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ИНОСТРАННЫЙ ЯЗЫК В ПРОФЕССИОНАЛЬНОЙ КОММУНИКАЦИИ – 16

Материалы
XVI Всероссийской научно-практической конференции студентов, магистрантов, аспирантов
(г. Уфа, 13-25 апреля 2026 г.)

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«Уфимский университет науки и технологий»

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В сборнике представлены материалы 16 Всероссийской научно-практической конференции студентов, магистрантов и аспирантов. Одной из основных задач конференции молодых ученых, помимо обмена информацией, является эффективное использование иностранных языков – английского, немецкого и французского – для осуществления профессиональной и научной коммуникации. В тезисах докладов обсуждается самый широкий круг проблем естественных, технических и гуманитарных наук.

Предназначено для молодых ученых, аспирантов, магистрантов и студентов, заинтересованных в совершенствовании навыков осуществления иноязычной профессионально-научной коммуникации.

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Секция 1

НАУЧНО-ТЕОРЕТИЧЕСКИЕ И ПРИКЛАДНЫЕ ПРОБЛЕМЫ ИССЛЕДОВАНИЙ (на материале кандидатских и магистерских диссертаций, выпускных квалификационных и научных работ студентов)

ГУМАНИТАРНЫЕ НАУКИ (КУЛЬТУРОЛОГИЯ, ПЕДАГОГИКА, ФИЛОЛОГИЯ)

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Self-translation in academic writing: bridging the gap

The 21st century's era is a definition of globalization. Nowadays, it is essential to communicate between cultures with clarity, credibility, and appropriate caution. This "effective communication" trend covers all aspects of our life and has become a cornerstone of academic writing. Research has consistently shown that academic writing traditions vary significantly across linguistic and cultural contexts. Among the stylistic conventions that shape scientific discourse, one of them is hedging. Along with others, it has been recognized as a central rhetorical strategy, particularly in the English-language academic tradition [2]. In particular, Russian academic discourse has historically been characterized by a more direct, categorical, and judgement-heavy style of presentation, which may conflict with the English-language preference for mitigation and non-categoricity [5]. While considerable attention has been paid to the differences in hedging practices between native and non-native writers of English, one specific area remains largely underexplored: self-translation. This unique kind of translation raises a set of intriguing questions. When a Russian-speaking researcher translates their own article into English, do they consciously adapt their hedging

strategies to meet the English-language stylistic expectations? Or do they retain the more categorical patterns of their native Russian discourse? Furthermore, what linguistic devices do they employ to "bridge the gap" between the two traditions, and how successful are these attempts?

The concept of hedging is primarily attributed to G. Lakoff, who introduced the term in 1973 to describe linguistic categories whose function is to express ideas in a non-categorical, tentative, and cautious tone. Lakoff's initial formulation focused on lexical items that blur the boundaries of propositional certainty, such as *"sort of"*, *"kind of"*, *"rather"*, and *"more or less"* [3]. However, as noted in Avkhacheva's (et al.) article "Hedging in Scientific Discourse: Comparative Analysis of English and Russian Traditions in Academic Writing", similar ideas emerged independently in Russian linguistics around the same period. Scholars such as G.A. Zolotova, A.N. Vasilieva, and N.M. Razinkina emphasized the importance of reducing the "subjective element" (as well as personal pronouns in order to reduce the author's presence) in scientific texts by limiting the scope of the author's judgements [1]. They also stressed the need to signal that certain statements convey only the speaker's or writer's opinion.

As for self-translation, this phenomenon was described by many researches, however the most common characteristic and the main feature of self-translation is that self-translators possess the "most intimate information" about the text's original intentions and the target audience's expectations. Therefore, they are free to choose a strategy to "reconstruct" the text by making more informed decisions about what to preserve, what to modify, and what to transform when moving a text across linguistic and cultural boundaries. In case of academic writing, self‑translation typically occurs when a scholar who is proficient in two (or more) languages prepares another version of a research article originally written in one of the languages. In this scenario, when translating their own work into English, the authors must therefore not only transfer propositional content but also re‑evaluate and, where necessary, restructure their own habitual ways of presenting knowledge. Such writers tend to add and omit different

pieces of information, depending on their vision of the relevance of said information.

In order to observe such shifts, we conducted a comparative analysis of an article in the field of biomedical engineering published in the Russian Journal of Biomechanics [4]. Created by a group of researches, with Yuri Nyashin included who is famous for self-translating his own works, the article represents a picturesque example for research. The analysis results are following:

1. Personalization. The English version adds personalizes sentences with an abstract subject "*one*" (as an "actor"): "*...one can conclude...*", "*...one can assume...*", while the Russian version is completely depersonalized: «*можно заключить*», «*можно предположить*»;

2. Omissions. Even though the texts' contents are basically the same, the English version lacks a paragraph on topic of relevance (in the conclusion section) and a sentence explaining the importance of mathematical modeling and analysis (the article's body last paragraph).

This comparative analysis of a Russian-English self-translated article on biomedical engineering reveals three key findings. Firstly, the English version contains significantly more hedging devices than the Russian one, indicating an effort to align with English traditional conventions. Secondly, the self-translator preserved first-person pronouns («мы» / "we") and some categorical claims, suggesting that native rhetorical habits persist. Thirdly, metacommentary passages present in the Russian text were omitted in the English version, pointing to strategic adaptation for a different readership. Thus, self-translation in academic discourse represents a partial rather than complete rhetorical reorientation. Future research should expand the corpus to determine whether these patterns hold across disciplines.

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Автоперевод в академическом письме: национально-культурные традиции

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ЕСТЕСТВЕННЫЕ НАУКИ

УДК 57

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Analyse des polymorphen Lokus rs1805010 des IL4RA-Gens bei der Bildung von Eierstockkrebs

Eierstockkrebs belegt in Russland den achten Platz unter allen Krebserkrankungen bei Frauen [2]. Diese Pathologie macht 3% der Gesamtzahl der krebskranken Frauen weltweit aus [7]. Die Fünf-Jahres-Überlebensrate von Patienten mit Eierstockkrebs beträgt 46,5%. Bei 1 von 70 Frauen wird im Laufe ihres Lebens Eierstockkrebs diagnostiziert. 45% der Fälle von RYA und 65% der Todesfälle durch

diese Krankheit sind bei Frauen über 65 Jahre alt [5]. Das von Tumorzellen produzierte IL4Ra fördert durch die Kontrolle von Makrophagen die Immuntherapieresistenz bei Eierstockkrebs [6].

Das Auftreten von Eierstockkrebs ist auf das Fehlen verschiedener wirksamer Früherkennungsmethoden, negative Statistiken auf der ganzen Welt und erhöhte Sterblichkeitsraten in der weiblichen Bevölkerung zurückzuführen. Am häufigsten wird die Krankheit in den Entwicklungsstadien III bis IV gefunden. Eierstockkrebs ist ein aktuelles Problem auf dem Gebiet der Onkoginäkologie [4].

Das epidemiologische Muster von Eierstockkrebs ist in verschiedenen Ländern unterschiedlich, was auf Unterschiede in den Risikofaktoren zurückzuführen ist, die durch die sozioökonomischen und geografischen Bedingungen bestimmt werden [1].

Die folgenden Histotypen gehören zu bösartigen Tumoren des Eierstockepithels: seröses Karzinom, Endometrioidkarzinom, mucinöses Karzinom sowie hellzelliges Karzinom [3].

Zweck der Studie: Analyse der Assoziation des polymorphen Locus ra1805010 im IL4Ra-Gen mit dem Risiko, bei Frauen aus der Republik Baschkortostan an RA zu erkranken.

Das Material für die Studie war DNA-Proben von Patienten mit Eierstockkrebs (n = 367) und bedingt gesunden Frauen (n = 289). Die Genotypisierung wurde mit Hilfe einer PDRF-Analyse durchgeführt.

Ergebnisse. Die Häufigkeit von Gasse A des polymorphen Ortes rs1805010 des IL4Ra-Gens bei Frauen mit Eierstockkrebs wurde gefunden, die Häufigkeit von Gasse A beträgt 40% und die Häufigkeit von Gasse G beträgt 60%. Der AA-Genotyp wurde mit einer Frequenz von 16%, AG – 48%, GG – 36% getroffen. In der Kontrollgruppe betrug die Häufigkeit des Allels A 41% und des Allels G 59%. Der AA-Genotyp wurde mit einer Häufigkeit von 14%, AG – 53% und GG – 33% gefunden. Bei der Analyse der Frequenzverteilung von Allelen und Genotypen des IL4Ra-Gens rs1805010 in der Gesamtprobe, bei der Trennung nach ethnischer Zugehörigkeit und klinischen Parametern wie dem menopausalen Status, wurde der

Differenzierungsgrad der Tumorzellen zwischen den untersuchten Gruppen nicht unterschieden (p>0,05). Wir haben jedoch festgestellt, dass das A-Allel dieser polymorphen Variante bei Patienten ohne Metastasen im Vergleich zu Patienten mit Metastasen signifikant häufiger auftrat, OR = CI (1,63 (1,03-2,57)); p = 0,04.

Folgerungen. Die von uns erhaltenen Daten deuten auf eine bestimmte Registerkarte des polymorphen Ortes rs1805010 des IL4Ra-Gens bei der Bildung von Ovarialtumormetastasen hin.

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Анализ полиморфного локуса rs1805010 гена IL4RA в формировании рака яичников

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Modern hydrological monitoring problems

Nowadays there are plenty of models, systems and methods in hydrology to estimate different characteristics for various needs. However, scientists are facing a problem that prevents use these methods to the fullest and extract maximal efficiency. This problem is caused by the lack and/or unreliability of the data obtained by the existing monitoring systems.

The problems of hydrological monitoring can be categorized in the following way:

1) Observation web: reduction of hydrological web; absence of some hydrological parameters monitoring; unsatisfactory high-altitude station base; poor web unit control; sparse observation net.

2) Methods: outdated measuring instruments; measuring bias.

3) Data processing: regime data mismatch; difference in sensors and equipment; lack of operative communication.

4) Funding: high cost; gap in the development of technological and personnel units; difficulty of updating and servicing of technologies.

The following steps can be offered to solve a number of problems:

1) Establishment of pattern for viable coordination between hydrological monitoring units and authorities;

2) Explicit separation of duties;

3) Providing the employees with the newest equipment and their training in new effective methods.

In conclusion, continuous collection of hydrometeorological data

characteristics, their operative transfer, processing and analysis are key factors in hydrological statistics and predicting, especially of natural hazards. Solution of this problem must be primary for people safety.

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Проблемы современного гидрологического мониторинга

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Analysis of genetic variants rs6265 (BDNF) and rs6994992 (NRG1) in the development of individual spatial reasoning

Spatial abilities possess evolutionary and adaptive significance in human life, representing a complex set of cognitive skills associated with the perception and processing of information regarding space and the objects within it. Spatial reasoning is characterized as an effective predictor of academic success for individuals in

advanced scientific fields categorized as STEM (Science, Technology, Engineering, and Mathematics). The formation of spatial reasoning depends on the combined influence of heredity and the environment.

In this regard, we undertook a study of the psychological and genetic aspects of the development and functioning of an individual's spatial abilities.

The aim of this study is to analyze the genetic variants rs6265 of the *BDNF* gene and rs6994992 of the *NRG1* gene in the development of individual spatial reasoning under the influence of various environmental factors. Research Objectives: To analyze the corresponding polymorphic variants of the *BDNF* and *NRG1* genes in the development of an individual's spatial reasoning.

The study involved 422 healthy individuals. The study utilized the necessary psychometric methods, including questionnaires, as well as standard molecular genetic analysis and statistical data processing.

Initially, the study conducted an analysis of intellectual and spatial abilities using a previously compiled battery of psychodiagnostic methods and psychometric units, specifically focusing on data obtained from the Mental Rotation test. Preliminary statistical processing identified outliers based on Mahalanobis distance (>95%) in 22 subjects; accordingly, they were excluded from further analysis. Thus, the final sample consisted of 400 individuals, comprising 76 males and 324 females.

In the first stage of the study, an assessment was made regarding the correlation between test performance and factors such as age and gender. No statistically significant relationship was observed ($p > 0.05$).

Consequently, we decided to evaluate the contribution of the genetic factors *BDNF* and *NRG1* to the development of the respondents' spatial abilities.

The *BDNF* gene encodes a protein from the nerve growth factor family, playing a key role in neuronal survival, growth, differentiation, and synaptic plasticity. In the brain, it is active in the hippocampus, cortex, and forebrain–regions responsible for learning, memory, and spatial abilities. Since the presented polymorphic variant leads to an amino acid substitution of valine (Val) with

methionine (Met) at position 66 of the BDNF neurotrophic factor, we performed «in silico» functional modeling of this substitution.

Although the selected bioinformatic software modeled a moderately neutral but variable effect for the p.Val66Met substitution in the *BDNF* biomarker «in silico», experimental studies indicate that this substitution affects neurotrophin expression levels.

