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ABSTRACT

of the dissertation for the degree of Doctor of Philosophy

**DEVELOPMENT OF METHODS FOR SOLVING
CORROSION AND SALT PRECIPITATION PROBLEMS IN
THE SUMQAYIT, BILGAH, PIRALLAHI, AND NEFTCHALA
REGIONS OF THE CASPIAN SEA**

Speciality: 3303.01 – Chemical technology and engineering

Field of science: Technical sciences

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Baku – 2025


The work was performed at “Optimisation and Mathematical Modelling of Chemical Processes” laboratory of the Academician Y.H.Mammadaliyev Institute of Petrochemical Processes of the Ministry of Science and Education of the Republic of Azerbaijan.

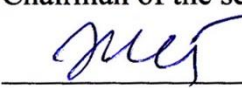
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GENERAL NATURE OF THE WORK

The relevance of the topic and the degree of development. It is known that the Caspian Sea makes a significant contribution to the energy supply of neighbouring countries such as Azerbaijan, Iran, Kazakhstan, Russia and Turkmenistan. The Caspian Sea, which is an important area for oil and gas production, has serious environmental challenges. Thus, the presence of corrosion in the Caspian Sea negatively affects the sustainability of industrial infrastructure and creates serious environmental and economic challenges. The region's variable temperature and high salinity increase the complexity of combating corrosion in the Caspian Sea. As the infrastructure deteriorates over time, the likelihood of failures such as pipeline leaks and platform failures due to corrosion increases. This can ultimately result in environmental disasters affecting marine life and coastal populations. Overcoming these challenges is essential to ensure the safety of oil and gas production.

In this regard, corrosion in the Caspian Sea in recent years has led to harmful economic and environmental consequences. As a result, maintenance and repair costs due to corrosion have increased significantly, and large amounts of money are allocated every year to reduce its impact¹. In addition, the environmental impacts of corrosion-related failures, such as oil spills and gas leaks, can result in serious ecological damage, alter marine ecosystems, and threaten the livelihoods of coastal residents.² Thus, slowing down and preventing corrosion processes is essential to ensure industrial productivity, environmental protection, and societal well-being in the Caspian littoral regions. In this regard, the presented dissertation is devoted to a topical issue - solving problems such as corrosion and salt precipitation on offshore oil platforms and pipelines.

¹ Терлеева, Н.В. Последствия и риски катастроф на морских месторождениях нефти и газа в Каспийском море. / Н.В. Терлеева, А.Ю. Иванов // Экология и промышленность России, – 2014. №11, – с.15-21.

² Mohialdin, S.N. Review on Corrosion Inhibitors for Oil and Gas Pipelines in Petroleum Industries. / S.N. Mohialdin, Ch.Dilshad // International Journal of Science and Research (IJSR), – 2022. Vol. 10, No. 10, – p. 754-764

Object and subject of research. Seawater from various regions of the Caspian Sea - Sumgayit, Bilgah, Pirallahi and Neftchala - was taken as the object, and the salt precipitation, corrosion, antimicrobial, microbiological and oil-accumulating properties of surfactants in the seawater taken as the subject were studied.

Goals and objectives of the study. The aim of the study is to comprehensively analyse the corrosion mechanisms specific to the Caspian Sea and evaluate the effectiveness of existing solutions to prevent or reduce corrosion. The aim was to study the methods for solving corrosion and salt precipitation problems in different regions of the Caspian Sea. The following issues were addressed to solve the problems:

- new substances were synthesised and spectrally analysed from the interaction of stearic acid with amines (monoethanolamine (MEA), diethanolamine (DEA), triethanolamine (TEA), ethylenediamine (EDA) and diethylenetriamine (DETA));

- The salt-precipitation, microbiological, antimicrobial and oil-accumulating properties of the synthesised substances were investigated;

- Computer Vision models have been created to increase the accuracy of laboratory research;

- The "Bag of SMILES" and "ChemGrams" artificial intelligence algorithmic library was created using the "SMILES" nomenclature to determine the effectiveness of corrosion inhibitors.

Research methods. The structure and properties of the substances obtained in the dissertation work and the prepared compositions were studied using modern research methods (IR-Fourier spectroscopy method, ^1H NMR, ^{13}C NMR and UV-spectroscopy, thermogravimetric (TG) and differential thermal analysis (DTA) methods). Thus, using physical research methods of the prepared compositions, the freezing point, pH indicator, the amount of water in the oil, mechanical impurities, chloride salts and various ions in the composition of the obtained samples were determined.

The main provisions put forward for defence:

- corrosion inhibitors;

- salt-precipitation inhibitors;
- bactericides against sulfate-reducing bacteria in seawater;
- antimicrobial properties;
- oil collector and SAM;
- Creation of artificial intelligence models.

Scientific novelty of the research.

New reagents have been developed to combat salt precipitation and corrosion in the Caspian Sea and its regions. For the first time, for example:

- MEA, DEA, TEA, EDA and DETA were synthesised with stearic acid and new compounds were obtained;
- Antimicrobial properties were investigated using the “Biotrac” device;
- The mechanisms of action of the synthesised substances against bacteria were studied using the “Docking” and “ChemInformatics” programs;
- The absorption properties of substances were investigated using the UV method;
- A model for identifying sulfate-reducing bacteria using computer vision models has been created;
- A computer vision model was created for observing oil reservoir properties;
- Algorithm libraries have been created to calculate the effectiveness of corrosion inhibitors to be synthesised in the future using artificial intelligence models.

Theoretical and practical significance of the study.

In various regions of the Caspian Sea (Sumgayit, Bilgah, Pirallahi and Neftchala), complex approaches have been taken to combat corrosion, salt precipitation and microbiological effects in seawater, and methods for solving this problem have been studied.

Reagents synthesized based on stearic acid and amines (MEA, DEA, TEA, EDA and DETA) can be used as multifunctional inhibitors. These reagents have also shown high results as salt precipitation, surfactant (SAM), microbiological, antibacterial agents.

The results of experiments conducted in laboratory conditions have been refined and widely applied with computer vision algorithms

developed by us. Thus, models have been created that localize oil spills, segment corroded metal parts in industrial facilities, identify sulfate-reducing bacteria (SRB) colonies (in test tubes), and automatically calculate the K-factor of SAMs using computer vision (CV) algorithms and satellite images.

The “ChemGrams” and “Bag of SMILES” libraries were created using the National Language Processing (NLP) model of artificial intelligence. With the help of these libraries, it is possible to calculate in advance how effective the selected inhibitor can be on the corrosion of target metals.

Molecular docking calculations were performed using modern computer programs such as Swissdock, Auto Dock Vina, and PyMol. As a result of these calculations, the probability of the ligand binding to the bacterial protein and which amino groups it can bind to were theoretically calculated .

Approval and implementation.

17 scientific works have been published on the main results of the dissertation work. 9 of them are articles, 8 are conference proceedings and a thesis.

The materials of the dissertation were discussed at the following conferences:

International Conference dedicated to the 60th anniversary of the establishment of the Department of Technology of organic substances and high-molecular compounds. "Modern problems of macromolecular compound technology", (Baku, 2024); Sustainable development of society: New scientific approaches and research collections of scientific papers on the materials of the IX International Scientific and Practical Conference, (Moscow, 2024); International scientific conference dedicated to the 100th anniversary of Academician Maharram Ali oglu Mammadyarov named "Modern problems of petroleum chemistry and oil technology" (Baku, 2024), Republican scientific and technical conference on "Water resources in Azerbaijan: problems and challenges" (Baku, 2024); VII International Scientific and Technical Forum on Chemical Technologies and Oil and Gas Processing, (Minsk, 2024); Third International Bilateral Workshop on Natural Science Between Dokuz Eylul University and

Azerbaijan National Academy of Sciences, (Baku, 2024); International scientific conference "Sustainable environment: transition to green energy" dedicated to the "Year of solidarity for a green world" (Baku, 2024); International scientific conference "Monomers and modern problems of petrochemicals" dedicated to the 110th anniversary of Academician Soltan Jafar oglu Mehdiyev (Baku, 2024).

