously, Azerbaijan partners with international consortia. As an example, the 240 MW Karabakh Solar Power Plant created by BP and deals with China Gezhouba fit with the designation of governmental-defined green energy zones in Karabakh, East Zangezur, and Nakhchivan. These zones will be set up with the modular power plants that are to solidify the energy security of both the rural and urban population. Moreover, the launch of the first ever initiative of the smart city and the smart village in Zangilan is the reflection of the innovative approach taken by Azerbaijan towards the tight collaboration of renewable energy with digital innovation. These efforts contribute to both environmental protection and sustainable development.

Socio-Economic Impacts

Renewable integration and smart grids have immense social economic impacts. Healthy economic growth is achieved through creation of workplaces in manufacturing, installation, and maintenance of renewable systems.^(65,66) Decentralized energy that is affordable raises the living standards and poverty levels among rural inhabitants. More so, smart grids can encourage innovation, investment and make nations more energy-secure. Nevertheless, initial MDV is expensive and socio-political issues demand the long-term financial instruments and people acceptance.⁽⁶⁷⁾

Aerial robotics and improved antenna technologies are devised in smart grids to establish the new industries and employment opportunities.^(34,59) Because of AI/IoT and machine vision, the digital transformation can be accelerated in industry, which enhances performance.^(41,44) The social effects linked to the cyber-physical environment represent the necessity of teaching the principles of ethics, digital skills, and digital literacy.⁽⁴⁴⁾ Reviews and monographs on nanomaterials^(40,51) foster innovation ecosystems and industrial applications.

CONCLUSIONS

The final conclusion in this chapter is that the introduction of renewable energy into modern

power systems will require another basic restructuring of the operation and management of the grid. The digital infrastructure, i.e. smart grid technologies, enable real time data tracking, control adaptations and customer interaction. The deployment of distributed generation and microgrids enhances system resilience and diminishes dependence on centralized fossil-fuel infrastructures. On the one hand, energy storage technologies cannot be ignored to damp the effect of intermittency and the stability of power delivery. Demand response programmers introduce flexibility where consumption is drastically coordinated to renewable generation patterns. The ever-growing input of power electronics enhances compatibility of grid with renewable outputs. Electric cars act as battery in motion more, thus also serving to balance the grids. Smart grids reduce environmental pollution, i.e. greenhouse gas emissions, and encourage the rational use of resources, which are factors that ensure sustainability. The pathway to successful integration is laid out by regulatory frameworks in Europe, the United States, Asia, China, India, Turkey and the Azerbaijan. Among the socio-economic benefits are that it will create jobs, initiate innovation, and increase energy access in the remote locations. Nevertheless, challenges such as cyber-security risks, substantial initial investments, and regulatory inertia persist. The future of smart-grid-implementation depends on the joint activities of policymakers, industry participants, and academically. Standardization and international collaboration will help fasten the implementation process and decrease the fragmentation in technology. The requisite is the balanced combination of technological innovation, favorable policy, and enthusiastic involvement of consumers. Smart grids are the key to the sustainable, resilient and the future-oriented energy infrastructure.

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Chapter 23

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Smart Cities and Environmental Water Pollution

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ABSTRACT

In this period, when the processes of industrialization and urbanization are accelerating, a number of environmental problems are manifested. Many sources used as energy in industry eventually have a negative impact on the environment, pollution occurs, and living organisms are also affected by them. Environmental pollution causes many different diseases in humans. Cancer is the most dangerous of them. The substances that cause this disease react with the environment inside various things and eventually spread to wider areas. One of them is organic pollutants, which are Polycyclic Aromatic Hydrocarbons. In the article, the urbanization process that causes ecological pollution, the factors affecting it, PAHs, which are organic pollutants, their discharge into the waters through oil, polluting the sea and ocean waters, and this process in general, over the Caspian Sea, were reviewed. Various analyzes were performed and the results were recorded. In addition, simple steps to prevent pollution are also mentioned at the end.

Keywords: Urbanization; Smart Cities; Industrialization; PAH; Environmental Pollution; Oil; Caspian Sea.