The study sought an association between the rs6265 *(BDNF)* polymorphic variant and the development of spatial reasoning in the analyzed cohort of 400 students after Mahalanobis distance correction. For the association analysis itself, gender, age, professional orientation, and the psychometric indicator (Mental Rotation test score) were selected as phenotypic correlates.

A statistically significant result was identified only when comparing groups of respondents categorized by their minimum and maximum scores on the "Mental Rotation" test ($\chi^2 = 4.67$, $p = 0.031$, $OR = 1.9$, $\beta = 0.67$, $p = 0.03$). A comparative analysis of the allele and genotype frequency distributions of the rs6265 (BDNF) polymorphic variant identified the contribution of the *A*G (29.76%) and *A*A (1.79%) genotypes, and the risk allele A * (16.67%), respectively, to the specific cognitive development patterns of individuals who achieved low scores on the test.

Neuregulin 1 (NRG1) is expressed in neurons and glial cells of the hippocampus and prefrontal cortex. The Neuregulin 1 protein, encoded by this gene, plays a vital role in the development and functioning of the nervous system. Neuregulin 1 is involved in myelination, synaptogenesis (synapse formation), neuronal migration, and cell survival. This specific genetic variant within the NRG1 gene may influence the expression or structure of the Neuregulin 1 protein and may be associated with general intelligence and working memory.

The experimental study and subsequent statistical processing of the significance of the rs6994992 (NRG1) polymorphic locus in the development of spatial abilities within our studied group of respondents did not yield significant results ($p > 0.05$). In our cohort, only a minor difference was observed in the allele

and genotype frequency distributions between groups categorized by their performance on the "Mental Rotation" test used in this study. This aspect may be attributed to the low prevalence of the minor allele T* among our subjects and suggests the need for an increased sample size in future research.

Conclusions

1. Association analysis of rs6265 in the ×BDNF× gene with the development of an individual's spatial intelligence revealed statistically significant differences in the studied group of respondents in correlation with "Mental Rotation" test scores ($\chi^2 = 4.67$, $p = 0.031$, $\beta = 0.67$, $p = 0.03$).

2. The search for an association between the rs6994992 (NRG1) polymorphic variant and the formation of an individual's spatial abilities did not reveal any statistically significant differences in the cohort under study.

Анализ генетических вариантов rs6265 (BDNF) и rs6994992 (NRG1) в развитии пространственного мышления индивида

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Pelargonium: medicinal properties and rooting methods

Pelargonium is a genus of flowering plants widely known by common names pelargoniums or sometimes geraniums. This genus unites about 280 species of perennial, succulent and shrubby plants. Initially, the taxonomist Carl Linnaeus

assigned all the species now known as Pelargonium and Geranium to the latter genus. However, in 1789, Charles Louis Héritier de Brutelle divided them into two separate genera [1].

As of 2017, there were approximately 10,000 varieties and hybrids of pelargonium in the world [2]. The initial classification of pelargonium singled out four main groups of varieties: zonal, ivy-leaved, royal and fragrant. However, the emergence of many varieties with unique characteristics of flowers and leaves required the development of a more extensive classification [3].

Pelargonium cultivation does not present significant difficulties if several basic rules are followed: for abundant flowering, it is extremely important to provide the plant with sufficient light and fresh air. Optimal temperature ranges from about +18 to +22°C in summer and from +10 to +15°C in winter [4],[5]. The soil should be light, well-drained and enriched with humus. Moderate watering is necessary in spring and summer, while in autumn and winter the frequency of watering should be reduced. For lush flowering, it is necessary to prune pelargonium twice a year with spring being the main one, held in late February – early March. It awakens dormant buds and causes lateral shoots to grow. Autumn pruning is done to prepare geraniums for the winter period and the subsequent flowering season. It is mainly carried out with royal geraniums – the rest of the varieties should be pruned only in spring [4]. Periodic application of mineral fertilizers helps to maintain color saturation and active growth. With proper care, pelargonium will delight with abundant flowering for many years, bringing comfort and benefit to the house.

Pelargonium is valued not only for its decorative appeal, but also for its pronounced medicinal properties. The leaves and stems of the plant are rich in essential oils, vitamins, tannins and flavonoids, which determine its beneficial effects: antiseptic property, anti-inflammatory effect, immunostimulating effect, soothing effect.

There are different ways of rooting pelargonium. Propagation of pelargonium by cuttings is an effective method that allows obtaining a significant number of

young plants in a short period of time. There are several ways of rooting, each of which has its own advantages and disadvantages. Classical soil rooting is a traditional and most affordable method suitable for most gardeners. A healthy shoot with a length of 8-12 cm and two or three nodes is selected. The lower leaves are removed, leaving only 2-3 upper leaves. A clean oblique cut is made with a clean tool directly under the node. It is recommended to dry the cut within half an hour. This helps prevent rotting. The stalk is planted in a light, breathable substrate (peat, sand, vermiculite), the soil around the base is carefully compacted. Greenhouse conditions are created by covering with a transparent bag or glass to maintain heat and humidity. The soil is regularly ventilated and moistened. The advantages of this method are the availability of materials, simplicity of execution, and a high probability of success. The disadvantage is the need for constant control of soil moisture, there is a risk of fungal diseases [4].

Water rooting is an alternative option convenient for those who prefer to visually observe the process of root formation. In the procedure a transparent glass or jar of water at room temperature is used. The lower end of the stalk is lowered into the water after removing excess greenery from below. The container is placed in a warm, well-lit place, away from direct sunlight. The water changes every 3-4 days, while the appearance of the first roots is monitored [4]. The advantages are the ease and clarity of the process, and the absence of the risk of drying out the substrate. But there may be difficulties with the development of weak roots, and subsequent transplanting into the ground is required.

Rooting in perlite or vermiculite is a modern method preferred by experienced gardeners. These materials provide excellent drainage and aeration, facilitating rapid rooting. The container is filled with sterile perlite or vermiculite. The prepared stalk is planted to a depth of 2-3 cm, the material around the base being slightly compacted. A greenhouse effect is created by covering it with a film or glass. Ventilation is carried out daily, the top layer of the substrate is moistened as it dries. The advantages are the high rate of root system formation, minimizing the risk of

infection. But it requires the use of specialized purchased materials, the cost of which is higher than that of conventional soil.

Agroperlite mixture is a more complex but highly effective method of rooting. A combination of agroperlite and coconut fiber or a mixture of agroperlite and vermiculite is used. The components are mixed in a 1:1 ratio, and a small amount of liquid fertilizer is added. The pot is filled with the resulting mixture, and a stalk is planted in it. Care is carried out in the same way as the previous option, with humidity and temperature control. The advantages of this method are rapid root growth and a high survival rate. However, it requires specific materials and knowledge of substrate processing technology [4].

The choice of rooting method depends on the individual preferences and the level of experience of the gardener. Beginners are advised to start with the classic soil method, while experienced hobbyists can experiment with options including perlite, vermiculite, or the water method. The key condition for success is the correct choice of the initial planting material and strict observance of rooting conditions.

In summary, it should be noted that pelargonium is a universal plant the healing and cosmetic properties of which have been known since ancient times. It helps to improve well-being, promote health and enhance attractiveness. Proper use of the beneficial properties of pelargonium allows you to fully enjoy the wealth bestowed by nature.

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Пеларгония: лечебные свойства и способы укоренения

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Wirkung von Salicylsäure auf Pflanzenenzyme

Salicylsäure (SS), auch bekannt als 2-Hydroxybenzoesäure, ist ein Phytohormon, dessen Biosynthese über den Phenylpropanoidweg oder den Isochorismatischweg erfolgt. SS-Moleküle befinden sich in Form von biologisch inaktiven Konjugaten mit Verbindungen wie Aminosäuren, Methylsalicylat, β-D-Glucoside, Glucosidestern usw. in der Pflanze, die bei Bedarf in eine freie aktive Form umgewandelt wurden. SS beeinflusst die Thermogenese von Pflanzen, die Keimung von Samen, Photosynthese, Transpiration ist ein Bestandteil von Signalsystemen, die für die Anpassung an die Wirkung von abiotischem Stress durch hohe und niedrige Temperaturen, Schwermetalle verantwortlich sind. Die Säure verbessert oft diese Prozesse, indem sie die entsprechenden Enzyme beeinflusst.

In diesem Zusammenhang der Zweck dieser Arbeit ist eine Überprüfung der wissenschaftlichen Literatur über die Auswirkungen der Verarbeitung von SS Pflanzen auf ihre enzymatischen Systeme.

Das durchgeführte Experiment hat in einigen wissenschaftlichen Arbeiten die

positiven Auswirkungen von SS auf die Synthese von antioxidativen Enzymen: Superoxiddismutase, Katalase und Guajakol-spezifische Peroxidase - bestätigt. Dieser Effekt kann vermutlich durch den Einfluss von SS auf die Erzeugung von Substraten dieser Enzyme (Wasserstoffperoxid und Superoxid-Ionen) und auf die Erhöhung der Expression der Gene, die für ihre Synthese verantwortlich sind, verursacht werden. So es gibt Hinweise, dass die SS die Aktivierung Superoxiddismutase, Katalase und Guajakol-spezifischer Peroxidase bei Kälte in Gurkenblättern (Cucumis sativus L.) bewirkt [4]. Die Behandlung von SS bei Gurkenpflanzen (Cucumis sativus L.) und Winterweizen (Triticum aestivum L.) bei niedrigen Temperaturen führte auch zu einer erhöhten Expression von eisenhaltigen manganhaltigen, Kupfer- / zinkabhängigen Superoxid-Dismutase und Katalase – Genen [1,4].

Es gibt jedoch Informationen, dass SS dagegen inhibitorisch auf die Katalase wirkt, da Katalase ein salicatbindendes Protein ist. Dies findet Bestätigung in der Arbeit von Belyh Yu. V., Kirillova N.V., Spassenkow A.I. [3] Niedrige SS-Konzentrationen führten zu einer Abnahme der Katalase-Aktivität (um 14 %) in der Gewebekultur Polyscias Polyscias filicifolia (Moore ex Fournter) Bailey. Die höheren Konzentrationen verursachten jedoch keine signifikanten Veränderungen des Aktivitätsniveaus des Enzyms. Daraus kann angenommen werden, dass dieser Effekt der Wirkung von SS auf die enzymatische Aktivität von Katalase eine dosisabhängige Wirkung hat.

Prolin ist auch an der Neutralisierung aktiver Sauerstoffformen (AFK) in Pflanzen unter Stressbedingungen beteiligt [2]. Es wurden neue Daten erhalten, dass Weizen– und Gurkenpflanzen bei niedrigen Temperaturen die Expression der Gene WP5CS und WP5CR verstärken, die für Prolinsyntheseenzyme kodieren - prolin-5-Carboxylat-Synthetase (P5X) und 1-Pyrolin-5-carboxylat-Reduktase (P5CR) [1].

So in der Arbeit von Abilova G.A. das Prolinniveau war bei Proben, die mit SS und $CdSO_4$ behandelt wurden, höher als bei Proben, die mit einem einzigen $CdSO_4$ behandelt wurden [2].

SS ist in der Lage, die Aktivierung nicht nur von Redoxenzymen, sondern auch von hydrolytischen Enzymen zu induzieren. So V.V. Chub schreibt, dass die Synthese von PR-Proteinen (pathogenesis related proteins), unter denen sich PR-2-Proteine als b-1,3-Glukanasen entpuppten und die PR-3-Protein als Chitinasen entpuppten, als Reaktion auf die Verarbeitung von Tabakpflanzen mit Salicylsäure begann [5].

Zusammenfassend betonen wir: die Salizylsäure ist für ihre breite Wirkung auf Enzyme interessant, die für das Pflanzenleben, ihre Gesundheit und ihren Ertrag, die Anpassung an ungünstige Bedingungen eine wichtige Rolle spielen: antioxidative Enzyme (Superoxiddismutase, Katalase und Guajakol-spezifische Peroxidase) und hydrolytische Enzyme (b-1,3-Glukanasen, Chitinasen), Enzyme der Prolinsynthese (prolin-5-Carboxylat-Synthetase und 1-Pyrolin-5-carboxylat-Reduktase). Der Einfluss von SS kann praktische Anwendung finden, ist von großem wissenschaftlichen Interesse und bietet Raum für das Studium.

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Влияние салициловой кислоты на ферменты растений

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Symbiotic Microbial Interactions in Pea: Ecology and Stress Resilience

In the context of intensifying agricultural production alongside with heightened demands for agroecosystem safety, the importance of research into the role of plant-associated microorganisms in shaping crop productivity and resilience is growing. Modern studies show that the productivity and stress tolerance of legumes are formed not only through nitrogen-fixing legume-rhizobial symbiosis but also via active involvement of endophytic microorganisms and arbuscular mycorrhiza, which regulate mineral nutrition, hormonal status, antioxidant protection, and plant resistance to abiotic and biotic stresses. Pea, as a key grain legume of temperate zones, serves as a model for analyzing complex symbiotic interactions, yet data on the coordinated functioning of endophytic, rhizobial, and mycorrhizal systems within

agroecenosis ecology remain fragmentary. The relevance of such research is amplified by the need to transition to ecologically oriented farming technologies and reduce reliance on mineral fertilizers and chemical protectants.