Name of the organization where the dissertation work was performed. The submitted dissertation work was performed at the Institute of Petrochemical Processes named after academician YHMammadaliyev of the Ministry of Science and Education of the Republic of Azerbaijan.

Personal participation of the author. The author personally participated in the formulation of the issues included in the dissertation, the generalization and interpretation of the experimental results obtained, the conduct of tests, and the writing of scientific works.

The total volume of the dissertation, indicating the volume of the structural sections of the dissertation separately: The dissertation consists of an introduction, 4 chapters, a conclusion, a list of references with 124 sources, and 163 pages, including 26 tables, 53 figures, and 3 diagrams. The dissertation consists of a total of 184965 characters (introduction 10415, chapter I 32530, chapter II 58355, chapter III 50150, chapter IV 31955, and conclusions 1560), excluding tables, figures, diagrams, and the list of references.

The introductory part of the dissertation provides information about the relevance of the topic, the goal, the scientific novelty and practical significance of the work.

The first chapter provides information on recently used inhibitors against corrosion and salt precipitation, as well as discusses existing bactericides against sulfate-reducing bacteria. The scientific literature on their mechanisms of action is reviewed, indicating their advantages and disadvantages.

In the second chapter, water samples were taken from four coastal areas of the Caspian Sea (Sumgayit, Bilgah, Pirallahi, Neftchala). The results of the studies of the physicochemical and ionic

composition of the taken water samples are given. The results of the thermal analysis of the dry residue remaining from the evaporation of water and the dynamic light scattering method are presented. The results of the X-ray phase analysis of the salt residue in the water samples are given. The bacterial composition of the water samples, microbiological analyses, and the analysis of corrosion and salt precipitation processes are given.

The third chapter presents information on the synthesis of amines (MEA, DEA, TEA, EDA and DETA) with stearic acid. The results of studying the composition of the obtained reagents by infrared and nuclear magnetic resonance spectral methods , and analyzing the absorption capabilities by ultraviolet methods are presented. The results of studying the molecular structures of the reagents by computer programs are presented. The possibilities of using the obtained reagents as inhibitors against salt precipitation , antibacterial and microbiological corrosion, and as surfactants against oil accumulation are analyzed.

The fourth chapter provides information about models that localize oil leaks from satellite images in a short time using artificial intelligence computer vision algorithms, detect the degree and location of corrosion zones on metal surfaces of industrial facilities, and determine the oil accumulation coefficients of SRB assemblies without human intervention inside the thermostat and SAMs from a camera installed on the experiment.

Information was presented on the creation of two new libraries that determine the effectiveness of corrosion inhibitors against metals from the "SMILES" nomenclature using artificial intelligence conversational language algorithms.

To better understand microbiological and antimicrobial properties through molecular docking calculations, the results of calculating the binding efficiencies of reagents to bacterial proteins and the theoretical study of the method of killing bacteria based on which amino groups of the bacterial protein can form bonds were presented.

At the end of the dissertation, results reflecting the research conducted, a list of cited literature, and appendices are included.

MAIN CONTENT OF THE WORK

Methods of analysis of waters brought from the basins of the Caspian Sea

After water samples were taken from the basins of the Caspian Sea (Pirallahi, Bilgah, Sumgayit and Neftchala), the pH, turbidity, salinity and electrical conductivity of these samples were examined.

According to the analysis results, the pH value varies from 7.6 to 7.9, which indicates the presence of a weak alkaline environment in all study areas. The results (6.5-8.5) are in line with the permissible concentration limits for drinking water and aquatic life and meet international standards.

The experimental results of electrical conductivity and salinity levels were quite high. The lowest electrical conductivity was determined in Sumgayit at 18120 $\mu\text{S}/\text{cm}$, and the highest in Neftchala at 18790 $\mu\text{S}/\text{cm}$. The salinity level varies in the range of 11.6-12.0 g/l. High electrical conductivity and salinity are directly related to the ionic composition of the water, and these indicators can also deteriorate as a result of seawater evaporation and human activities. High electrical conductivity and salinity levels indicate the presence of major ions that can affect the suitability of water for drinking, agricultural and industrial applications.

The amount of calcium ions in the water bodies studied varies from 320.64 mg/l to 360.72 mg/l, and the amount of magnesium ions varies from 680.96 mg/l to 814.72 mg/l.

Chloride ions are present at high levels in all of the studied water bodies. The highest concentration among these bodies was observed in Neftchala (5751.4 mg/l).

The concentrations of sulfate ions in water bodies vary from 3110.6 mg/l to 3244.2 mg/l, which depends on industrial pollution or mineral deposits. Such high sulfate ions can be associated with the presence of industrial or agricultural activities in these areas. The high concentration of sulfate ions in the environment leads to the formation and increase in the number of sulfate-reducing bacterial colonies in these areas.

the evaporation of seawater samples taken from four main areas

of the Caspian Sea - Bilgah, Sumgayit, Pirallahi and Neftchala - and the residues obtained after drying were studied using thermogravimetric (TG) and differential thermal analysis (DTA), X-ray phase (RF) and dynamic light scattering (DLS) methods.

In general, TG/DTA analyses of the residues obtained after evaporation of seawater samples taken from the Caspian Sea show that their chemical composition varies depending on the area and these changes affect the mass variability and thermal stability under the influence of heat. The higher crystal water content of the Bilgah and Sumgayit samples caused them to lose more mass during the thermal decomposition process. On the other hand, the Pirallahi and Neftchala samples were richer in SiO_2 and CaSO_4 compounds, so their thermal properties were different. These results provide important information for a better understanding of the nature of salts in the Caspian Sea and their impact on the ecology.

IDS analyses of samples taken from the Caspian Sea show that the particle size and distribution of salts in each area depends on the ecological state of those areas and anthropogenic impacts. Since industrial pollution is higher in the Sumgayit and Pirallahi areas, more diverse and inhomogeneous particles are observed in the samples taken from these areas. On the other hand, the Bilgah and Neftchala areas are less polluted, which led to the presence of less homogeneous particles in their composition.

Overall, X-ray phase analyses of samples taken from different areas of the Caspian Sea show that there are differences in chemical composition in each area, and these differences are closely related to the ecological situation and industrial impacts of those areas. The results of the analyses allow us to reveal similarities and differences between samples taken from the four main areas and provide important information for a deeper understanding of the causes of these differences.

Statistical approaches were used to analyze the obtained results in more depth. Considering the non-normal distribution of the results and the limited number of samples, the Kruskal-Wallis test was chosen as the appropriate statistical test method.

Statistical analysis confirmed that there was a significant

difference between the studied water bodies in terms of “Coliform” and “E.Coli” bacteria. This is due to the fact that the “p-value” was lower than 0.05. Additional “post-hoc” tests revealed a significant difference between Neftchala and the other three studied regions. No association was found for the Entrecocc bacteria. These results confirm the role of local factors in bacterial contamination, which increases the need for local approaches for bacterial cleaning.

H_2S), a metabolic product of SRB in the Pirallahi region, was also studied. It was determined by analytical titration that the amount of H_2S was 256 mg/l. Such a high amount of H_2S is one of the main factors stimulating the corrosion process of metals in the environment in an acidic environment.