INTRODUCTION

The processes of ruralization and urbanization have recently been developing at an equal speed. In the very recent past, the acceleration of the urbanization process and the migration of people to cities have had many negative effects on agriculture. Countries probably took this into account and began to pay attention to the development of agriculture.

Many important factors were manifested in the desire of people to move to cities. Many of them went to the cities out of necessity rather than desire. This, in turn, led to the increase and acceleration of the urbanization process.

We can mention some of the factors influencing the acceleration of this process.

It is known that the birthplace of industrialization is cities, or in other words, the places where industry has set foot become urbanized later. Employment—most likely in the recent past—before agricultural innovations—was greater in cities, and that was the factor that most attracted people. Socialization was another key factor in accelerating urbanization. And also, other factors.

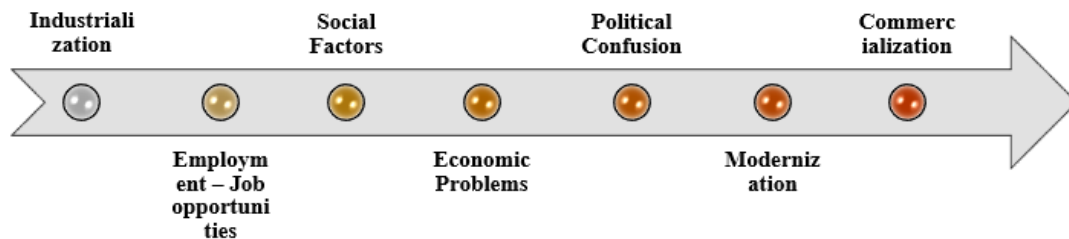


Figure 1. Some factors affecting the urbanization process

According to forecasts, at least 70 % of the world's population will live in cities in the near future - around 2050.

But the introduction of innovations - the introduction of smart village projects along with the application of smart technologies - in agriculture still makes people hopeful about the villages. However, there is still a stronger project than the smart village project. This is the Smart City concept.

The era of industrialization, the increase in human influence, and the further acceleration of urbanization cause many problems. So, along with industrialization, there has been a huge increase in the percentage of environmental pollution. Such pollution eventually leads to a decline in the quality of life of humans and other living beings, and unfortunately continues to this day.

However, continuous technological advances help to prevent pollution and improve the quality of life.

The Smart City project is a concept that combines the capabilities of ICT, that is, using its capabilities, aims to increase both public services and the quality of life of people. From this point of view, various innovations are constantly presented in order to reduce environmental pollution within Smart Cities.

Given that environmental pollution also causes cancer, one of the greatest scourges of our time, it is now the most global problem. With the help of technological possibilities applied in the Smart City, it is estimated that in the near future it will be possible to prevent environmental pollution - to a large extent.

In the article, the following directions are considered:

Environmental Pollution: Impact Of PAH on Human Health

Polycyclic Aromatic Hydrocarbons (PAHs) are persistent organic pollutants (POPs) with two or more benzene rings in their chemical structure.⁽¹⁾

Organic compounds such as polycyclic aromatic hydrocarbons (PAHs) are a global environmental concern as they cause inflammation and skin cancer. As you know there are two types of anthropogenic sources of hydrocarbons: petrogenic and pyrogenic sources. Petrogenic sources include crude oil and petroleum-derived hydrocarbon compounds. Pyrogenic sources of hydrocarbon compounds are formed as a result of incomplete combustion of organic substances

such as oil, wood, coal. About 6,1 million tons of oil products are thrown into the ocean annually most of which are of anthropogenic origin. It is known from the literature that according to the latest indicators every year 6 mln tons of oil and oil products are discharged to the world ocean. Pyrogen and petrogen pollution of sea water contamination with ballast water and so on causes pollution of common water basins. These hydrosphere segments are a dynamic system which leads to a decrease and depletion of fresh water supplies over time.^(2,3)

More than 100 Polycyclic Aromatic Hydrocarbons can be found in nature. However, 16 of these are designated as specific pollutants by the United States Environmental Protection Agency. These are the following:

Table 1. 16 EPA PAHs	
№	PAHs' names
	acenaphthene,
	acenaphthylene,
	anthracene,
	fluoranthene,
	fluorene,
	naphthalene,
	phenanthrene,
	pyrene,
	benz(a)anthracene,
	benzo(b)fluoranthene,
	benzo(k)fluoranthene,
	benzo(ghi)perylene,
	benzo(a)pyrene,
	chrysene,
	dibenz(a,h)anthracene,
	indeno(1,2,3-cd)pyrene.