To date, scientific literature has formed a comprehensive understanding of microorganisms' roles in plant life and agroecosystem functioning. The concept of plant-microbial communities views the plant as a holobiont–a complex organism intimately linked with microorganisms inhabiting the rhizosphere, rhizoplane, and internal tissues [1]. The mechanisms of legume-rhizobial symbiosis formation and function have been studied most thoroughly, including regulation of nitrogen fixation, nodule development, and mineral nutrition's impact on interaction efficiency [2]. Substantial data exist on arbuscular mycorrhiza, particularly regarding plant phosphorus nutrition, water regime, and enhanced abiotic stress tolerance [3]. In contrast, endophytic microorganisms are often addressed fragmentarily, typically within descriptions of specific taxonomic groups or strains with growth-promoting and protective properties [4]. Information on the biodiversity of endophytic communities in various pea organs and tissues, colonization pathways, and ecological factors determining their abundance and functional activity remains limited [5, 6]. Interactions between–endophytic bacteria, rhizobia, and mycorrhizal fungi within a unified plant symbiotic system are also underexplored [7].

Ecological patterns of changes in the structure and functional roles of various symbiotic systems depending on environmental conditions and plant ontogenetic stages are particularly underexamined. Under stressful conditions, legume-rhizobial symbiosis efficiency declines [8], while endophytic bacteria's potential emerges, providing protective effects by enhancing cellular barrier and osmotic properties, influencing the plant immune system, improving mineral nutrition efficiency, and producing phytohormones–ultimately boosting biomass and reducing yield losses [9, 10]. Recent studies indicate that inoculating with endophytic bacteria also positively affects the soil microbiome [11]. Furthermore, these bacteria can modulate microbial community dynamics in the rhizosphere, fostering a more resilient soil ecosystem

that supports long-term plant health. This interplay becomes especially critical during key developmental phases, such as flowering and pod formation in pea, where stress impacts are most pronounced. Experimental evidence from field trials suggests that combined inoculants could amplify these benefits, offering practical solutions for marginal soils.

Scientific works only partially address the redistribution of contributions from legume-rhizobial, endophytic, and mycorrhizal systems in ensuring plant resilience under stress factors. The lack of comprehensive studies integrating microbial biodiversity analysis, plant physiological-biochemical indicators, and soil microbiota status necessitates further development of this issue within agroecosystem ecology. Such integrated approaches could reveal synergistic effects, paving the way for biofertilizers tailored to specific agroclimatic zones.

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Симбиотические микробные взаимодействия в горохе: экология и устойчивость к стрессам

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Comparative characteristics of acute and chronic leukemia

1. The concept and general characteristics

Leukemia is a heterogeneous group of malignant diseases of the hematopoietic system caused by the pathological proliferation of atypical leukocytes, leading to disruption of normal hematopoiesis and immune function of the body [2].

The main clinical division of leukemia is based on the rate of flow and the degree of cell maturity into acute and chronic forms:

Acute leukemia is characterized by a rapid spread of the disease and the predominance of immature blast cells, leading to rapid inhibition of normal hematopoiesis.

Chronic leukemia progresses slowly and is characterized by the accumulation of more mature partially functional cells [2].

2. Cellular morphology and pathogenesis

Acute leukemia:

The pathology is caused by the proliferation of cloned immature blasts (>20% in the brain/blood), unable to differentiate. The rapid growth of blasts leads to suppression of normal hematopoietic function; subsequently, symptoms of anemia, bleeding, and infectious complications occur.

These include, in particular, acute myeloid leukemia (AML) and acute lymphoblastic leukemia (ALL).

Chronic leukemia:

The cells are more mature and retain partial functionality in the initial phases, which leads to a slow progression. Examples include chronic myeloid leukemia

(CML) and chronic lymphocytic leukemia (CLL).

In CML, a specific cytogenetic abnormality is often diagnosed - the Philadelphia chromosome, reflecting the fusion of BCR-ABL1 genes [3].

3. Clinical manifestations and course

Acute leukemia has pronounced symptoms: rapid development of anemia, tendency to bleeding, severe intoxication, frequent infections, organ damage due to infiltration by leukemic cells.

Chronic leukemia in the early stages is often diagnosed accidentally by blood analysis without a pronounced clinical picture; symptoms can develop gradually over the years.

4. Diagnostic criteria

In case of acute leukemia the main diagnostic signs are a high percentage of blasts in the blood/bone marrow, specific immunological and cytogenetic markers detected by immunophenotyping and molecular genetic analysis [1].

Chronic leukemia diagnosis is based on the detection of cloned mature cells with a characteristic phenotypic structure, often using cytogenetics and molecular technologies (for example, detection of BCR-ABL1 in CML).

5. Modern approaches to research and treatment

The progress of molecular technologies, including next-generation sequencing (NGS), has significantly expanded the possibilities of diagnosis, risk stratification and disease monitoring in both acute and chronic leukemia providing more accurate targeted treatment and prediction of outcomes [2].

The treatment of acute and chronic forms of leukemia differs: acute forms require aggressive chemotherapy and often allogeneic bone marrow transplantation, whereas chronic forms can be monitored for a long time and treated with targeted therapy taking into account the molecular profile [4].

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Сравнительная характеристика острых и хронических лейкозов

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Secrets of metabolism: the microbiome as a regulator of protein and hormonal metabolism

It is generally believed that the splitting of undigested food residues is the main and almost the only function of human intestinal microorganisms. Of course, the microbiome makes a significant contribution to the "digestion" of exogenous

proteins, processing 25 times more of its own weight of food substances per year, but other equally important functions can be noted [3, p. 214].

Firstly, microorganisms are able to modify amino acids entering the host's body, as well as synthesize them *de novo*, thereby replenishing the pool of compounds essential for the body. This operation is carried out using intricate and often overlapping chains of biochemical reactions, when one chemical precursor can yield several different compounds. It is important to note that microbial amino acids are full-fledged participants in metabolism and are effectively integrated into proteins and peptides [1, p. 303].

Secondly, the fermentation of protein agents allows microorganisms to turn them into peculiar energy sources that they can use when the oxygen balance changes, or create a number of special by-products that are actively involved in the general metabolism. Perhaps the most significant metabolites of microbial origin include short-chain fatty acids, hydrogen sulfide, ammonia, a number of indole compounds, hormonal peptides and neuroactive compounds.

In this issue, it is worth noting the role of diet, and most importantly the composition of the consortium of microorganisms, since this is one of the decisive factors in which product will be obtained at the exit: an important metabolite or a toxin dangerous to the body, which in turn determines what physiological effect will be exerted on the body [3, p. 225].

The previously mentioned microbial metabolites, and especially short-chain fatty acids, may also have a regulatory function in relation to the synthesis of many hormones, which essentially transforms the collection of microorganisms colonizing the gastrointestinal tract into another "endocrine organ".

Some might think that the contribution of these small bacteria is negligible, but their morphological and biochemical diversity surpasses any other endocrine organ in complexity, and the complexity of organization and symbiotic interaction is comparable to the complexity of the structure and functioning of the brain [2, p. 1223].

It is possible to describe a number of hormones that are under the control of the intestinal microbiota, for example, glucagon-like peptides, serotonin, melatonin and other tryptamines, a number of neurotransmitters, as well as hormones that regulate the feeling of satiety.

This can be done in several ways. One of them is that microbial metabolites activate cellular receptors and thereby trigger cascades of reactions that are aimed at changing ion exchange or regulating gene transcription, which contributes to the initiation of synthesis of a substance of hormonal nature. At the same time, other microbial metabolites act as inducers or inhibitors of synthesis in this process, preventing excessive accumulation of substances [4, p. 302].

The second approach is that a number of microorganisms, which are quite common in probiotics, are able to synthesize these hormones on their own.

Another interesting option is a situation in which the regulating factor is not the microbial metabolites themselves, but the components that make up the bacterial cell walls [1, p. 3].

Ending the conversation about the human gut microbiome, we can safely say that its metabolic activity goes far beyond the gastrointestinal tract, it is not just a system for processing undigested residues, it is a full-fledged "regulatory body" on the effectiveness of which human health depends.

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Тайны метаболизма: микробиом как регулятор белкового и гормонального обмена

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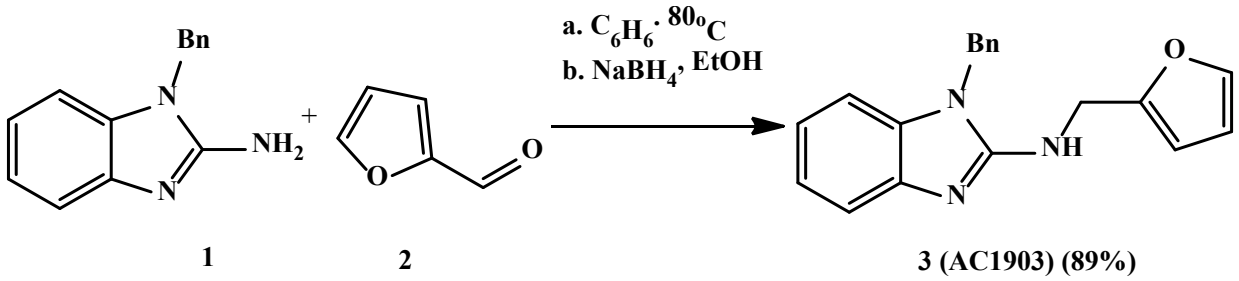
A novel method for the synthesis of TRPC5 inhibitor – compound AC1903

Chronic kidney disease (CKD) is a global healthcare challenge, characterized by a steady increase in prevalence and high rates of population disability. A key pathogenetic factor in the progression of CKD is podocyte injury–damage to the cells that form the filtration barrier of the renal glomerulus. In recent years, the TRPC5 ion channel has been considered a promising molecular target for the development of pathogenetically based therapy, as its activation triggers a cascade of intracellular events leading to cytoskeletal remodeling and podocyte death [1, 2]. Biological studies have demonstrated that AC1903 is a highly selective blocker of TRPC5. Notably, the compound did not affect currents induced by carbachol in TRPC4-expressing cells or currents activated by OAG in TRPC6-expressing cells, even at high micromolar concentrations [3, 4]. This distinguishes AC1903 favorably from the previously known inhibitor ML204, which exhibits activity against TRPC4 and

weakly blocks TRPC6 [3]. In standard kinase activity profiles, AC1903 did not demonstrate significant off-target effects [3].

In this work, a preparative method for the synthesis of the highly selective TRPC5 inhibitor – N-(2-furanylmethyl)-1-(phenylmethyl)-1H-benzimidazol-2-amine (AC1903) – was developed using commercially available starting material, 1-benzyl-2-aminobenzimidazole 1 (Scheme 1).



Scheme 1. Synthesis of N-(2-furanylmethyl)-1-(phenylmethyl)-1H-benzimidazol-2-amine (AC1903) based on commercially available 1-benzyl-2-aminobenzimidazole

The synthesis of AC1903 3 was carried out using a one-pot method, involving the condensation of 1-benzyl-2-aminobenzimidazole 1 with furfural 2 in benzene under conditions of azeotropic water removal (Dean-Stark apparatus, 2 h, reflux temperature), followed by the reduction of the formed Schiff base with sodium borohydride ($NaBH_4$).

Thus, a preparative method for the synthesis of compound AC1903 has been developed, based on the reaction of commercially available 1-benzyl-2-aminobenzimidazole with furfural in benzene, followed by reduction with sodium borohydride.

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Новый метод синтеза ингибитора TRPC5 – соединения AC1903

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Comparative analysis of automated provisioning methods for mass deployment of IP phones

Provisioning in the context of IP telephony is the process of automated setup, configuration, management, and updating of endpoint devices.

TFTP-Based Provisioning

Provisioning based on the Trivial File Transfer Protocol (TFTP) is historically one of the first and most widespread methods for automated configuration of IP phones, particularly in isolated corporate networks. Its operation is based on a simple request-response model for file downloads.

The architecture of this method consists of three key components: a DHCP server, a TFTP server, and an IP phone. The process is initiated by the phone after it receives basic network parameters from the DHCP server. A critical role is played by DHCP Option 66, through which the DHCP server provides the phone with the IP address or domain name of the TFTP server. Alternatively, a pre-configured address in the phone may be used. The phone then requests a configuration file from the server using TFTP (which operates over UDP on port 69). The file name is typically hardcoded in the phone's firmware and is based on its MAC address (e.g 'SEPXXXXXXXXXXXXX.cfg 'for Cisco,' y000000000000.cfg 'for Yealink) or device model. After successfully downloading the file, the phone parses its contents (often in XML or proprietary text format) and applies the settings [1].

HTTP/HTTPS-Based Provisioning

Provisioning using HTTP and its secure version HTTPS is a modern, flexible, and secure approach that is gradually replacing TFTP in corporate environments. It is based on web technologies, opening up extensive possibilities for integration and dynamic configuration generation.