Investigation of the corrosion process in samples taken from the coastal regions of the Caspian Sea.

The data on corrosion rates clearly demonstrate the variation in water chemical composition between regions and its effects on the corrosion process. The highest corrosion rate was recorded in Pirallahi as 1.3724 g/m²·h. Thus, the results obtained show that it is more aggressive in terms of corrosion. In Neftchala, the corrosion rate was 1.3586 g/m²·h, in Bilgah 1.3448 g/m²·h, and in Sumgayit, the corrosion rate was the lowest and was recorded as 0.8345 g/m²·h. It can be said that here this corrosion process mainly depends on environmental factors and industrial waste discharge.

The highest corrosion rate observed in Pirallahi is due to the geographical factors of this region. and industrial waste. Since this region has active oil production, the water is likely to contain hydrocarbons, heavy metals, and other industrial waste. This can cause the water to have more aggressive corrosive properties.

Salt precipitation in the Caspian Sea water problem.

Experimental results conducted in the coastal regions of Neftchala, Bilgah, Pirallahi and Sumgayit of the Caspian Sea indicate that the salinization rates in these areas are at different levels. The salinization rates were measured in milligrams per square meter per hour and the values ranged from 0.000012 to 0.00002 mg/m²·h.

Table 1.**Salinization rate of samples taken from the coastal zones of Neftchala, Bilgah, Pirallahi and Sumgayit regions**

An experiment was conducted. territory	Salt precipitation rate mg/m ² ·h
Neftchala	0.000013
Wise	0.000014
Pirallahi	0.00002
Sumgayit	0.000012

The research conducted allows for the creation of more effective means of protection against corrosion of oil and gas extraction equipment in various regions of the Caspian Sea, technical installations on the coast that use Caspian Sea water, and in particular, seawater transport pipes to maintain stable pressure in the formation .

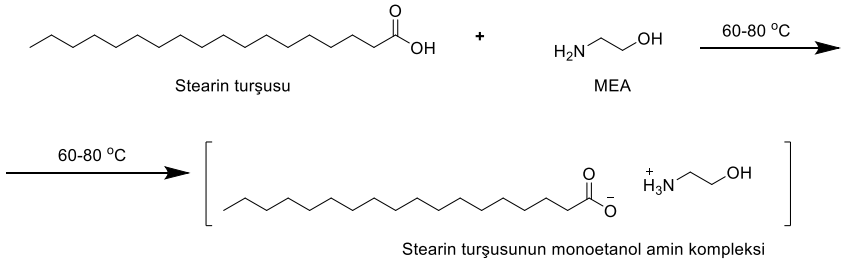
Study of the possibilities of using amine complexes as reagents in solving the problems of salinization, corrosion and microbiological corrosion in the waters of the Caspian Sea

New amine complexes have been synthesized and their various properties analyzed to solve the problems of salt precipitation , corrosion, and microbiological corrosion encountered in the waters of the Caspian Sea .

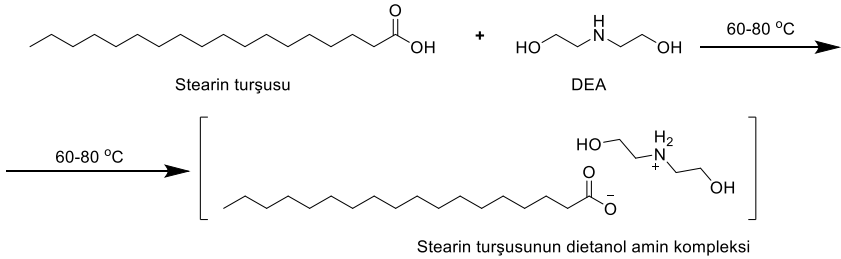
Obtaining new substances from the reaction of amines with stearic acid.

We considered it appropriate to use stearic acid as a basis for our study . One reason for this is that there is large-scale industrial production of synthetic stearic acid [C₁₇H₃₅-COOH], as well as a mixture of C₁₇-C₂₀ fatty acids. On the other hand, there are natural triglycerides that are mainly triglycerides of stearic acid, and stearic acid can be obtained from these triglycerides by hydrolysis. This creates opportunities for the use of renewable raw materials.

1. Scheme of the reaction for obtaining the monoethanolamine complex of stearic acid:

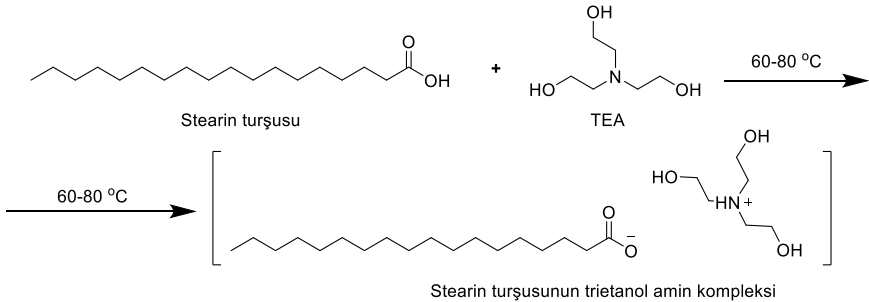


2. Scheme of the reaction for obtaining the diethanolamine complex of stearic acid :



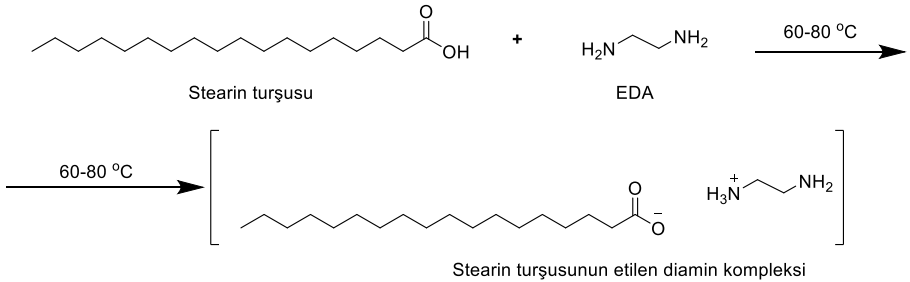
The reaction of stearic acid with triethanolamine (TEA) occurs as a more complex reaction due to the presence of three hydroxyl and amine groups in the triethanolamine molecule.

3. Scheme of the reaction for obtaining the triethanolamine complex of stearic acid:



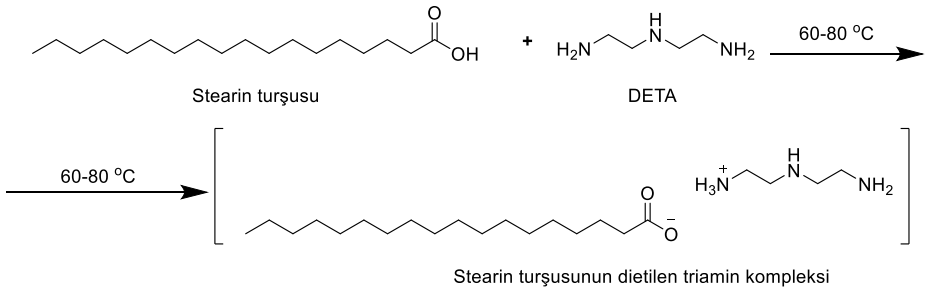
During this reaction, triethanolamine protonates the carboxyl group of stearic acid, resulting in the formation of a carboxylate ion and a protonated form of triethanolamine. The presence of three active groups in triethanolamine increases the functionality of this product.