These 16 EPA PAHs were identified in the 1970s.⁽⁴⁾

- These compounds are among the priority pollutants as reasons.⁽⁵⁾
1. Having more information about these compounds than others.
 2. More harmful PAHs are suspected to be harmful and demonstrate effects.
 3. The risk of exposure to these PAHs is higher than others.
 4. In America, these PAHs have the highest indicators on the list of national priorities (National Priorities List, NPL) can be considered.

Human exposure to PAHs can occur through inhalation, skin contact, or ingestion of food contaminated with PAHs. PAHs in air pollution are primarily associated with particulate matter; When PAHs are in the gas phase, their lifetime is less than a day. Overall, current scientific evidence suggests that PAHs in ambient air are associated with increased cancer incidence in

exposed populations. A positive association between environmental PAHs and breast cancer, uterine cancer and lung cancer has been reported. Epidemiological studies have shown that PAHs are associated with decreased lung function, exacerbation of asthma, obstructive pulmonary disease, and increased cardiovascular disease. Limited epidemiological evidence also suggests adverse effects on cognitive or behavioral function in children.⁽⁶⁾

Here we will take a look at PAHs in water pollution - more precisely in the waters of the Caspian Sea.

There are many ways to treat wastewater. Since these treatment methods are not completely effective therefore, they become a serious threat to the flora and fauna of the Caspian Sea. We know that after treatment wastewater from the oil refining industry is discharged into the Caspian Sea. Wastewater from the oil industry negatively affects the biota of the sea. The Caspian Sea is a very sensitive ecosystem. Over the past decades under the influence of anthropogenic and biochemical factors the state of ecosystems in general has deteriorated sharply and especially in the northeastern part of the sea.⁽⁷⁾

Industrialization and urbanization in the Caspian region have developed rapidly over the past several decades and the associated increase in hydrocarbons is a concern in the region. Offshore production and accidental oil spills, industrial waste, wastewater, discharges flowing down from river water are considered the main source of anthropogenic hydrocarbons in the marine environment.⁽⁸⁾ Industry is believed to be the main source of oil pollution in the Caspian Sea.⁽⁹⁾ The total amount of industrial waste discharged into the Caspian Sea averages 2342,0 million m³ per year. Such waters contain 122,5 thousand tons of oil, 1,1 thousand tons of phenols, 9,9 thousand tons of organic chemistry products. The total content of hydrocarbons in the North-Western part of the South Caspian was small - 32-54,2 µg/g. In this area in the vicinity of oil fields the concentration of phenol was 0,002-0,003 µg /g.^(10,11)

The main volume of pollution (90 % of the total) enters the Caspian Sea with river runoff. After purification these waste waters are discharged into the Caspian Sea and even in small quantities these harmful substances are dangerous for the flora and fauna of the sea and the environment. As is already known PAHs are very dangerous for the environment for living organisms in aquatic ecosystems and therefore the identification of hazardous substances and the application of methods for their destruction is very important.^(12,13)

METHOD

The quantitative analysis of polycyclic aromatic hydrocarbons (PAHs) also of phenol and its derivatives were carried out in a system including an Agilent 6890N gas chromatograph which has an interface with an Agilent 5975 high-performance mass-selective detector manufactured by Agilent Technologies (USA). The chromatograph was equipped with a splitless injector and a ZB-5 capillary column (Phenomenex, USA). Column ZB-5 has the following specifications: 5 %-biphenyl 95 %-dimethylpolysiloxane copolymer length-60 m inner diameter 0,25 mm film thickness 0,25 µm. Helium (99,999 % purity) with a flow rate of 1,5 ml/min was used as a carrier gas. The temperature rise was programmed from 40 °C to 310 °C. The extracts were introduced using an automatic sampler in a volume of 1 µl (Dettmer-Wilde, 2014). Quantitative analysis was performed against a seven-point calibration against standard reference solutions. A mixture of deuterated polycyclic aromatic hydrocarbons: naphthalene-d₈, phenanthrene-d₁₀ (Cambridge Isotope Laboratories, Inc., Andover USA) was used as an internal standard for calculating the obtained results of chromatographic analysis.⁽¹⁴⁾

At first PAHs were analyzed in water samples discharged from the oil industry into the Caspian Sea. The results of the analyses and chromatograms for each sample are given below.