The architecture is similar to the TFTP method, but instead of a TFTP server, a standard web server (e.g., Apache, Nginx) is used. The server address can be provided via DHCP (Option 66) or preconfigured. The key difference lies in the interaction process. The IP phone contacts the web server via HTTP(S), sending a GET or POST request to a specific URL. The request often includes device identification parameters (MAC address, serial number, model), which the server uses to generate a personalized configuration file "on the fly." This allows a single script (in PHP, Python, etc.) to serve thousands of different devices. After

downloading, the configuration is applied by the phone. The use of HTTPS (HTTP over TLS) ensures encryption of the entire communication session.

Provisioning Using TR-069

TR-069 (Technical Report 069) is a comprehensive device management protocol for Customer Premises Equipment (CPE) developed by the Broadband Forum, also known as CWMP (CPE WAN Management Protocol). Unlike file-oriented methods, TR-069 defines an object-oriented management model and provides a complete set of functions for remote administration.

The TR-069 architecture is client-server and consists of two main components: the ACS (Auto-Configuration Server) and the CPE (Customer Premises Equipment – in this case, the IP phone). Communication between them is typically initiated by the CPE and takes place over a secure HTTPS channel. The ACS address can be preconfigured, obtained via DHCP Option 43, or from a configuration file downloaded via TFTP/HTTP (so-called "bootstrap"). Once the session is established, the ACS can perform a wide range of operations: configure parameters (using a standardized hierarchical object model), initiate firmware downloads and updates, request diagnostic information (status, statistics), and reboot the device [2].

The comparative analysis based on a system of criteria confirmed that there is no universal "best" method. Each protocol is optimal for its target environment:

- TFTP is effective for rapid deployment in isolated local networks with a small number of devices, where simplicity and speed of implementation are priorities.

- HTTP/HTTPS serves as a balanced standard for corporate networks that require security, flexibility, and the ability to manage remote devices.

- TR-069 is a specialized solution for telecom operators where full centralized control and automation of management for thousands of distributed devices are necessary.

Thus, the study confirmed that the choice of provisioning technology is a pragmatic engineering task, the solution of which is determined by the specific

boundary conditions of the project, rather than by the abstract technical advantages of any given protocol.

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Сравнительный анализ методов автоматизированного provisioning для массового развертывания ip телефонов

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СОВРЕМЕННЫЕ ТЕХНОЛОГИИ ПИЩЕВОЙ ПРОМЫШЛЕННОСТИ И БИОИНЖЕНЕРИИ

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Functional bakery products enriched with plant antioxidants

The bakery industry in the Russian Federation is one of the most important sectors of the national economy, continuously developing towards expanding the

assortment of functional food products. The modern concept of a healthy lifestyle dictates the necessity of creating food products with specific technological and functional properties that ensure the correction of nutritional value, which includes the antioxidant effect. The relevance of developing sweet baked goods is due to their inherent technological properties, particularly the flexibility of the formulation, allowing for the potential inclusion of various functional ingredients with specific characteristics related to their origin [1,3].

The technological features of the semi-finished product (dough), characterized by a significant content of sugar and fat, allow for the enrichment of the product with components such as dietary fiber and antioxidants without substantial deterioration of organoleptic properties. Furthermore, there is a possibility of modifying the nutritional value through the partial replacement of traditional raw materials with healthier alternatives (e.g., whole-grain flour or sugar substitutes). This allows for the creation of products with an improved nutrient profile to satisfy specific dietary needs, successfully combining a desirable sensory profile with health benefits.

In Russia, particular attention is given to the development of low-waste technologies in the food sector, which allow for the use of grain processing by-products as secondary raw material resources, as well as in the form of functional ingredients. Raw materials of plant origin possess greater antioxidant activity. Plant antioxidants that could be applied in the technology of bakery and sweet baked goods include green tea extract, fermented sea buckthorn pomace, flaxseed flour, quinoa flour, and some others. In addition, plant products grown in the depths of the world's oceans exhibit enhanced antioxidant activity. For example, the microalga spirulina and powders from kelp (Laminaria) and Fucus have become widely used in the food industry due to their high content of flavonoids (specific polyphenols – phlorotannin’s) [4].

Flavonoids are an extensive class of natural phenolic compounds with potent antioxidant activity. Their specific mechanism of action lies in the ability to neutralize free radicals, chelate metal ions, and participate in the regulation of cellular

signaling pathways. The aim of this study is to investigate the feasibility of using seaweed, flaxseed processing products, green tea, and black cumin in the technology of enriched bakery products to correct their chemical composition and enhance their bioactive (antioxidant) properties.

The main plant antioxidants used for bread samples were Kelp/Laminaria, Black Cumin, Green Tea and Flaxseed Flour (Figure 1). The standard Russian bread recipe was used as a control sample for the antioxidant-enriched bakery product. Bakery products produced according to the classic recipe (control sample) and experimental samples (with various replacements of raw materials with alternatives) were checked for compliance with the quality requirements presented in GOST 31805-2018 [2]: organoleptic indicators (appearance, crumb condition, taste and smell, color), physic-chemical indicators (crumb moisture, crumb acidity, mass fraction of sugar and fat in terms of dry matter, mass fraction of filling, specific volume, and volumetric yield).

Fig. 1. View of baked products in cross-section

The organoleptic evaluation of experimental samples demonstrated positive influence on quality of the final product.

Sample No. 1. Seaweed (**Kelp/Laminaria**) Enriched Bread

Shape: The product appears relatively dense, retaining the typical rounded shape characteristic of enriched bread. *The colour* of the product is deep dark brown, exhibiting an orange or clay-like hue. This dark coloration is attributed to the natural pigments of brown algae (e.g., fucoxanthin), as well as to Maillard reactions and sugar caramelization processes, which are influenced by the minerals present in Laminaria. *Crumb/Porosity:* The pores appear denser and less uniform compared to

standard bread. The complex fibers and polyphenols (phlorotannin's) found in Laminaria may have partially inhibited the gluten network structure and yeast activity. A distinctive marine/iodine aftertaste is anticipated, which may require the application of flavor-masking technologies or the use of precisely determined concentrations to enhance consumer acceptability.

Sample No. 2. Green Tea Enriched Bread

Shape: The shape is assessed as good and uniform. *Color*: Olive-green or yellowish-green, the green color is a direct result of the presence of chlorophyll and its derivatives originating from the green tea powder. *Crumb/Porosity*: The crumb exhibits adequately good porosity; it is lighter and more uniform than the seaweed-enriched sample. The effect of the green tea powder on the gluten structure may be less pronounced than that of Laminaria, allowing for a better volume increase in the dough. *Aroma and Taste*: A fresh herbal aroma is expected, along with a slight bitterness caused by the high concentration of potent catechin compounds (EGCG).

Sample No. 3. Flaxseed Flour Enriched Bread

Shape: The product is dense, but with good overall volume. *Color*: Light golden-brown, reminiscent of whole-grain or light rye bread, the color is a direct result of the presence of the ground flaxseed hull, which is rich in fiber, phenolic compounds (lignans), and fats. *Crumb/Porosity*: The crumb appears softer and less dense compared to the Laminaria sample. An improvement in moisture or texture softness is possible due to the high content of water-retaining soluble fibers (mucilage). *Aroma and Taste:* A slight nutty aroma is expected, and the presence of Omega-3 fatty acids in the flaxseed may generally enhance the product's palatability.

Sample No. 4. Black Cumin (Press Cake) Enriched Bread

Shape: The shape is good, but shows a tendency toward slight compression. *Color:* Dark-gray or black with visible speckles/inclusions, the very dark color is due to residual oil and the dark hulls of the black cumin seeds (press cake) remaining after oil extraction. *Crumb/Porosity*: The pores appear non-uniform with clear black points (seed residues), indicating that the large press cake particles may have structurally

weakened the gluten network. *Aroma and Taste*: A pungent and intense aroma is anticipated, which is the characteristic feature of thymoquinone and the volatile oils of black cumin, lending a strong and distinctive flavor to the product.

Consequently, the introduction of plant components influences the formation of the organoleptic properties of the final product, and no foreign odors or aftertastes were observed. The choice of ingredients for the antioxidant-focused bread formulation demonstrates a positive effect on quality indicators. However, the introduction of laminaria contributes to the deterioration of the organoleptic and physic-chemical properties of the finished products.

The functional value of the bread is determined by the antioxidant capacity of the key phenolic compounds in each of the utilized components (Table 1):

Table 1

Groups of antioxidants in the used plant raw materials and functions for the human body

Raw material name	Active compound (Antioxidant)	Mechanism of action and main property
Seaweed (Kelp)	Phlorotannins	Unique marine polyphenols. They are more effective than vitamin C in neutralizing free radicals, and also have antihyperglycemic properties (aimed at lowering blood sugar levels).
Green Tea	Catechins (EGCG)	(Epigallocatechin gallate is one of the most powerful antioxidants in tea. It acts as a highly effective "free radical scavenger" and supports the health of the cardiovascular and nervous systems.
Flaxseed Flour	Lignans	Powerful phytoestrogens. They have pronounced antioxidant and hormone-regulating properties, playing a role in cell protection.
Black Cumin (Cake/Meal)	Thymoquinone	The key active ingredient. It has strong anti-inflammatory and antioxidant properties, and is effective in supporting the immune system and respiratory system.

Antioxidant-rich additives have a direct impact on the quality of the final product (as observed during the organoleptic analysis).

Table 2

Influence of antioxidants on the dough formation process and the quality of the finished bread

Technological property	Expected change	Assessment of technological problem
Fermentation and Dough Volume	Reduction of specific volume (especially in samples 1 and 4).	Fiber and Fat: Insoluble fibers (in kelp and black cumin cake) "dilute" the gluten network, which reduces the ability of the dough to retain gases released by yeast.
Color and Appearance	Radical and desirable change (green, dark brown, gray).	Phenolic Compounds: Natural pigments (chlorophyll, fucoxanthin) change color. Polyphenols also interact with proteins and carbohydrates during baking, enhancing Maillard reactions and affecting the color of the crust and crumb.
Crumb Structure (Porosity)	Increased density and irregularity (especially in the laminaria sample).	Water absorption: Sticky fibers (in flax) can increase moisture retention and texture softness, while coarse fibers (in cake) lead to gluten mesh rupture and uneven porosity.
Expiration date	Noticeable improvement in resistance to staling.	Antioxidant Effect: Antioxidants delay the oxidation of fats present in flour and additives, which slows down the appearance of a "rancid taste" and improves the preservation of bread.

The utilization of bioactive additives (seaweed, green tea, flaxseed, black cumin) is an effective strategy for developing "functional food products" capable of modifying the chemical composition of standard bread and significantly enhancing its antioxidant activity. The research has showed that the technology of enriching bread with antioxidants represents a promising and technologically feasible direction. Nevertheless, success in this area depends on a delicate balance between: biological efficacy including ensuring the preservation of the antioxidant activity of sensitive compounds during the heat treatment process and technological/organoleptic acceptability including developing formulations that balance the health benefits with the sensory challenges (color, taste, and texture) introduced by the additives.

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Функциональные хлебобулочные изделия, обогащенные антиоксидантами растительного происхождения

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The effect of fermentation duration and flour type on the properties of homemade bread

Bread is one of the oldest prepared foods known to humanity. It provides a dense source of energy through complex carbohydrates and, depending on the grain type, can also supply dietary fiber, protein, vitamins, and minerals. Whole-grain breads are especially valuable, they retain the bran and germ of the grain, which are rich in fiber, essential minerals like magnesium and zinc, and bioactive compounds.

Bread quality is a complex trait influenced by many interacting variables: the type of flour, fermentation time, method and the biochemical and physical processes that happen during dough development. Scientists and food technologists are particularly interested in how these factors affect three main aspects of bread: texture,

flavor, aroma and nutrition. A comprehensive analysis of the effects of flour type and fermentation duration on the physical, chemical, and organoleptic characteristics of bread was conducted in the study. The physical processes applied in this study aim to evaluate the structural and mechanical properties of bread, which are crucial indicators of quality. In bread quality evaluating, parameters such as bread loaf volume, volumetric yield, specific volume, shape stability, crust colour and crumb structure play a fundamental role.

The successful breadmaking requires detailed comprehension of the materials used. Standard ingredients and components including water, flour, salt and baker's yeast are commonly applied in experimental and artisanal bread production. Two types of flour, different in technological functionality and biochemical content were chosen as the primary raw materials. Refined white wheat flour is known to serve as the conventional basis due to its higher gluten forming capacity, which ensures good gas retention properties and the development of light, aerated crumb.Whole grain flour was added to another dough test object, which is a more nutritious alternative enriched with bran and grain germ, which is abundant in additional amounts of dietary fiber, minerals and antioxidants. Dry baker's yeast (Saccharomyces cerevisiae), examined in the laboratory was used as a biological leavening agent due to gas production capacity of bread during fermentation process and widespread accessibility in controlled baking experiments. Water performs fundamental functions in breadmaking process shaping dough structure and gluten fermentation as well as serves as a hydration medium. Food-grade sodium chloride was added to strengthen gluten, regulate fermentation, improve flavour, while granulated sugar is used in formulations to support yeast activation during the process of initial mixing.