4. Scheme of the reaction for obtaining the ethylenediamine (EDA) complex of stearic acid:



As a result of this reaction, ethylenediamine protonates the carboxyl group of stearic acid to form an ammonium salt. The functionality of the product is increased due to the two active groups of ethylenediamine.

5. Scheme of the reaction for obtaining the diethylenetriamine complex of stearic acid:



The reason for the high functionality of diethylenetriamine is that it contains several active groups.

The IR spectra of the reaction products were recorded at room temperature on an ALPHA IR-Fourier spectrometer (Bruker) manufactured by the German company BRUKER (Figures 1 and 2). E-1 is the reaction product of MEA with stearic acid, E-2 is the reaction product of DEA with stearic acid, E-3 is the reaction product of TEA with stearic acid, E-4 is the reaction product of EDA with stearic acid, and E-5 is the reaction product of DETA with stearic acid.

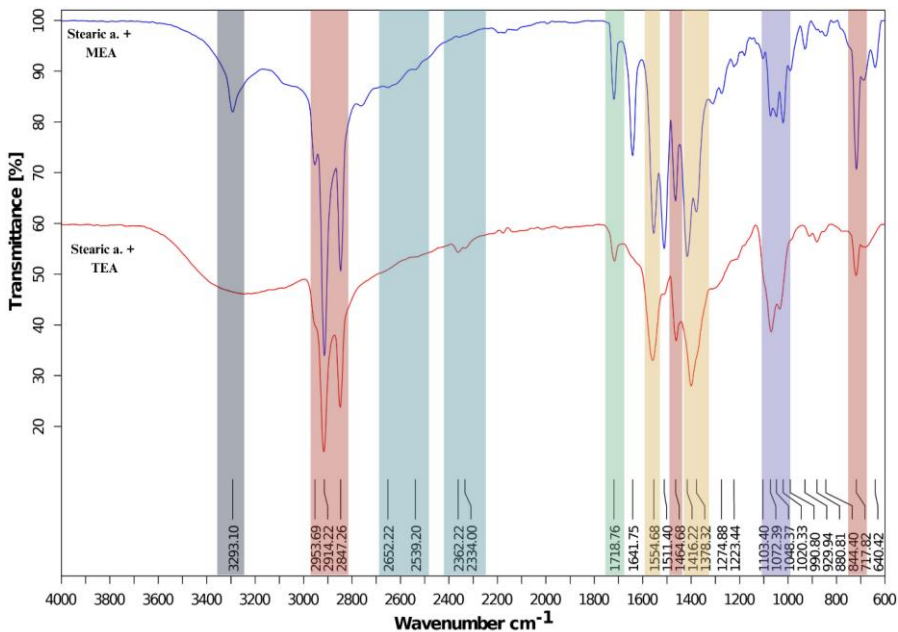


Figure 1. Graphical representation of the IR spectra of reagents E-1 and E-3.

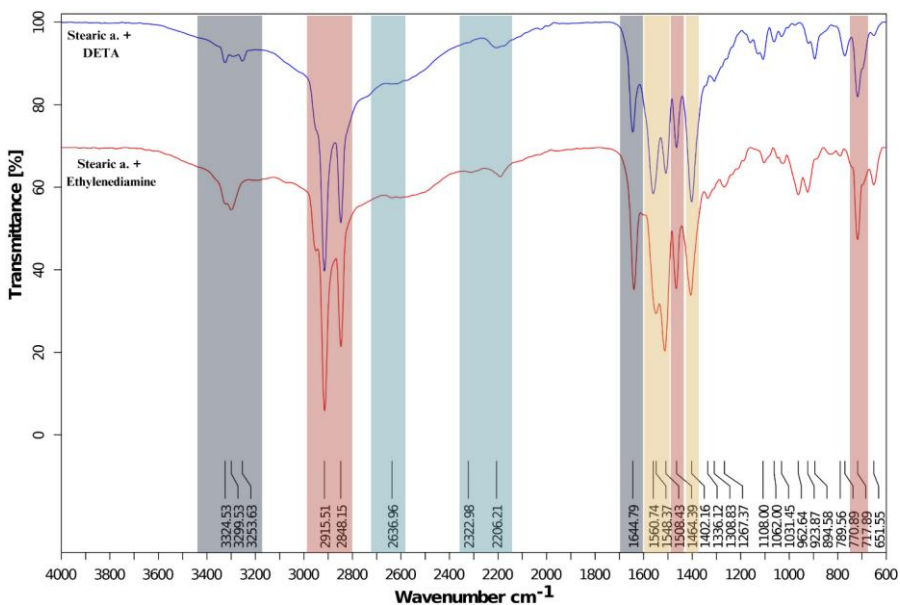
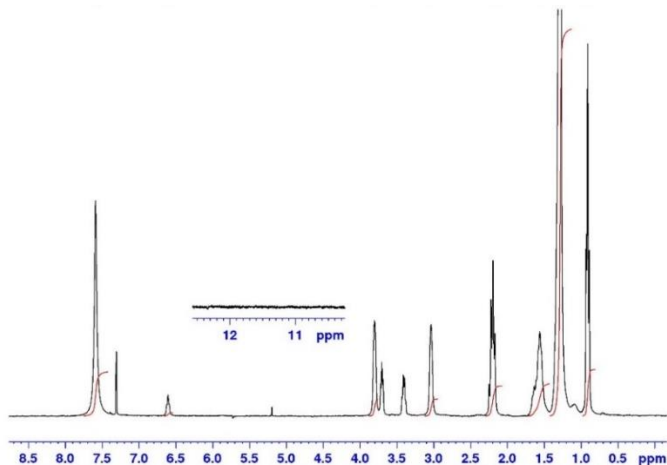
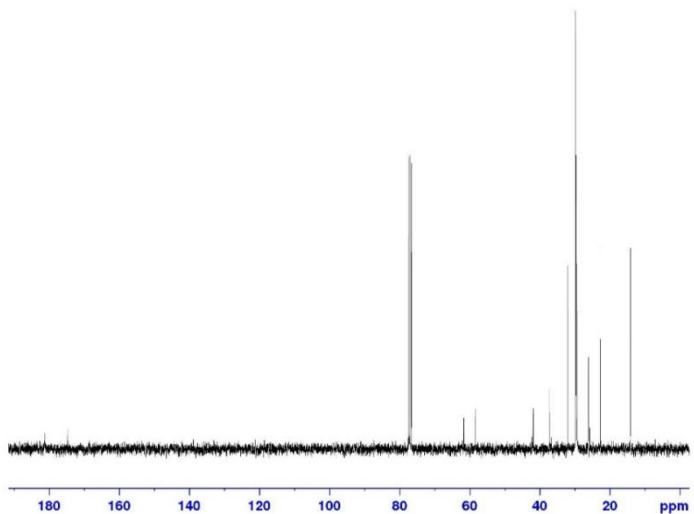


Figure 2. Graphical representation of the IQ spectra of reagents E-4 and E-5

of the reaction products were recorded on a LUMOS IR-Fourier microscope in the wavelength range of $600\text{-}4000\text{ cm}^{-1}$, and on a 300 MHz spectrometer manufactured by "BRUKER" (AFR) at room temperature (Figures 3-4).



^1H NMR spectrum of the complex obtained from stearic acid with MEA



^{13}C NMR spectrum of the complex obtained from stearic acid with MEA

Study of a complex based on triethanolamine and stearic acid as a surfactant.

In this study, the effectiveness of a reagent obtained from the reaction of triethanolamine (TEA) and stearic acid as a surfactant (SAM) was evaluated. The reagent used was E-3, which is obtained from the reaction of triethanolamine with stearic acid.