Table 2. Determination of Polycyclic Aromatic Hydrocarbons in Water Samples Taken from the Oil Refinery					
№	PAH, mg/l	Standard indicator	Sample 1	Sample 2	Sample 3
	Naphthalene	≥0,01	0,08	0,23	20
	Achenthylene	≥0,01	0,02	0,51	15
	Acenaften	≥0,01	0,04	0,33	43
	Fluorene	≥0,01	0,24	0,81	80
	Phenanthrene	≥0,01	0,29	4,32	298
	Anthracene	≥0,01	0,04	0,33	26
	Fluoranthene	≥0,01	0,03	3,01	15
	Piren	≥0,01	0,05	13	66
	Benz (a) anthracene	≥0,01	0,01	3,5	17
	Chrezen	≥0,01	0,02	15	41
	Benz (b + j + k) fluoranthene	≥0,01	<0,01	2,2	5,0
	Benz (a) pyrene	≥0,01	<0,01	1,3	5,0
	Inden (1,2,3-cd) pyrene	≥0,01	<0,01	0,37	1,5
	Benz (ghi) perilen	≥0,01	<0,01	0,63	1,7
	Dibenz (ah) antracen	≥0,01	<0,01	0,57	1,8

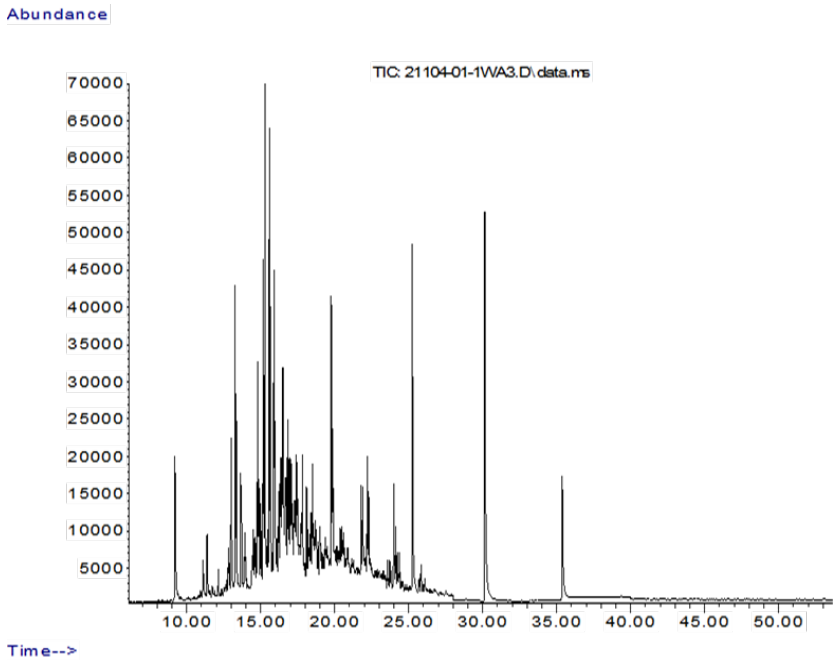


Figure 2. GC-MSD spectroscopy of sample 1

It should be noted that excess PAHs are expected to be present in refinery wastewater. Wastewater of this type is biologically treated and then discharged into the Caspian Sea. Below are the chromatograms taken for 3 water samples of the oil industry.