The materials for bread samples were prepared and analyzed in the standard laboratory to ensure accuracy, reproducibility, and controlled experimental conditions. The ingredients were mixed in stainless-steel bowls, providing a non-reactive surface suitable for ultimate dough development. They were measured by digital laboratory scales with ±0.01 g precision to ensure consistency and

reproducibility across all experimental batches. Flours used were kept under controlled conditions to avoid from excessive humidity and thermal fluctuations. The uniform distribution and quality of the dough components were critical to ensure the reliability of the experiment and make sure that observed differences in bread characteristics could be attributed to the independent variables investigated, flour type and fermentation extension. Bread was baked in an electric, temperature-controlled oven to ensure precise regulation of baking temperature and timing, critical for achieving consistent crust and crumb characteristics. The internal temperature of bread was measured by a food-grade thermometer to ensure complete baking. Physical measurements of the bread such as volume and crumb structure were conducted using a combination of a digital caliper and ruler to accurately evaluate size and porosity of a product.

Table 1

Bread preparation formulations

Raw materials	Classic wheat flour bread (3 hours in 35°C)	Mixed wheat-whole grain bread (3 hours in 35°C)	Classic wheat flour bread with extended fermentation (12 hours in 5-6 °C)	Mixed wheat-whole grain bread with extended fermentation (12 hours in 5-6 °C)
Flour, g	Wheat - 100	Wheat – 80, whole grain - 20	Wheat - 100	Wheat – 80, whole grain - 20
Water, g	65	68	65	68
Salt, g	2	2	2	2
Yeast, g	1	1	0,5	0,5

To evaluate structural and mechanical properties of bread, the crucial indicators of its quality, physical methods were applied in the study. Parameters such as specific volume, volumetric yield and shape stability play an important role in assessing of the quality of bakery products.

The specific volume of bread, defined as the ratio of product's volume to its weight is the most crucial external feature of bread and is considered as an indicator of porosity and lightness of the crumb structure.

A higher specific volume indicates a lighter and porous texture, which is directly related to the physical properties of the dough, including its ability to retain gas bubbles formed during fermentation and baking.

Volumetric yield characterizes the efficiency of converting the dough mass into a finished product and allows for the assessment of the technological rationality of the process. This parameter reflects the degree of dough expansion under the influence of gases produced during fermentation and determines the economic efficiency of production [4]. Particular importance is attached to the shape stability of hearth bread, which characterizes the product's ability to maintain its intended shape after baking and cooling. This indicator determines the elasticity and resilience of the crumb, its resistance to deformation under its own weight and external mechanical forces.

Shape stability is a critical criterion for the physical integrity and visual quality of bread. The moisture content of dough is one of the key parameters determining its quality and technological properties. It is primarily classified as a physicochemical characteristic, as it reflects both the physical state of the dough mass and the molecular interactions occurring among its components. From a physical standpoint, moisture content characterizes the amount of water present in free and bound forms and determines the consistency, plasticity, and rheological behavior of the dough.

Organoleptic analysis is an integral part of assessing the quality of bread. According to GOST 31805-2018 (State Standard) «Bakery products made from wheat baking flour» the general technical specifications governing the rules for the acceptance of bakery products, as well as methods for sampling and determining organoleptic parameters, such characteristics as shape, surface, color, crumb condition, taste and smell are important. When evaluating the surface of a crust, it is important to pay attention to its smoothness or the presence of cracks, elasticity and thickness. The surface of the molded bread should be smooth, without large cracks and explosions, and incisions or punctures are allowed in the hearth. The color of the crust and crumb is also analyzed: the standards provide for a range of shades

characteristic of this type of bread - from light yellow to brown. The condition of the crumb is one of the most important criteria. According to GOST 31805-2018 (State Standard), baking quality is evaluated (the crumb should not be wet to the touch, should be elastic, return to shape after light pressure and porosity should be developed, without air pockets and hardened crusts, without separating the crust from the crumb). Taste and aromatic characteristics should also be taken into account [5]. The taste and smell of bread should be pleasant, corresponding to the type of bread, without foreign or undesirable odours.

Experiments have shown that incorporating whole-wheat flour increases the nutritional value by raising fiber, mineral, and protein content, while slightly reducing loaf volume and crumb uniformity. Extended fermentation, applied both to white bread and to the wheat–whole-grain blend, has improved aroma and flavor characteristics, imparting a mild acidity and a more complex flavor profile without substantially affecting texture. Careful selection of flour type and fermentation time allows for severe control of bread quality, ensuring a balance between technological, organoleptic and nutritional parameters. The results of the research can be used the development of bread formulations both in laboratory conditions and in industrial bakeries, taking into account the preferences of various consumer groups and current nutritional requirements.

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Влияние длительности брожения и типа муки на свойства домашнего хлеба

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Development of functional food products based on young walnut leaf extract

The modern world is marked by evident decline in population health indicators and constant increase in the incidence of age-related pathologies. Widespread dietary deficiencies, in particular concerning the intake of essential micronutrients like iodine and bioactive compounds having antioxidant properties useful for human health are considered as a significant contributing factor to the development of various health problems. Lack of iodine is reported to remain a public health issue in various regions, linked to thyroid dysfunction and impaired cognitive development. Simultaneously, the accumulative damage caused by oxidative stress, a consequence of insufficient antioxidant defence, plays an important role in the pathogenesis of numerous chronic diseases, including cardiovascular pathologies, cancer, and neurogenerative disorders. The relevance of this research is underscored by ongoing need for development of innovative food products fortified with these essential

substances. There is a noticeable tendency toward using natural, plant-based ingredients which are considered as safe and synergetic sources of nutrition compared with synthetic additives. Young walnut leaves (Juglans regia L.) represent a promising source for such functional food applications due to their phytochemical composition.

The walnut tree has been revered for centuries, not only for its prized nuts but also for the medicinal properties attributed to its leaves, bark, and green husks in traditional pharmacopoeias. Within the modern food industry, the walnut is valued for its exceptional nutritional qualities, high-quality lipids, proteins, and dietary fibre. Its enduring popularity and versatility align perfectly with contemporary consumer trends that emphasize whole, natural, and health-promoting foods. Walnut history demonstrates a consistent capacity to adapt to evolving consumer demands, from a staple energy source to a recognized component of heart-healthy and anti-inflammatory diets [1]. The positive walnut perception creates its value and becomes the basis for development of value-added products. A comprehensive understanding of the physiological importance of iodine and antioxidants is fundamental to appreciating the value of their dietary supplementation.

Iodine is an essential trace element, serving as a critical constituent of thyroid hormones (thyroxine (T4) and triiodothyronine (T3) in the body. They are known for regulating micronutrient metabolism, thermogenesis and neurological development, especially in utero and during early childhood. Insufficient dietary supply of iodine disrupts the synthesis of these hormones, leading to a spectrum of disorders collectively known as iodine deficiency disorders (IDD). They are classified into goitre (enlargement of the thyroid gland) and hypothyroidism–manifesting as fatigue, weight gain, and cognitive slowing to severe and irreversible intellectual disability in children [2]. Ensuring adequate iodine intake is known to be a cornerstone of preventive healthcare.

Antioxidants comprise a diverse group of compounds that mitigate oxidative damage by neutralizing reactive oxygen species (ROS) and free radicals. This

oxidative stress, resulting from an imbalance between pro-oxidants and antioxidants in the body, causes cell damage, accelerating the ageing process and increasing the susceptibility to chronic diseases. Dietary antioxidants, such as polyphenols, flavonoids, and vitamins C and E, found abundantly in plants, supply electrons to stabilize free radicals, thereby interrupting destructive chain reactions. Epidemiological and clinical studies have consistently associated high dietary intake of antioxidants with a reduced risk of conditions like atherosclerosis, certain cancers, and age-related macular degeneration [5]. The combination of iodine and dietary antioxidants, offered by a natural source like walnut leaves, can have synergistic health effect, increasing body resistance to environmental toxins and psychological stressors.

The global food industry is witnessing a paradigm shift, moving beyond mere sustenance towards the delivery of specific health benefits. This has given rise to the robust functional food and nutraceutical sectors. Modern fortification strategies are increasingly sophisticated, focusing not only on replacing deficient nutrients (e.g., iodized salt) but also on foods with bioactive compounds that can positively influence physiological functions. There is a clear consumer-driven preference for "clean-label" products, which requires the use of natural supplements like plant extracts, fruit concentrates, and so-called "superfoods." The incorporation of these nutrient-dense ingredients into everyday staples such as baked goods, dairy products (e.g., yogurts, cheeses), beverages, and snacks is becoming a mainstream practice [3]. This trend is supported by scientific research aimed at optimizing the stability, bioavailability, and sensory compatibility of these functional ingredients within complex food systems.

The integration of young walnut leaf powder or extract into food products is a high degree of sophistication in food science and technology. The primary challenge lies in achieving a significant level of fortification without compromising the sensory attributes such as flavour, aroma, colour, and texture that determine consumer acceptance. The initial phase of product development involves testing various recipes and conducting thorough sensory evaluations using trained panels. Walnut leaves can

impart a slightly bitter, astringent, and herbaceous flavour, which must be balanced with other ingredients. Masking agents, flavour modulators, or combining the extract with complementary ingredients (e.g., honey, spices, or strong-flavoured fruits) may be necessary. Following the establishment of a palatable prototype, it is important to validate its nutritional claims through analytical chemistry. The techniques like ICP-MS (Inductively Coupled Plasma Mass Spectrometry, ICP-MS (Inductively Coupled Plasma Mass Spectrometry and spectrophotometric methods are used to measure iodine content, antioxidant capacity and total phenolic and flavonoid content. These analyses not only confirm the nutritional enhancement but also provide critical data for accurate labelling and health claim substantiation, which are vital for building consumer trust and complying with regulatory standards [4, 5].

A growing body of in vitro and in vivo research provides a scientific basis for the health-promoting properties of walnut leaf extracts. In vitro studies on cell cultures have demonstrated the potent free-radical-scavenging activity of these extracts, effectively reducing markers of oxidative stress. Furthermore, research involving model organisms has suggested that bioactive compounds in walnut leaves can upregulate endogenous antioxidant defence systems, such as the activity of superoxide dismutase (SOD) and glutathione peroxidase (GPx). Some studies have indicated an anti-apoptotic effect and an extension of cellular lifespan in certain models, providing a plausible mechanism for the purported anti-ageing benefits [6,9]. While clinical trials are still limited, the preclinical research strongly supports the concept that regular consumption of foods fortified with standardized walnut leaf extract can contribute to reducing systemic oxidative stress and mitigating associated health risks.

The distribution of a new functional food product extends far beyond the laboratory and requires effective market strategy. Different groups of consumers will include health-conscious customers, individuals with specific dietary preferences, e.g, those consuming natural sources of iodine or antioxidants, fitness enthusiasts, and elderly population aimed at improving quality of life and healthy ageing. A

comprehensive marketing strategy should effectively provide the unique selling proposition (USP)–the dual benefit of natural iodine and antioxidant fortification. Communication transparency, scientific basis and healthcare compliance regulations can improve the marketing strategy actions. Appropriate distribution channels including health food stores, premium supermarkets, online retail platforms, specializing in healthy products and clinical settings as a part of recommendations ensure the efficient flow of products from manufacturer to the consumers. An initial launch can be supported by a targeted promotional campaign, including informative content marketing, event sampling, and collaborations with nutritionists or fitness influencers. The legal and regulatory environment is essential, it comprises obtaining all necessary food safety certifications, compliance with food additive and innovating food regulations, and providing accurate nutritional data labelling that includes the declared content of iodine and antioxidants.

Significant potential of young walnut leaf extract highlights promising possibilities for development of fortified food products. Public health challenges driven by nutrient deficiencies and the crucial impact of oxidative stress require proactive approaches, practical solutions and science-based research in food industry. Young walnut leaves offer a sustainable and bioavailable source of both essential iodine and a complex mixture of potential antioxidants. The incorporation of young walnut leaves into functional foods presents a reliable pathway to the development of products that not only meet but also respond to growing consumer demand for clean label products, health promoting options, young walnut leaves also possess enhancing human health capacity. This approach taking into account key aspects starting with phytochemistry and product formulation to market strategy and regulatory compliance can make substantive contribution to improving dietary quality, maintaining metabolic health, promoting healthy aging. Further application, particularly robust human intervention studies will enable to fully elucidate the long-term health benefits and strengthen the position of walnut leaf fortified foods in the global functional food market.

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Разработка функциональных пищевых продуктов на основе экстракта молодых листьев грецкого ореха

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Prospects for the development of iron-enriched confectionery

Iron is an essential element that performs various physiological functions to support human health and maintain life. Its fundamental role is in transporting oxygen to organs, producing energy and regulating immune system activation. Chronic iron deficiency results in the development of iron deficiency anemia, a condition in which hemoglobin level and number of red blood cell are reduced. The main signs of iron deficiency anemia are known to include fatigue characterized by constant tiredness and lack of energy, depression, weakness, paleness, shortness of breath, concentration difficulty and decreased mental and physical activities, irritability, and maintaining constant body temperature difficulty. During pregnancy, severe cases of anemia can lead to health complications and an increased risk of premature birth. In addition, lacking of sufficient intake of iron enriched foods can also cause neurological problems, gastrointestinal disturbances, decreased immunity and high absorption and accumulation of toxic micronutrients affecting human life. The relevance of this problem is underscored by ongoing need for iron deficiency evaluating and innovating with this indispensable element.