The results of the study show that E-3 reagent can be used as an effective surfactant in various environmental and industrial conditions. The high oil recovery efficiency achieved with a distilled water sample and an oil sample taken from the “Oil Rocks” field makes the use of this product more appropriate for the cleaning of oil spills in marine environments. On the other hand, the effectiveness of the product remains quite high even in environments with high salinity levels, which makes it promising for widespread use in various industrial sectors, especially in complex processes such as offshore oil extraction and oil spill management.

Verification of synthesized reagents in the solution of the salt precipitation process .

In our previous studies, we determined that the salinization process on the shores of the Caspian Sea is very high. For this reason, among the substances we synthesized, we initially investigated the elimination of this problem using the E-3 reagent, which we considered more suitable due to its physicochemical properties. The direct effect of triethanolamine stearate and its esters on the salinization process can be explained by three main mechanisms:

1. Weakening of the crystallization process: Triethanolamine stearate and its complex compounds weaken the interaction between ions, delaying the precipitation process of salt ions in the form of crystal structures. This prevents the formation of precipitates by allowing the salts to remain in a metastable state for a longer period of time.

2. Acceleration of the dissolution process of ions: The reagent interacts with water molecules, ensuring the stability of dissolved ions in a suitable environment. This has led to an increase in the solubility of salts and a decrease in the likelihood of precipitation.

3. Prevention of the formation of precipitation centers: The salt precipitation process initially begins with the formation of precipitation points. E-3 reagent slows down the formation of these points, thereby reducing the rate of precipitation formation.

These mechanisms are of particular importance in the salt precipitation process, as research has shown that even in systems that produce minimal levels of sediment, the application of such substances can dramatically reduce the amount of sediment.

The results of the study show that different amounts of E-3 reagent can significantly reduce the salt precipitation process. Experiments conducted with water samples collected from different regions have determined the precipitation prevention potential of E-3 and the dependence of this potential on the composition of the solution (Table 2).

Table 2.
The effect of solutions of substance E-3 on the salt precipitation process according to water bodies

Experimental area	Example	Salt precipitation coefficient	Impact rate
Neftchala	Inhibitor-free	0.000013	
Neftchala	E3 IPS 50:50	0.0000011	92%
Neftchala	E3 IPS	0.0000009	93%
Wise	Inhibitor-free	0.000014	
Wise	E3 IPS 50:50	0.0000013	91%
Wise	E3 IPS	0.0000017	88%
Sumgayit	Inhibitor-free	0.000012	
Sumgayit	E3 IPS 50:50	0.00000035	97%
Sumgayit	E3 IPS	0.000001	92%
Pirallahi	Inhibitor-free	0.000016	
Pirallahi	E3 IPS 50:50	0.0000055	66%
Pirallahi	E3 IPS	0.0000032	80%

In the water sample taken from the Bilgah coastal area, compared to the alkaline solution, the E3 IPS 50:50 mixture reduced the salt precipitation process with a 91% effectiveness rate (coefficient 0.0000013), and the pure E3 IPS reduced the salt precipitation process

with a 88% effectiveness rate (coefficient 0.0000017). This shows that although both the 50:50 mixture and pure IPS provided high effectiveness in the Bilgah sample, the 50:50 mixture showed a better result.

The highest effects were observed in the water sample taken from the Sumgayit coastal region. While the alkali solution had a salinity coefficient of 0.000012, the E3 IPS 50:50 solution reduced this indicator to 0.00000035, providing a 97% effect. The pure E3 IPS solution also demonstrated high effectiveness with a 92% effect (coefficient of 0.000001). This indicates that the E-3 substance has the highest potential in preventing the sedimentation process of the water sample taken from the Sumgayit coastal region.

In the water sample taken from the Pirallahi coastal region, lower impact effects were observed compared to other regions. While the salinity coefficient in the alkaline solution was 0.000016 , the E3 IPS 50:50 solution reduced this indicator to 0.0000055, providing a 66% impact effect. The pure E3 IPS solution showed a better result with an 80% impact effect (coefficient of 0.0000032). These indicators confirm that the Pirallahi sample differs from other samples due to its high salinity and ionic composition.

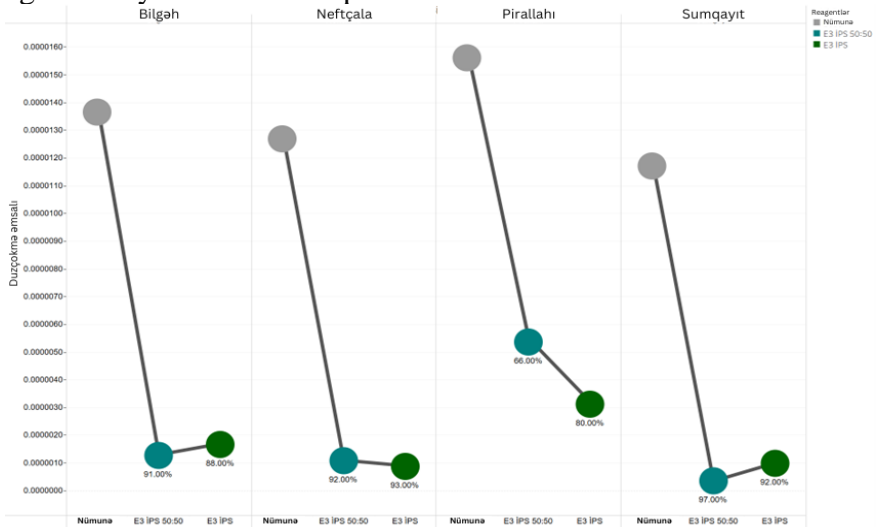


Figure 5. Efficacy of inhibitors in preventing salt precipitation by region.

As can be seen from the results, E-3 reagent was able to significantly reduce the formation of sediment in all samples. Among the two main structures, a 50:50 mixture of IPS and water showed higher efficiency in some samples (Sumgayit and Bilgah), but pure IPS achieved high results in Neftchala and Pirallahi samples. This indicates the wide application potential of E-3 reagent and its efficiency in various environmental conditions. Thus, this substance is an effective method for managing salt precipitation problems and has broad prospects for use in industrial applications.

Investigation of the bactericidal effect of synthesized reagents on sulfate-reducing bacteria.

The bactericidal properties of the inhibitor were determined using FOCT 18963-80. The test used the SRB strain "Desulfovibrio desulfuricans" isolated from a water sample taken from the Pirallahi coast of the Caspian Sea. The nutrient medium for the development of bacteria is Postgate B medium.

The number of bacteria in the inhibitor-free medium is $n_b \approx 10^3$. From this we can conclude that thousands of bacterial cells (10^3) developed in the reagent-free medium. In the reagent-containing medium, the number of bacteria in the samples taken at concentrations of 50, 100 and 200 mg/l changed as follows: Sample I reduced the number of bacteria from 10^3 to 10^2 at a concentration of 50 mg/l, while the other samples reduced the number of bacteria from 10^3 to 10^1 at the same concentration, except for sample VI at a concentration of 100 mg/l, all other samples reduced the number of bacteria from 10^3 to 10^1 , and at a concentration of 200 mg/l, all samples reduced the number of bacteria from 10^3 to 0, thereby completely stopping the development of bacterial cells.

As can be seen from Table 3, the bactericidal effect of the samples at a concentration of 50 mg/l varies between 90-98.6%, and at a concentration of 100 mg/l - between 95.8-99.4%. All samples showed 100% bactericidal effect at a concentration of 200 mg/l, and sample VI showed 100% bactericidal effect at all concentrations, completely stopping the life activity of sulfate-reducing bacteria.