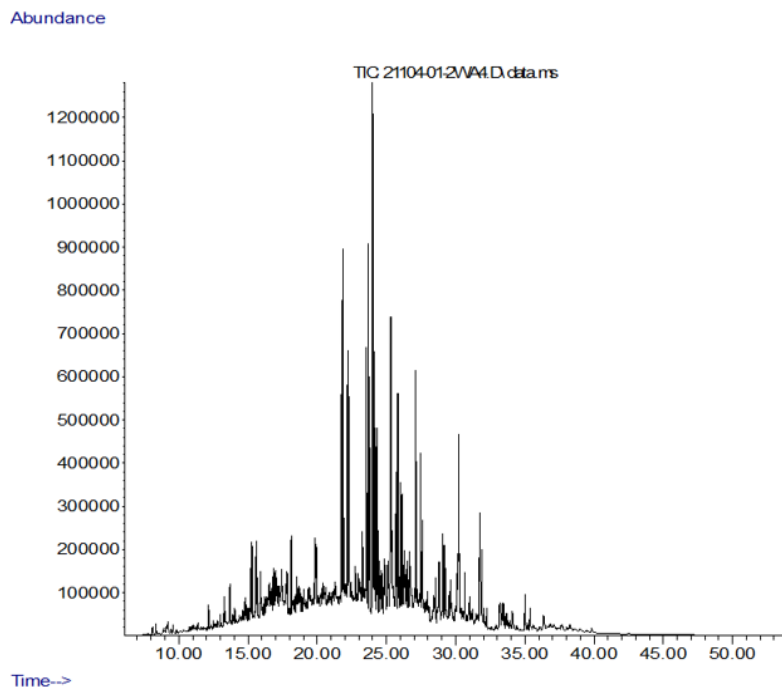


Figure 3. GC-MSD spectroscopy of sample 2

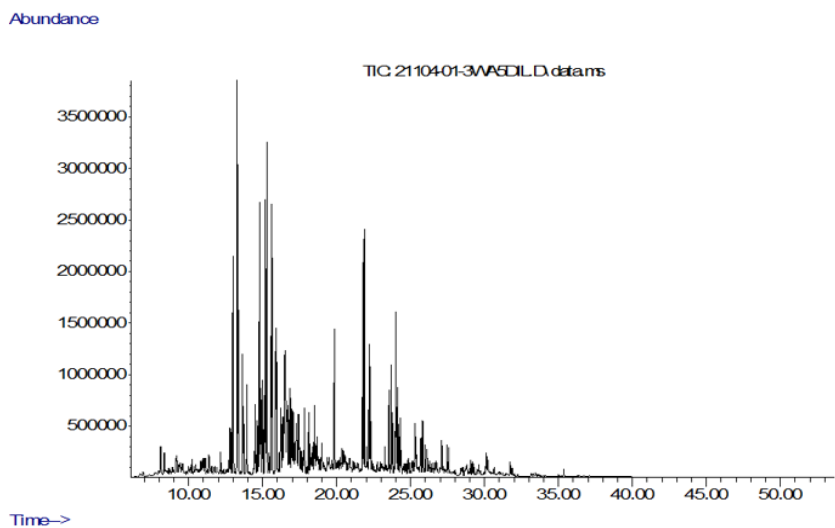


Figure 4. GC-MSD spectroscopy of sample 3

Phenol and its derivatives were also determined in the water samples of the oil industry and the results are given in table 3.

Table 3. Determination of phenol and its derivatives in water samples taken from the Oil Refinery

Nº	Compounds (mg/l)	Standard indicator	Sample 1	Sample 2	Sample 3
	phenol	$\geq 0,04$	5,34	5,65	1,44
	o-cresol	$\geq 0,04$	0,76	0,26	0,16
	2-nitrophenol	$\geq 0,04$	0,59	0,48	0,08
	2,4-dimethylphenol	$\geq 0,04$	31,99	8,71	0,20
	m,p-cresol	$\geq 0,04$	20,59	3,81	0,85
	2,6-dichlorophenol	$\geq 0,04$	1,14	0,67	1,80
	4-chloro-3-methylphenol	$\geq 0,04$	0,63	0,43	0,69
	2,4,5-TCP	$\geq 0,04$	0,48	0,28	0,18
	2,4,6-TCP	$\geq 0,04$	0,14	0,04	0,25
	2,3,4,6-tetrachlorophenol	$\geq 0,04$	0,27	0,18	0,002
	2-methyl-4,6-dinitrophenol	$\geq 0,04$	<0,04	<0,04	<0,04
	pentachlorophenol	$\geq 0,04$	0,27	0,25	0,06
	2-sec-Butyl-4,6-dinitrophenol	$\geq 0,04$	<0,08	<0,08	<0,08
	Compounds (mg/l)	Standard indicator	Sample 1	Sample 2	Sample 3
	phenol	$\geq 0,04$	5,34	5,65	1,44