The prevalence of iron deficiency anemia in the Russian Federation remains consistently high. Data on the prevalence of iron deficiency anemia vary by region and population group, but the general picture is as follows (Table 1).

Table 1

Prevalence of Iron Deficiency Anemia in the Russian Federation

Population group	%	Complication
Pregnant women	20% - 40%	The most vulnerable group due to increased physiological needs
Young children	20% - 30%	Period of intensive growth and depletion of neonatal reserves
Teenagers (girls)	15% - 25%	Combination of growth spurt and onset of menstruation
Women of reproductive age	15% - 20%	Regular physiological blood loss. Latent iron deficiency can reach 50-60%
Older adults	10% - 15%	Often associated with chronic diseases and poor nutrition

According to the Russian Ministry of Health, the incidence of anemia has increased more than sixfold over the past 20 years, with iron deficiency anemia accounting for approximately 90%. According to the World Health Organization (WHO), iron deficiency anemia is the leading cause of 38 of the most common human diseases. In Russia, it affects 6-30% of the population [1].

Iron deficiency anemia is the most common pregnancy complication worldwide. According to the World Health Organization (WHO), approximately 40% of all pregnant women worldwide suffer from anemia. In some developing countries, this figure can reach 60-80%. In Russia, iron deficiency anemia among pregnant women ranges from 20% to 40%, according to various sources. Anemia is reported to develop in the second and third trimesters.

The daily iron requirement was shown to vary and depend on gender, age, and physiological condition. (Figure 1)

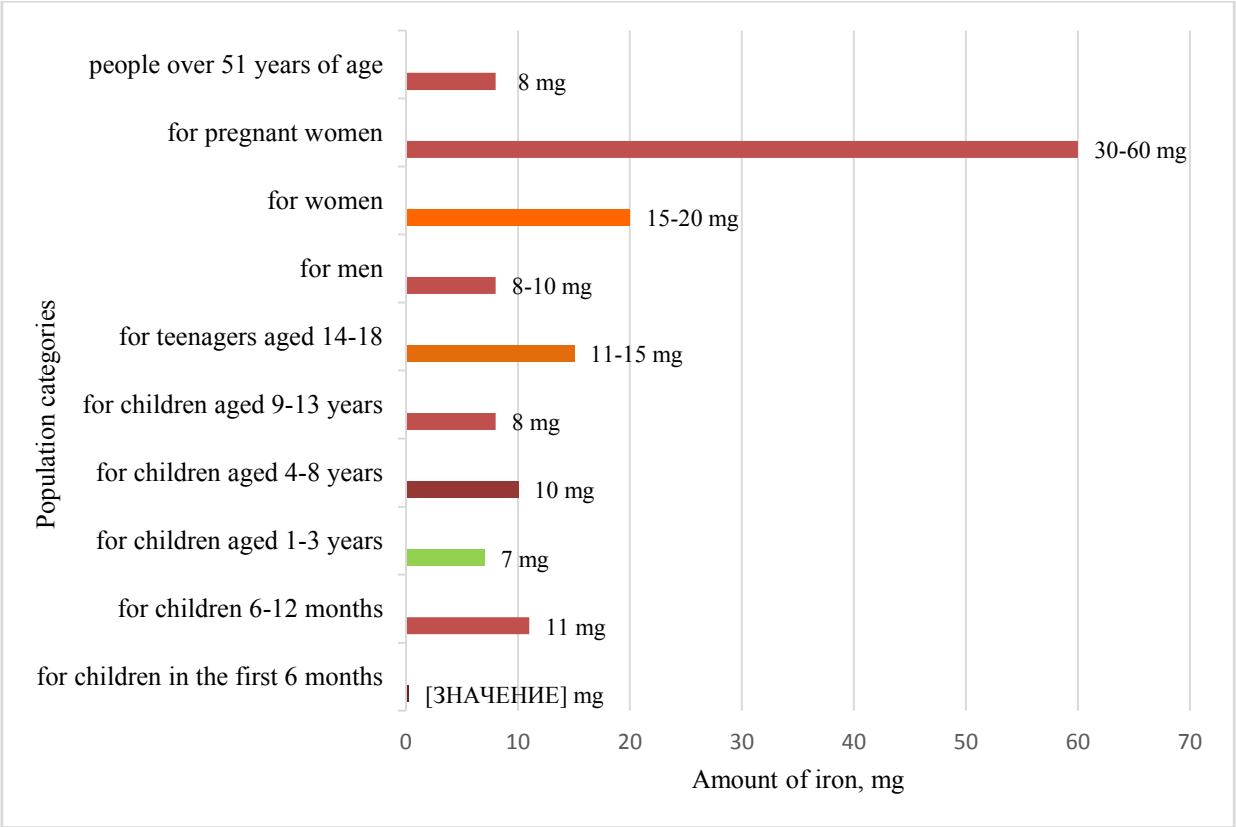

Fig. 1. Daily Iron Requirement, mg

Pregnant women are at the highest risk. During pregnancy, decreased hemoglobin levels are recorded in 41.8% of cases, with iron deficiency the cause of anemia in the vast majority of cases, and 40% have iron metabolism disorders prior to pregnancy [3]. Maternal iron deficiency directly threatens the health of the fetus, increasing the risk of developmental delays, premature birth, and low birth weight. It is virtually impossible to meet the requirement of 30-60 mg of iron through diet alone, making it necessary to take specialized supplements or fortified foods. For example, confectionery products can be fortified. The main challenge in fortifying confectionery products with iron is the choice of the iron form and its impact on the product organoleptic properties.

The most suitable iron form was selected based on a number of factors, including bioavailability, stability, safety, and changes in organoleptic properties (Table 2).

Table 2

Comparison of Iron Forms

Iron form	Positive effects	Side effects	Population group
Ferrous Sulfate (Most Common)	High bioavailability (easily absorbed); Low cost; Proven effectiveness	Severe gastrointestinal side effects: nausea, constipation, pain; metallic taste in the mouth; reacts with food, may oxidize other components	For healthy adults with severe deficiency who do not have stomach problems and who are willing to tolerate side effects
Ferrous Gluconate and Fumarate	Better tolerated than sulfate; Relatively high bioavailability; Reasonable price	May still cause gastrointestinal discomfort; metallic taste possible	For those who are sulfate intolerant but looking for a budget option
Ferrous Pyrophosphate	No gastrointestinal side effects; No metallic taste; Stable in foods, does not oxidize them; High bioavailability (especially encapsulated)	Higher cost; Less common in pure form in pharmacies	Ideal for: children, pregnant women, people with sensitive digestive tracts, and fortifying foods (cereals, drinks)
Iron Bisglycinate (Chelated Form)	Better tolerability (minimal side effects); Very high bioavailability; Does not interact with food, can be taken with food; No aftertaste	The highest price among similar products	Best choice for: people with very sensitive stomachs, those for whom comfort is critical, and long-term preventative use
Heme Iron (From Animal Hemoglobin)	Absorbed 2-3 times better than non-heme forms; Not dependent on other foods; Virtually no side effects	Very expensive; Rare on the market; Not suitable for vegans/vegetarians	For those who are looking for the most effective and safe form and are willing to pay for it

Of the forms of iron reviewed, ferric pyrophosphate is the most bioavailable and stable. Numerous clinical studies [3] have shown that ferric pyrophosphate is among the salts that provide the best results even in the most severe deficiencies. Ferric pyrophosphate has the following characteristics:

– High bioavailability. Especially in the form of submicron particles, it is absorbed as well as, and sometimes even better than, sulfate, but without the side effects.

– Neutral taste and color. It does not have a characteristic metallic aftertaste, which is critical for creating tasty products.

– Stability. It does not oxidize fats and other product components, significantly extending its shelf life and preserving its original flavor.

– Gastrointestinal safety. It does not irritate the stomach or intestines, making it ideal for children, pregnant women, and those with sensitive digestion.

Iron pyrophosphate (especially in encapsulated form) is the gold standard for food fortification, as it does not affect the flavor or color of foods. This modern, technologically advanced form is ideal for most people, including children and pregnant women. It is effective yet safe for the gastrointestinal tract.

The encapsulated form of iron pyrophosphate creates a protective shell around each iron particle, preventing unwanted interactions with other product ingredients (acids, vitamins, and fats) before it enters the body. This ensures that the iron is released precisely in the gastrointestinal tract where it is most absorbed. The encapsulated form of iron masks any potential aftertaste, providing a pure and pleasant taste of marmalade [5].

Marmalade is a confectionery product loved by both children and adults. It is associated with pleasure, not treatment, which increases adherence to regular consumption. Each gummy bear or wedge can contain a precisely defined, safe, and effective dose of iron, adapted for different target groups–in our case, pregnant women.

Considering all of the above, the development of a functional confectionery product – gummy bears enriched with encapsulated iron pyrophosphate is an extremely useful alternative for managing iron deficiency anemia. The creation of bioavailable gummy bears based on iron encapsulation is not just a marketing ploy, but a real step toward improving the quality of life and health of all segments of the population, including pregnant women. This product combines a scientific approach, impeccable taste, and effectiveness, making iron deficiency prevention truly accessible and enjoyable.

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Перспективы разработки кондитерских изделий, обогащенных железом

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Cactus seed oil: Nutritional benefits and pharmacological properties

The prickly pear cactus (Opuntia ficus-indica) is a perennial plant, cultivated throughout Mexico, the Mediterranean region, northern Africa, Chile, South Africa,

the Middle East, California, and other parts of the Southwestern United States. The fruit of this cactus is known to contain about 9-10% seeds by weight, which represents a substantial byproduct of cactus fruit processing. The seeds contain 5-16% oil by weight, depending on the variety, growing conditions, and extraction methods used. The growing interest in cactus seed oil parallels increased consumer demand for natural, plant-based oils with both nutritional and functional properties. Cactus seed oil meets this demand as it is rich in unsaturated fatty acids as well as natural antioxidants. Interaction of fatty acid composition and antioxidant components contribute to the stability and biological activity of the oil.

Unsaturated fatty acids, tocopherols and phenolic compounds in cactus seed oil provide cardioprotective effect including reducing oxidative stress, enhancing lipid profiles, and modulating inflammatory pathways through various mechanisms. Regular introduction of oil enriched with these components into the human diet has been concerned with decreased risk of cardiovascular diseases investigated by the scientists. Linoleic acid has been reported to reduce low density lipoprotein cholesterol levels when substitute dietary saturated fats with unsaturated ones in the diet. In addition, cactus seed oil contains phytosterols, especially B-sitosterol which contribute to decreasing cholesterol absorption competing with dietary cholesterol with absorption in the small intestine.

Cactus seed oil is abundant in natural antioxidants, including vitamin E, particularly y-tocopherol and different phenolic compounds which neutralize free radicals and reactive oxygen species, protecting cell components from oxidative damage. The antioxidant capacity of cactus seed oil has been shown in both in vitro and in vivo studies. The presence of these natural antioxidants not only provide health benefits of the oil but also enhances its oxidative stability, extending shelf life of the product without using any synthetic preservatives [1]. This natural stability is advantageous for both food and cosmetic applications where oxidative rancidity can negatively influence the quality of the product and its safety.

Beyond its nutritional value, cactus seed oil is known for its several

pharmacological properties that support its potential applications in medicine. These properties are attributed to the unique combination of fatty acids and biologically active compounds found in the oil.

Cactus seed oil exhibits significant anti-inflammatory activity through different mechanisms. The high levels of linoleic acid in the oil serves as a precursor for anti-inflammatory eicosanoids, while inflammatory signaling pathways are modulated by its phenolic compounds. Isorhamnetin, a flavonoid found in the oil of cactus seed has been reported to regulate HF-kB, PI3K/AKT, and MARK signaling pathways, which are integral to inflammatory responses. The results of in vivo research have demonstrated an ability of antioxidants to reduce inflammation in different models, suggesting the potential of cactus seed oil for controlling chronic inflammatory conditions. The anti-inflammatory effects of the oil complement its antioxidant properties, providing dual protection against oxidative damage and inflammation, which are often interconnected in chronic diseases.

The antioxidant capacity of cactus seed oil has been extensively documented through both in vitro and in vivo research. Tocopherols, particularly y-tocopherol, and phenolic compounds found in the oil effectively neutralize free radicals and reactive oxygen species, decreasing oxidative damage to cellular components. Research has shown that consumption of cactus pear fruit positively affects body redox balance, decreases oxidative damage to lipids, and improves antioxidant status in healthy humans.

Cactus seed oil may offer benefits for blood sugar management and diabetes complications. While most research on antidiabetic effects has focused on cactus pads and fruits, the seed oil contains similar bioactive compounds that may contribute to glycemic control [1, 2]. The soluble fiber pectin found in cactus components has blood-sugar-lowering properties and beneficial effects on blood fat levels.