Table 3.
Results from the analysis of the bactericidal properties of 20% solutions of aminostearates

Complexes conventional name and composition	Density of the substance, C- mg/l	Bacterial count (cell count/ml)	H₂S quantity mg/l	Bactericidal effect, Z-%
I E-1 (20% in ethanol)	50	10 ²	86.4	77
	100	10 ¹	23	94
	200	-	-	100
II E-1 (20% in water-ethanol (50:50))	50	10 ¹	42	89
	100	10 ¹	20.4	94.5
	200	-	-	100
III E-1 (20% in IPS)	50	10 ¹	40.1	89.3
	100	10 ¹	19	95
	200	-	-	100
IV E-1 (water-IPS (50:50)20%)	50	10 ¹	37.5	90
	100	10 ¹	15.7	95.8
	200	-	-	100
V E-2 (20% in IPS)	50	10 ¹	31	92
	100	10 ¹	14.8	98.3
	200	-	-	100
VI E-3 (20% in IPS)	50	-	-	100
	100	-	-	100
	200	-	-	100
VII E-3 (water-IPS (50:50) 20%)	50	10 ¹	10.6	97.1
	100	10 ¹	4.4	98.8
	200	-	-	100
VIII E-3 (water-IPS (70:30) 20%)	50	10 ¹	7.4	98
	100	10 ¹	4.1	99
	200	-	-	100
IX E-3 (20% in ethanol)	50	10 ¹	7.5	98
	100	10 ¹	3.6	99.04
	200	-	-	100
X E-3 (20% in water-ethanol (50:50).	50	10 ¹	5	98.6
	100	10 ¹	2.2	99.4
	200	-	-	100
Control-I H₂S content in SRB-free environment 24 mg/l				
Control -II H₂S content in SRB medium 256 mg/l				
Control - III - Analysis done water bacteria in the sample number 10³ cell count / ml				

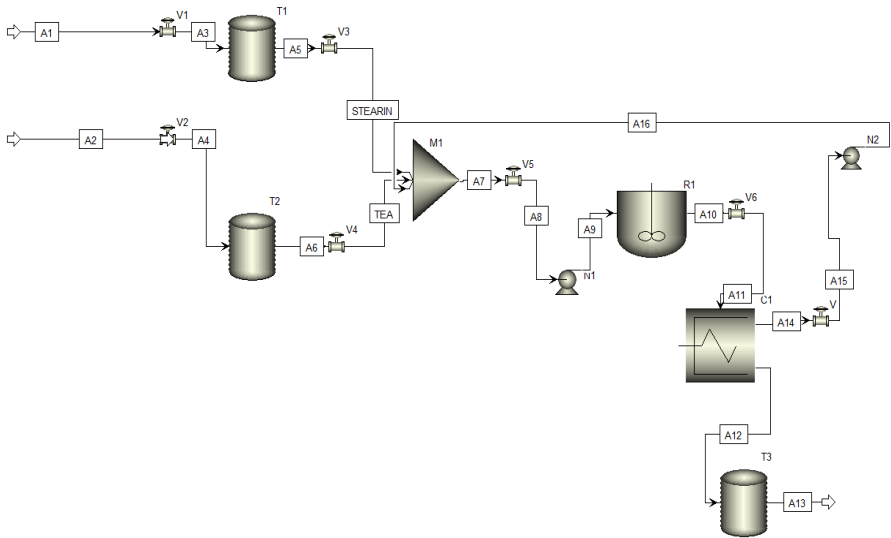
Thus, synthesis of salts made high bactericide characteristic their in the composition of active groups of who is it reaction participation in mechanisms to do with an explanation is being done. That is, active groups bacteria to the cell wall and cytoplasmic membrane impact to do membrane by disrupting its functions metabolism processes to brake reason Carboxyl and amen groups, interactions at the cell surface creating bacteria structure destruction does this if they are life of the activity It results in a stoppage.

The main technological scheme of the E-3 complex production process.

Since our synthesis product, the E-3 complex, is not included in the basic software package, the reagents are included in the UNIFAC system.

After the reagents were entered into the UNIFAC, MUNIFAC (Dortmund) and NIST systems, the JSON format of their molecular structure was prepared. With the newly added molecular structure, stearic acid, triethanolamine and water used in another process were added to the system. Suitable systems for the simulation system were formed and introduced into the program. The simulation process is given in Scheme 1. During the process, along with the main product By-products that can be obtained as a result of the reaction were added to the system.

The new reagent was added to the program, the process and equipment were added to the Aspen Plus program according to the technological scheme. During the process, tankers with a volume of 1000 l were selected as the raw material capacity. The flow containing stearin and TEA was determined to be at a temperature of 25 °C. The ratio and initial temperature of the substances fed to the reactor, the residence time in the reactor and the temperature in the reactor were optimized using artificial intelligence and mathematical models. At the end of the process, a triethanolamine stearate complex with a purity of 99.8%, E-3 reagent, was obtained. This also indicates that the proposed technological scheme can be successful in industrial application.



Scheme. 1. Simulation of the technological scheme with the Aspen Plus program.

In order to carry out the optimization process in a comprehensive manner, it is necessary to select the right test points. The Latin Hypercube Sampling LHS statistical method was used to collect the correct sample data. The main reason for choosing this method is that it can comprehensively consider all possible combinations without repeating the method of traditional factorial selection and random sampling. The main parameter ranges during sample collection were selected based on the reactor temperature and the residence time of the raw material in the reactor. The residence time of the raw material in the reactor was between 3 and 6 hours, and the reactor temperature range was between 60-90 °C. After the sample collection was collected, the “Decision Tree Regression” model, which has high accuracy, was selected. This model, compared to traditional regression models, divides the data into parts and builds a stepwise regression model, which allows studying the effect of all parameters separately.

Figure 6 illustrates the surface analysis and decision-making process based on our model.

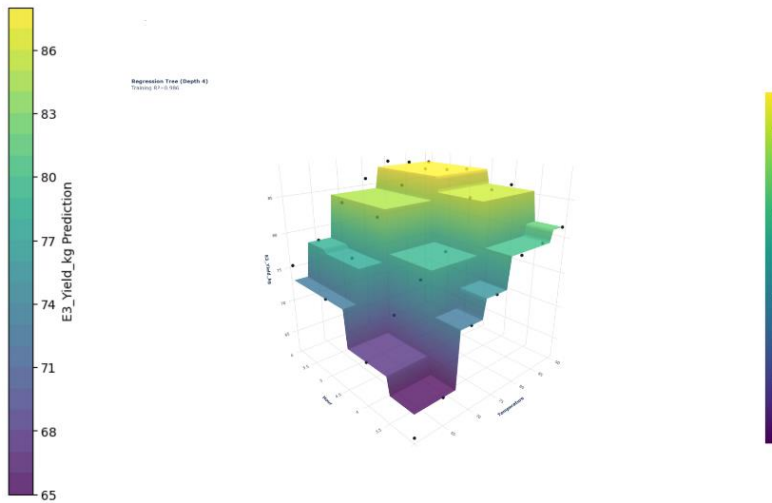
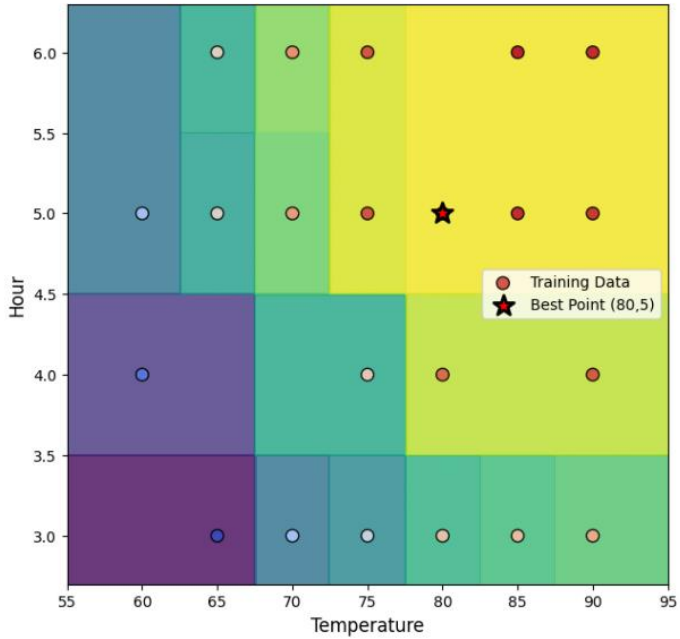


Figure 6. 2D and 3D surface analysis of the “Decision Tree Regression” artificial intelligence model for the reactor.