The high amount of phenol in the 2-water sample is due to sampling from a water tank located closer to the production site. At the same time heavy metal ions were identified in the water samples examined. Heavy metals enter aquatic living organisms and enter the human body through the food chain. Determination of heavy metals was performed by ICP-OES, Optima 2100DV emission analysis method. The results are shown in the table 4.

Table 4. Number of heavy metals in wastewater samples of the Oil Refinery			
Heavy metals, mg/l	Sample 1	Sample 2	Sample 3
Fe	0,048	0,047	0,042
Zn	0,143	0,078	0,023
Cu	0,023	0,028	0,020
Mn	0,021	0,105	0,038
Pb	0,022	0,017	0,009
Cd	0,007	0,006	0,008
Cr	0,004	0,003	0,004
Co	0,009	0,014	0,012
Ag	0,009	0,010	0,008

All these metals are dangerous if they exceed the MPC norm, but Cd is more dangerous. Norm for Cd is 0,001 mg/l (mg /dm³). As can be seen from the table the amount of Cd in the studied samples is higher than the norm.

Combating Water Pollution in Smart Cities

We gave an analysis of PAHs in waters polluted by oil spills in the previous chapter.

Oil has become one of the main sources of energy since the 1950s, on the eve of the industrialization period. And it still remains so. Although the concept of Smart Cities is an “Environmentally friendly” project, there is still a need for oil-derived energy. However, the use of oil inevitably causes major environmental pollution. Most importantly, it causes ocean and sea water pollution.

We first analyzed PAHs and their effects on water pollution due to oil, as well as subsequent PAH levels in these waters.

Such environmental problems should be minimized through the Smart City concept. Harmful sources of energy such as oil should be replaced with more efficient ones. However, although we cannot completely prevent water pollution in general, we can control it nowadays with a number of smart technologies.

We can look at this chapter in two directions:

1. Prevent water pollution with simple efforts.
2. Steps to combat water pollution and depletion of freshwater resources through smart technologies.

Prevent pollution with simple efforts

The entire responsibility for preventing pollution cannot be placed on smart technologies. People can prevent pollution by simple efforts. By first protecting our own little world from pollution, we can significantly minimize environmental pollution as a whole.

Before the technological approach, people can implement a number of methods to prevent pollution:

Disposal of toxic chemicals

We use many chemical products for daily processes like cleaning etc. Various bleaches and dyes cause serious problems. When such products are subsequently disposed of in the sewers, their harmful effects increase.

The best way to avoid this is to apply recycling.

Proper disposal of medical waste

Medicines should not be thrown into the sewer or into any water such as a lake or the sea. Because it affects the animals living there, it causes various diseases, and in the end, the water that people and cattle drink becomes polluted. This again poses a threat to a person's own health.

Do not pour oil down the drain

Many experts repeat this many times. Products such as oil should not be thrown down the drain. This again has a very heavy impact on water pollution.

Try to avoid using plastic containers

Plastic is one of the things that have a negative impact on nature. It continues to exist in

nature for a long time. Similarly, thousands of plastics thrown into the seas have a negative effect on the creatures there. The main effort that can be made here is either not to use plastic items at all or to send plastic items to recycling.

Help clean up beaches and rivers

Unfortunately, 75 out of 100 people make efforts to protect nature, while the other 25 do the opposite. In this regard, whenever possible, people should help to regularly clean the banks of rivers and seas from garbage thrown by other people. In fact, that garbage should not be thrown there. On the other hand, it is the duty of every person to fight against the perpetrators, as well as to clean up. Because this nature is the abode of every living being.