A 2022 review suggested that prickly pear consumption may decrease fasting blood sugar levels in both healthy adults and those with type 2 diabetes. The effects appear to depend on the form of consumption and the part of the plant used, with

further research needed to determine the specific contribution of seed oil to these antidiabetic effects.

The unique composition and beneficial properties of cactus seed oil have led to its exploration in various industries, including food, cosmetics, and pharmaceuticals. Its combination of nutritional value and bioactive properties makes it a versatile ingredient with multiple applications.

In the food industry, cactus seed oil can be used as a nutritive edible oil with potential health benefits. Its high linoleic acid content and favorable fatty acid profile make it nutritionally superior to many conventional oils. The natural antioxidant content of the oil also provides oxidative stability, potentially reducing the need for synthetic preservatives in food products. Specific food applications include:

Salad oils and dressings: The pleasant flavor profile and nutritional benefits make cactus seed oil suitable for cold applications where its bioactive compounds are preserved.

Functional food ingredients: Cactus seed oil can be incorporated into various functional foods designed to provide health benefits beyond basic nutrition.

Food supplements: The oil can be encapsulated or otherwise formulated as a dietary supplement to deliver its concentrated health benefits [4].

Despite these potential applications, the relatively low yield and high production cost of cactus seed oil currently limit its widespread use in the food industry. Advances in extraction technology and increased cultivation of cactus for dual purposes (fruit and seed production) may help address these limitations. Several factors must be considered for the successful commercial application of cactus seed oil:

Standardization: Variations in composition based on geographical origin, species, and extraction methods necessitate standardization processes to ensure consistent quality and efficacy [3].

Stability: While the oil contains natural antioxidants, additional stabilization measures may be required for certain applications to maintain quality during storage.

Cost-effectiveness: The relatively low oil yield from seeds makes production expensive compared to conventional oils. Development of efficient extraction methods and valorization of seed cake byproducts could improve economics.

Regulatory status: Depending on the intended application and market, cactus seed oil may need to comply with various regulatory requirements for food, cosmetic, or pharmaceutical ingredients.

Cactus seed oil represents a promising natural resource with significant nutritional and pharmacological potential. Its unique content, characterized by high levels of linoleic acid, phytosterol, y-tocopherol and different phenolic compounds, contributes to different health benefits such as antioxidant, anti-inflammatory, hypolipidemic, and hepatoprotective effects.

Despite the growing number of scientific publications supporting the potential use of cactus seed oil, several areas require further investigation. The scientists should focus the research on standardization of extraction techniques to increase yield while preserving bioactive compounds, clinical human studies to provide the health benefits noted in preclinical studies, creation of value-added products on the basis of cactus seed oil for food, cosmetic, and pharmaceutical industries, sustainability evaluation of cactus cultivation and production. The potential of cactus seed oil extends beyond its current applications, enabling the development of new functional foods, nutraceuticals, and cosmeceuticals. As research continues to clarify its mechanisms of action and optimal applications, cactus seed oil may become an increasingly valuable commodity in the global market for natural health products.

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Масло семян кактуса: пищевая ценность и фармакологические свойства

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Experimental study of fluid mineralization based on frequency

Operational monitoring of reservoir fluid mineralization is of practical interest for preventing salt deposits in well equipment. Existing contact methods have a number of limitations, which makes it relevant to develop non-contact approaches to assessing mineralization. The physical basis of the proposed method is the dependence of the electromagnetic properties of the solution on the concentration of

ions. As mineralization increases, the parameters of complex dielectric constant (ε' and ε'') and specific electrical conductivity (σ) change, which should be reflected in the amplitude-frequency characteristic of the signal passing through the medium under study. The purpose of the work is to study the effect of mineralization of aqueous solutions on their amplitude-frequency characteristic (AFC) in the high-frequency range. The main objective is to provide a practical basis for assessing mineralization based on changes in the parameters of the high-frequency electromagnetic field.

To conduct the research, the following was collected

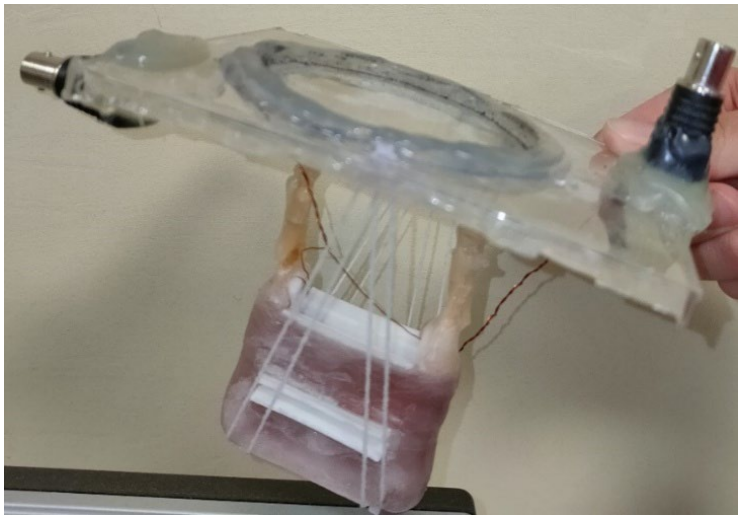

Fig. 1. The developed dual-coil sensor

A 1-liter sample of liquid was placed in the space between the coils. A sinusoidal signal was applied to the emitting coil, and the received signal was recorded by an oscilloscope. The measurements were conducted for distilled water and solutions of sodium carbonate (Na_2CO_3) and potassium sulfate (K_2SO_4) with concentrations up to 1 g/L.

The analysis of the obtained oscillograms allowed for the construction and comparison of the frequency response for the studied media (Figure 2). The results of the experiments confirm that the magnitude of the output signal depends on the specific electrical conductivity of the salt solution: as it increases, the attenuation parameter decreases. In addition, the frequency of the artificial EM field also affects the dielectric constant of the medium, which affects the measurements.

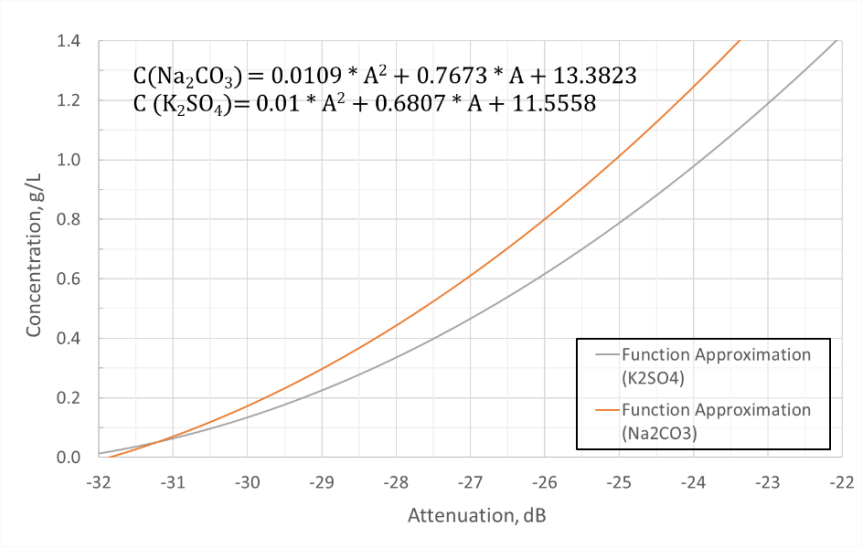

Fig. 2. Comparison of the dependencies of the dissolved salt fractions Na2CO3 and K2SO4

The conducted studies have confirmed that the proposed laboratory model is capable of registering changes in the amplitude-frequency response when the mineralization of the liquid changes. The quantitative results obtained demonstrate the effectiveness of the approach and its sensitivity to the ionic strength of the solution, but more comprehensive studies are needed to use solutions of other salts and consider changes in temperature.

The results of my work can be integrated with geophysical measurements in wells, contributing to the optimization of production and the prevention of emergencies in ESPs.

Экспериментальное изучение минерализации флюида по частотному отклику

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Analysis of pressure distribution in the wellbore during water injection

This paper addresses the question of how pressure changes with depth in an injection wellbore during water injection. Under static conditions, pressure increases with depth due to the hydrostatic effect; however, during dynamic flow, hydraulic friction losses play a significant role. Depending on the flow rate, pressure can either increase or decrease with depth. The study includes a theoretical analysis based on fundamental hydraulic laws and numerical simulations carried out using a proprietary software code developed by the author. The numerical results confirm that pressure decrease with depth is theoretically possible and occurs under certain wellbore geometries and flow regimes. Specific quantitative values have been obtained; only qualitative patterns are presented. Practical recommendations for designing reservoir pressure maintenance systems are given.

For a stationary fluid, the bottomhole pressure P_{bh} is related to the wellhead pressure P_{wh} and depth H by $P_{\text{bh}} = P_{\text{wh}} + \rho g H$, where ρ is water density, g is gravity, and H is depth. This linear increase is valid only when there is no fluid motion. In reality, water is continuously pumped down the tubing, and energy losses due to viscous friction and local resistances must be accounted for. The frictional pressure drop along a pipe of length L and internal diameter D is given by the Darcy–Weisbach equation: $\Delta P_{\text{fric}} = \lambda \cdot (L/D) \cdot (\rho v^2/2)$, where λ is the friction factor and v is the average flow velocity. Local losses can be added as $\Delta P_{\text{local}} = \sum \xi_i \cdot (\rho v^2/2)$, so the total loss is $\Delta P_{\text{loss}} = \Delta P_{\text{fric}} + \Delta P_{\text{local}}$.

Taking losses into account, the bottomhole pressure becomes $P_{\text{bh}} = P_{\text{wh}} + \rho g H - \Delta P_{\text{loss}}$. If $\Delta P_{\text{loss}} > \rho g H$, then $P_{\text{bh}} < P_{\text{wh}}$, meaning pressure decreases with

depth. The differential form clarifies this: $dP/dz = \rho g - dP_{\text{loss}}/dz$. When the loss gradient exceeds the hydrostatic gradient, the pressure derivative becomes negative. To verify these theoretical predictions, a numerical simulation was performed using a software code developed by the author (in collaboration with the scientific supervisor). The code solves the one-dimensional steady-state flow equations in a vertical wellbore, accounting for variable fluid properties and realistic friction models. A series of calculations was carried out for typical injection well parameters (depth range 1000–2500 m, tubing diameters 50–100 mm, flow rates 200–2500 m^3/day). The results clearly demonstrate that pressure can indeed decrease with depth when the flow rate is sufficiently high and the tubing diameter is relatively small. In such cases, the frictional pressure drop dominates over the hydrostatic gain, leading to a negative pressure gradient along the wellbore. However, the key qualitative conclusion is robust: pressure may either increase or decrease with depth depending on the operating conditions. The transition occurs when $\Delta P_{\text{loss}} = \rho g H$. The numerical results are in excellent agreement with the theoretical analysis, confirming that the phenomenon is not merely theoretical but practically observable.

Injectivity of a well is defined as $Q = K_{\text{inj}}(P_{\text{bh}} – P_{\text{res}})$, where K_{inj} is the injectivity coefficient and P_{res} is the reservoir pressure To achieve a desired flow rate, the required wellhead pressure is $P_{\text{wh}} = P_{\text{res}} + \Delta P_{\text{loss}} - \rho g H + Q/K_{\text{inj}}$. If $\rho g H > \Delta P_{\text{loss}}$, the wellhead pressure needed may be lower than the reservoir pressure; if losses are high, a significantly higher wellhead pressure is required. Therefore, accurate prediction of pressure distribution is essential for selecting surface equipment and avoiding over pressurization. In conclusion, in a static fluid column pressure always increases with depth. During water injection, hydraulic friction losses oppose the hydrostatic effect. Pressure decreases with depth when the loss gradient exceeds ρg. This is possible at high flow rates, small tubing diameters, or high fluid viscosities. Numerical simulations using custom-developed software confirm the theoretical possibility of pressure decrease. Quantitative results have

been obtained. For practical engineering, the key is to compute the actual bottomhole pressure accurately, as it determines well injectivity.