The process was re-simulated with optimal input parameters based on the proposed technological scheme . During the process, the raw material is transferred from the tank to the mixer and from there to the reactor. The reaction products from the reactor are fed to the precipitator. In the precipitator, a triethanolamine complex with a purity of 99.8% is obtained and the target product yield of the reactor is calculated to be 88% based on stearic acid.

The step-by-step material balance of the triethanolamine stearate complex production process is as follows:

I. Neutralization

Enters :	Weight , kg	%
1) Stearin acid	655.9	65.5
2) TEA	344.1	34.5
<hr/>		
Plural :	1000	100.0
Purchased :		
– Complex + unreacted raw material	1000	100.0
<hr/>		
Plural :	1000	100.0

II. Precipitator

Enters :		
– Complex + unreacted raw material	1000	100.0
<hr/>		
Plural :	1000	100.0
Purchased:		
1) Unreacted stearin acid	78.6	4.2
2) Unreacted TEA	41.3	2.2
3) complex	880.1	93.6
<hr/>		
Plural	1000	100.0

The yield of the target product was 88% based on the extracted stearic acid, and the purity of the final raw material was 99.8% based on the target product.

Modeling corrosion problems in seawater with artificial intelligence and computer algorithms

Problems arising from metal corrosion in industrial areas can lead to equipment failure, reduced structural strength, and life-threatening risks. Therefore, timely detection and elimination of such problems is a very responsible and important task.

Automation of monitoring processes will not only help prevent human errors, but will also be able to detect corrosion processes as soon as they begin to occur, by integrating with IoT (Internet of Things) devices in areas where humans cannot access. For this reason, we have developed a modeling process based on the data set obtained by new computer vision and classification models to further improve the existing system.

Preparing image samples for vision detection models.

A cross-approach structure (K-folds) was created to regulate the learning of the model. This method prevents the memorization of models, as well as prevents errors that may occur during the verification cycles of the models. During the cross-approach, the shortcomings that may arise due to the small number of image samples are also indirectly eliminated. The cross-approach method is a traditional learning method, is significantly different from the validation partition. In the traditional method, image samples were randomly divided into validation and training parts. The model learns to identify with the training data and then makes predictions based on these criteria on the validation sample.

In order to create conditions for a comprehensive study of the process, the latest updated and modern model architectures were used. Thus, the linear levels of previously studied results were eliminated and, in general, deeper learning was achieved. SqueezeNet, GoogLeNet, ResNet-18, ResNet-101, Wide ResNet-50, Wide ResNet-101 model architectures were used at the modeling stage. The number of parameters in these models is 1,266,344, 6,656,160, 11,000,000, 44,609,088, 69,943,168, 126,946,624, respectively. It should be noted that the parameters are the number of filters used in the study of the

model, the values of the variables k and b . The “Python” programming language and deep learning libraries such as “FastAI”, “Pytorch” were used for modeling. Before entering the models, each image was scaled to 512*512 pixels, which is necessary for learning the model filters. The learning speeds of the models differ significantly depending on the architecture size. The learning speeds of the models were 8, 9, 8.25, 51, 61, 111 minutes, in order of name. The graph of the dependence of the number of parameters of these models on the estimation result of the image set is given in Figure 7.

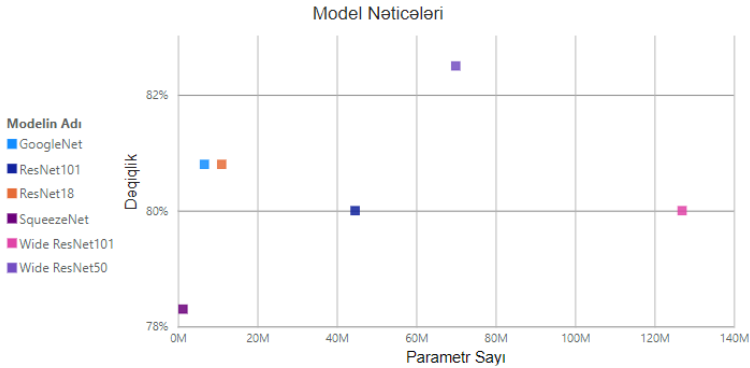


Figure 7. Results of the models used.

The Wide ResNet-50 model performed the highest without changing the structure of the images in the format used, with an accuracy of 82.5%. The GoogleNet and Resnet 18 models, despite having a small number of parameters, showed an accuracy of 80.5%, the Wide ResNet-101 and Resnet-101 models showed an accuracy of 80%, and the SqueezeNet model showed an accuracy of 78.3%.

Modeling on a satellite image collection.

Among the image localization algorithms, nano, small, medium and giant models of the Yolo v8 model were developed. The results obtained were recorded and the most optimal model architecture was investigated in terms of both learning detection speed and accuracy criteria.

F1, accuracy, completeness, object error, and classification error

were used as the main validation criteria.

$$F1 = (\text{precision} \cdot \text{recall}) / (\text{precision} + \text{recall})$$

The highest performance among all models was observed in the large-sized Yolo v8 model. The results are shown in Figure 8.

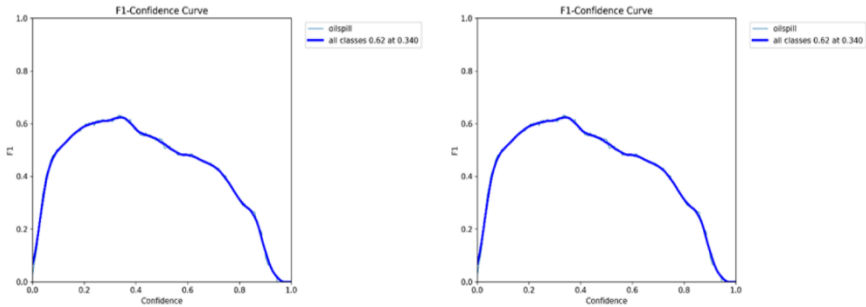


Figure 8. F1 and precision-completeness curves of the large-scale YOLOv8 model.

Development of oil recovery properties of surfactants using visual models.

Surfactants have oil-collecting and dispersing abilities in the oil sector. These abilities of new substances synthesized in our laboratory were investigated. During the research, petri dishes with an outer diameter of 9 cm and an inner diameter of 8.8 cm were used.

As a result of the model, we obtained a segment of the oil-containing parts for each petri dish, the pixel coordinates of which were stored in a separate matrix. The oil-containing zones and the total petri dish part were separated from the segmented images.

This calculation was performed individually, as it depends on the camera we use, the angle and distance from which the images were taken. As a result of the calculation, it was found out how many cm of information 1 pixel represents. Thus, it was determined by the conversion functions how many cm² each oil image segment is. The calculation process is shown in Figure 9 below.