Control your cars: people who use cars should regularly have their cars checked (monitored). Thus, the oils and various liquids leaking from the car flow into the sewers, from where they can eventually go to other water sources.

These are just some of the steps that need to be taken. And they are the simplest ones. People can use hundreds of different methods to prevent pollution.

On the other hand, it is possible to prevent pollution through smart technologies:

Steps to combat water pollution and depletion of freshwater resources through smart technologies

In fact, in a simple case, the main step here is: the proper use of smart technologies.

Due to water pollution, fresh water resources are in danger of diminishing. This eventually leads to drought. In order to prevent this, fresh water resources should be constantly monitored. This is a relatively difficult process without the help of technology. Internet of Things-based devices, especially applied in smart cities, are the ideal smart tools that can help people in such processes.

In general, the following smart technology projects have been proposed:

Data collection systems or Monitoring systems

First, data collection systems are created for any system. Thus, changes in the amount and composition of water are constantly monitored, data is collected and analyzed. At the same time, various data analysis technologies are used for this. Big Data Analytics is also applicable.

IoT-based water distribution systems to monitor water flow, quantity and leakage

Smart Water, Shap technological innovations are among the main helpers in this direction. For irrigation systems, HydroPoint's Weather TRAK irrigation system applies.

ED technology

Electrodialysis (ED) is notable for removing chromium and arsenic from water contaminated by sources such as textile dyeing, leather tanning, dye and pigment industries.^(15,16) ED technology can recover wastewater and reclaim water through concentration, dilution, desalination, regeneration and valorization.

Efficient water management systems

Water management is important in terms of developing water-energy interconnection. For example, SCUBIC is an IoT smart energy management solution that uses data to improve the

functionality of water utilities. By deploying sensors and collecting data, pumping schedules can be simplified to reduce costs and improve water safety.⁽¹⁷⁾

Different countries adopt different acts to prevent water pollution. Accordingly, they use both the above-mentioned and a number of other technologies and build factories.

In Belin, for instance, a phosphorus elimination plant was built to treat the effluent of the pharmaceutical industry in order to limit the quantity of phosphorus discharged into the rivers.
(15,18)

CONCLUSIONS

It is known that the waste water of the oil industry is very dangerous for the aquatic ecosystem. Thus, it causes serious damage to flora and fauna of water ecosystem. For this purpose, 3 waste water samples were taken from the oil industry and analyzed. The goal was to determine their composition. For this purpose, PAHs, phenolic organic compounds and heavy metals were determined in water samples. Chemical analysis of water samples was carried out on a GC-MSD gas chromatograph 6890N with a highly efficient mass-selective detector-Agilent 5975. In water samples heavy metals were analyzed on a PerkinElmer ICP/OES-2100DV. A total of 15 PAHs, 13 phenolic and heavy metals compounds were analyzed in water samples. As in the analysis of PAHs the most dangerous naphthalene were observed in the water samples 2 and 3. As can be seen from the Table 2, the MPC limit for PAHs is 0,01 mg/l. Naphthalene belongs to a class of high-risk substances and is considered the most hazardous among PAHs. Therefore, the main focus was on which areas of the water samples had the highest levels of naphthalene. The amount of phenol was higher in water samples 1 and 2. In general, the permissible concentration of phenol for industrial water in the maximum case should be 0,1 mg/l. As can be seen from the Table 2, in this 3, 1, 2 samples the amount of phenol gradually increases: 1,44-5,34-5,65 mg/l. As for heavy metals most of them (mainly Cd) have exceeded the limit.

In general, we can briefly note the following results:

1. Environmental pollution is one of the most global problems of the time. One of the main reasons for this is the acceleration of the urbanization process. As people came to cities, industry became more developed, and of course, one of the reasons for pollution is the era of industrialization.
2. Environmental pollution is mainly in 3 forms: air, soil and water pollution. In the article, we looked at water pollution and its contamination with PAHs. Various methods were applied and analysis was carried out here.
3. In order to prevent pollution, at least to reduce it to a minimum level, people need to apply various methods. A few of them were mentioned. On the other hand, several technological innovations applied in smart cities have been mentioned.

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ADDITIONAL INFORMATION

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