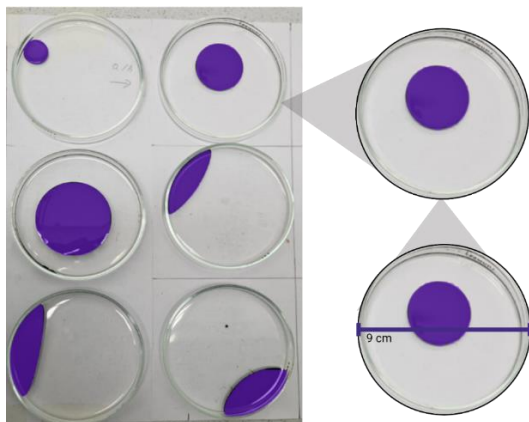


Figure 9. Segmentation of oil-bearing zones and pixel counting based on petri dish diameters.

During the segmentation modeling, we used three main indicators: accuracy, completeness, and average numerical accuracy. These parameters are the criteria that control both the correct selection of oil-bearing sections and the selection of all oil-bearing zones. The results of the segmentation model verification criteria are as follows:

- Accuracy: 98.6%
- Completeness: 100%
- mAP (Mean Numerical Accuracy Limits 0.50:0.95): 99.5%

High precision and recall indicate that the model exhibits high accuracy in accurately identifying oil fields.

Calculating inhibitory effectiveness with spoken language models

In this work, we have developed two new segmentation algorithms to improve the predictive performance of machine learning models on chemical databases. We have modified and tested the algorithms, which we call “Bag of SMILES” and “ChemGrams”. “Bag of SMILES” is a segmentation method based on understanding the atomic and bond structure of molecules represented in the “SMILES” format and explaining the meaning of each symbol. This method segments individual “SMILES” names into atomic and symbol-level tokens, which allows us to combine both token counts and their positional information. Additionally, we can use the information obtained to evaluate the atoms and symbols in the molecule based on

their location and repetition frequencies. Therefore, new parameters have been added to the “Bag of SMILES” algorithm to take these approaches into account.

Calculating the effects of ligands on bacteria using molecular docking calculations.

The interaction of the E-3 ligand with the protein of the anaerobic type of sulfate-reducing bacteria "Desulfovibrio desulfuricans" was calculated using the "docking" program. As a result of the study, the most suitable docking positions and their energies were calculated.

In the next stage, the key amino acids at the ligand binding site to the protein were identified using the PyMOL program.

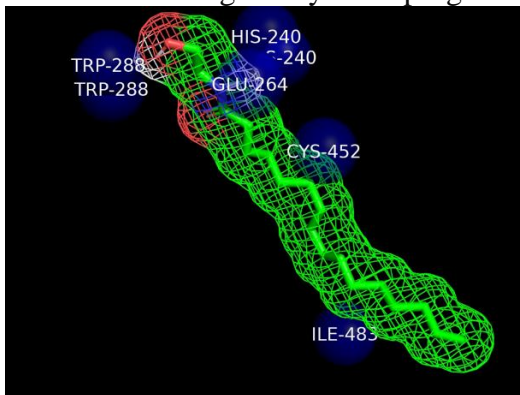


Figure 10. Close-up of the ligand binding to the amino acids of the bacterium.

Based on the results, it was determined that the ligand is compatible with the protein of the bacterium “Desulfovibrio desulfuricans”. The tight binding affinity in Model 1 indicates the possibility of using this ligand as an inhibitor (blocker) to exert antibacterial effects.

Molecular docking analyses were performed to elucidate the interactions of the synthesized E-1 reagent with bacterial proteins and to elucidate the mechanism of its antibacterial action at the molecular level. The binding affinity of three major bacterial proteins was determined using the AutoDock Vina program: “3bgc” for “Coliform”, “1vly” for “E.coli” and “1fu0” for Entrecoccyx. These

docking studies provided important information to explain how E-1 attenuates and destroys bacterial life. Figure 11 shows the optimal binding regions of the molecule to bacteria.

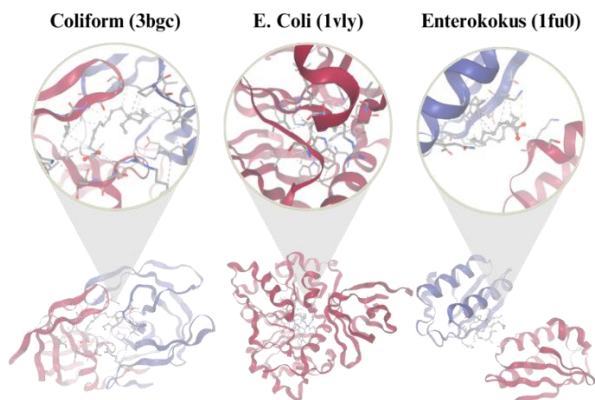


Figure 11. Best-fit approximations of E-1 to Coliform, E.Coli, and Enterococcus bacteria.

Docking assays showed that E-1 reagent showed high specificity and strong binding to protein structures of various bacteria. The high degree of binding observed for coliform bacteria ensured their complete destruction. Slightly weaker binding was observed for E.coli, but still resulted in complete bactericidal activity. However, binding was slightly weaker for enterococci, resulting in only partial destruction of these bacteria.

These docking results are directly related to experimental results and explain the specific interactions of the E-1 reagent with different bacterial species. Molecular docking confirms how E-1 acts on different bacteria and its high antibacterial potential.

RESULTS

1. Complexes of stearic acid with amines and ethanolamines (EDA, DETA, MEA, DEA, TEA) were synthesized, their physicochemical properties were studied, and their structures were studied using modern computer programs [13, 17].

2. Water samples were taken from the Sumgayit, Bilgah, Pirallahi and Neftchala coastal basins of the Caspian Sea, and their physicochemical properties, salt and microbiological compositions were studied [3, 7, 9, 15].

3. 20% solutions of the synthesized complexes in water-ethanol, water-isopropyl alcohol mixtures were prepared, and their effects on salt precipitation and corrosion were investigated. It was found that when a 20% solution of the complex formed by stearic acid and TEA in a mixture of IPS: water 50:50% was used, it provided protection against salt precipitation in water samples taken from 4 areas (97% in Pirallahi water) [6, 11].

4. The effect of the prepared samples (E-1, E-2, E-3, E-5) on pathogenic microbes was studied. It was found that the prepared solutions, especially E-1, have a high antimicrobial effect. E-1 reagent destroys 100% of "Coliform" and "E. Coli" bacteria [5, 10].

5. The effect of the prepared complex products on the development of SRB was studied. It was found that when all the solutions were added to the medium in an amount of 200 mg/l, the vital activity of SRB completely stopped (100%), there was no SRB in the medium. At the same time, there was no H₂S in the medium (it decreased from 256 mg/l to 0) [12, 14].

6. The possibilities of modeling corrosion problems in seawater using artificial intelligence and computer algorithms have been explored [1, 2, 4, 8, 16].

7. A technological scheme for obtaining E-3 reagent was developed and prepared, the parameters of this scheme were optimized using mathematical models and artificial intelligence models, and simulated using computer programs [17].

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The defense will be held on «30» June 2025 at 10⁰⁰ at the meeting of the Dissertation council ED 1.17 of Supreme Attestation Commission under the President of the Republic of Azerbaijan operating at the Institute of Petrochemical Processes of Azerbaijan Republic MSE

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Abstract was sent to required addresses on: «26» May 2025.

Signed for print: 23.05.2025

Paper format: A5

Volume: 38543

Number of hard copies: 20 copies