Анализ изменения давления в стволе нагнетательной скважины при закачке воды

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Experimental study of the peculiarities of liquid droplet generation using a microfluidic device

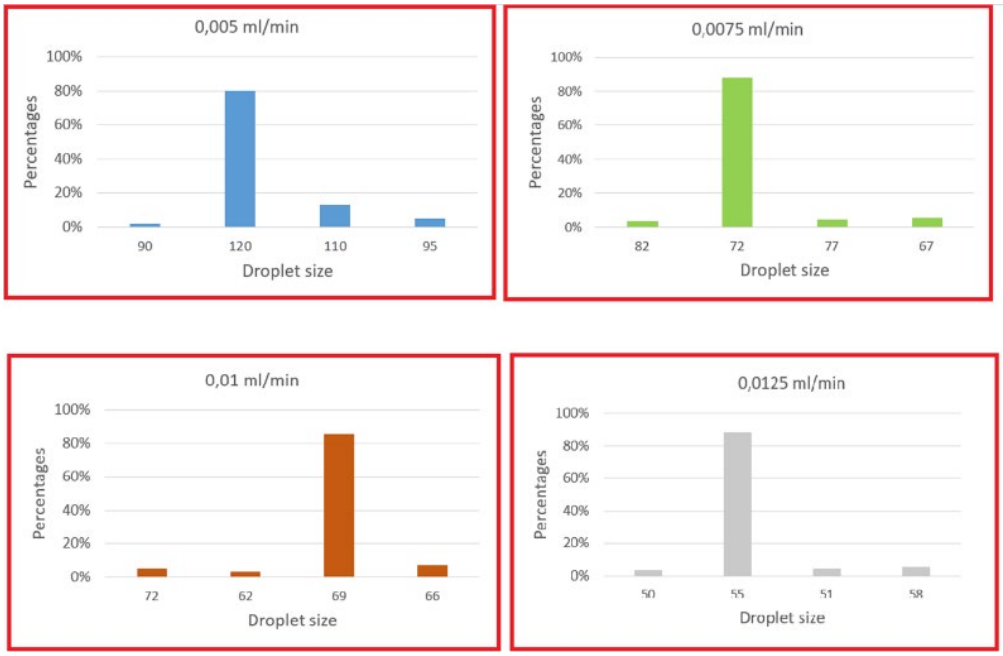
Despite significant progress in the field of microfluidic technology, important scientific and technological issues remain unresolved, such as optimising droplet formation conditions, increasing process productivity and improving the stability of droplet structures [1].

The purpose of this study was to experimentally study the process of droplet formation depending on changes in geometry.

The experimental setup consisted of a microfluidic chip [2], a chip cell, «COLE PALMER» syringe pumps and an inverted optical microscope «Olympus IX-71». An Infinity camera was installed on the optical microscope, which transmitted images and videos in real time to a computer using the Infinity Capture program for further processing.

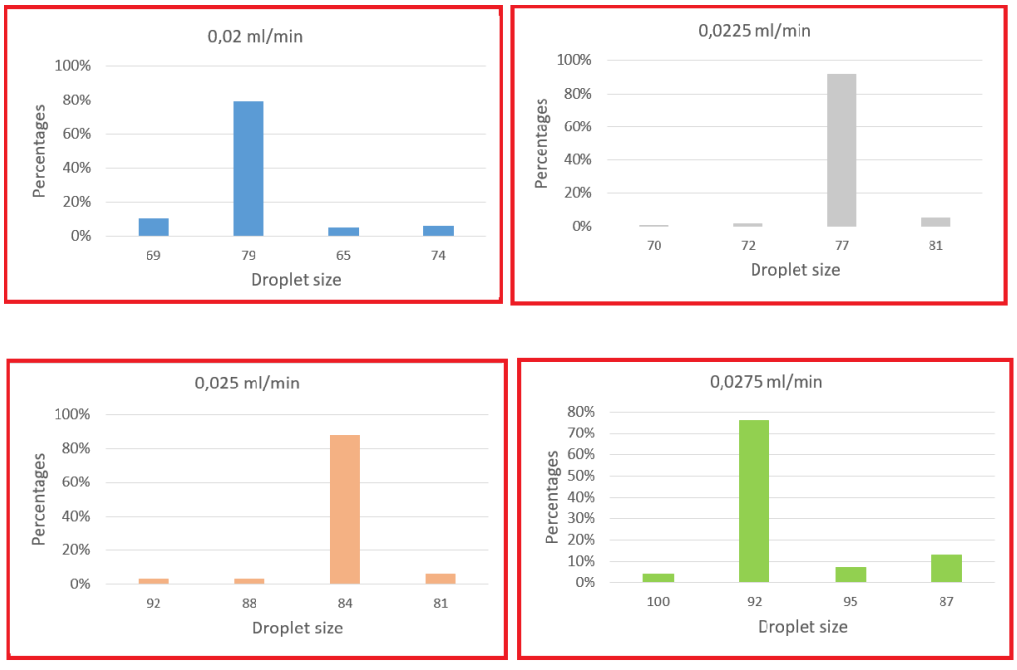
In the first series of experiments, the water consumption remained constant at 0.02 ml/min, and the oil consumption varied from 0.005 to 0.0125 ml/min in

increments of 0.0025 ml/min. In this case, it was possible to achieve the main droplet volume of the entire emulsion in the range from 53 microns to 121 microns.



Graph of emulsion droplet distribution at a constant water flow rate obtained with a syringe pump experimental setup

In the second case, the oil consumption remained constant 0.01 ml/min, and the water consumption varied from 0.02 to 0.0275 ml/min in increments of 0.0025 ml/min. In this case, with an increase in water consumption, the droplet size increased from 75 microns to 92 microns.



Graph of emulsion droplet distribution at a constant oil flow rate obtained with a syringe pump experimental setup

The average deviation of droplets in all cases amounted to 3 μm. During experiments on creating emulsions on microfluidic chips, key factors affecting the stability and uniformity of droplets were identified. The geometry of the chip also had a significant impact on the process. It can also be noted that by regulating oil consumption, it was possible to achieve a much larger range in changing the size of droplets than by regulating water. Accordingly, oil flow control allows you to vary the droplet size over a wider range than changing the water flow.

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Экспериментальные исследования особенностей генерации монодисперсных капель жидкости с помощью микрофлюидного устройства

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Analysis and technology of research in cementing quality control using various acoustic instruments

Acoustic logging is one of the most informative well logging methods, enabling a wide range of applications – from geological section evaluation to well

integrity monitoring. A key role is played by acoustic cement logging, which evaluates isolation quality by measuring cement height, annular fill, and cement bond to casing and rock. As well construction conditions become more geologically and operationally challenging and reliability requirements increase, selecting the optimal equipment and investigation techniques is critical–impacting both data accuracy and cost-effectiveness. The objective of this study is to perform a techno-economic analysis of geophysical investigations using acoustic cement logging and to formulate recommendations for choosing equipment suitable for different operational environments.

In carrying out investigations, a critical stage is the calculation of labor effort and work costs, providing the foundation for developing budget norms and staff payroll. Total labor input comprises several elements and is determined by the formula [1]: $T_{total} = T_t + T_{pfr} + T_{sv} + T_{aux} + T_{to}$, where T_{tr} – travel time; T_{pfr} – preparatory and final work time; T_{sv} – survey time; T_{aux} – auxiliary work time; T_{to} – tripping operations time. Based on a standard geophysical crew trip, the following time was calculated: travel time (accounting for various road classes) – 123.4 min; preparatory and final work at base and well – 112.0 min; actual logging over a 416 m interval – 44.93 min; tripping to 3616 m – 42.67 min; total operation time (labor input) – 343 min. The cost of operations was calculated in the same way, using hourly rates [1]: $C_{total} = C_{tr} + C_{pfr} + C_{sv} + C_{aux} + C_{to}$. The direct cost of the well logging operation, based on unit pricing, was 7362 rubles. However, the total estimate additionally comprises overheads (24.76% of direct costs), planned savings (14%), and data processing/interpretation expenses, which account for 182% of the direct survey costs. Consequently, the full cost of acoustic cement logging operations, covering all related expenditures and interpretation, was 23872.59 rubles based on revised 1990 norms. This amount provides a foundation for budgeting and can be updated to present-day values through indexation.

The contemporary market for geophysical instrumentation provides a broad spectrum of devices for acoustic logging. The main factors in choosing a device

include the casing diameter, the type of logging operation (wireline or drill-pipe conveyed), and the necessary data resolution and equipment reliability. During the analysis, various instrument types were examined, grouped according to their application range based on casing diameter. For small casing diameters (up to 70 mm), the MAK-42 and MAK-42Ts instruments are the best choice, with the selection depending on the conveyance method (wireline or drill pipe). For intermediate casing sizes (70–120 mm), the MAK-4 and MAK-4-SKA instruments are appropriate, ensuring dependable signal acquisition in typical environments. For casing diameters ranging from 120 to 245 mm, the MAK-9M instrument represents the most versatile and up-to-date choice for wireline operations, outperforming earlier models due to its enhanced features and innovative engineering. The MAK-2 tool is suggested as an alternative, provided that the transmitter type is carefully selected to match the particular casing. When working on drill pipes for casings of this diameter, the AKS-AK-80-150/100 system is recommended. Field experience indicates that the AKS system offers greater data integrity (with no flash memory errors) and features a more convenient, user-friendly interface than competing devices such as the "Horizontal" system. The MAGIS-AK system is advised for use in modular assemblies, providing a blend of robustness and simple tuning. The MAK-3 tool was selected for use with large-diameter casings (up to 426 mm), owing to its long-standing reputation as a robust and reliable device for challenging conditions involving large drill pipes. A separate analysis was conducted on instruments that are not part of the core recommendations for routine cement bond logging. The 4AK-T-60-120/80 series instruments and AVAK variants are more focused on applications involving scanning acoustic logging and the diagnostics of horizontal well integrity. Although the MAK-100SK instrument was state-of-the-art when introduced, it has since become outdated. Its role has been effectively taken over by the new MAK-9-SKU device, which is intended for integral-scanning acoustic logging.

Based on the results of the analysis, a number of conclusions can be formulated. The economic efficiency of applying acoustic cement logging consists

not only of the costs of direct measurements, but also of associated expenses (transportation, preparatory and final work, overhead costs, data interpretation), which necessitates careful budget planning. The labor intensity (343 minutes) and total survey cost (23,872.59 rubles) calculated according to the 1990 standards can be used as baseline references when drawing up modern estimates using current conversion factors. The selection of an acoustic tool that matches the specific measurement conditions is of fundamental importance for obtaining reliable results. A selection matrix for equipment has been developed, based on the casing diameter and the method of deployment (wireline or drill pipe). Modern digital systems (AKS, MAGIS-AK) and new tools such as the MAK-9-SKU outperform outdated models in terms of reliability, data quality, and ease of operation. Therefore, a well-founded choice of equipment and correct work standardization contribute to improving the quality of cementing control, which directly affects the long-term reliability and productivity of oil and gas wells.

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Анализ и технология исследования при контроле качества цементирования различными акустическими приборами

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Study of the morphology of a polyalinine derivative film on an aluminium substrate by atomic force microscopy

Electrically conductive polymers, including polyaniline, are an important class of materials that combine the properties of polymers and electrically conductive substances [1].

Atomic force microscopy (AFM) has become one of the key tools for studying the surface of films, allowing for high-resolution imaging [2-3]. This study used a sytall substrate on which a layer of aluminum about 300 nm thick was deposited using thermal evaporation in a vacuum using UVP-250. The same method was used to deposit a layer of polyaniline on an Al substrate. The approximate thickness of this film was about 100-150 nm.

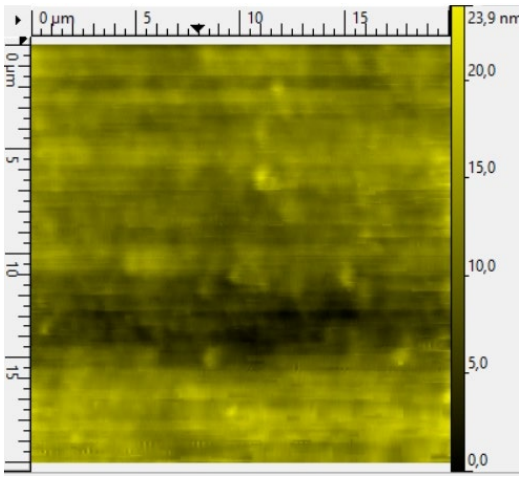

Fig. 1. Surface morphology of polyaniline obtained by atomic force microscopy: 2D image, scale 20x20 µm

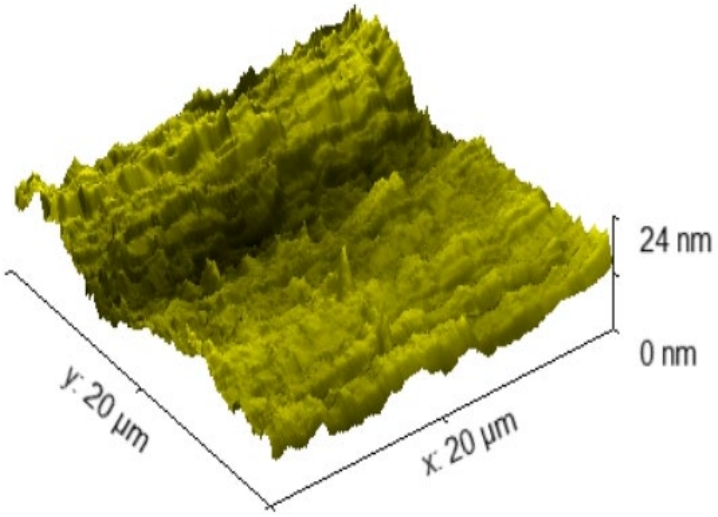

Fig. 2. 3D visualization of the surface topography of polyaniline obtained by atomic force microscopy

The surface morphology of the polyaniline films was analyzed using atomic force microscopy (AFM) in a semi-contact mode. The scanning was performed on a 20×20 μm area, which allowed for the assessment of the coating's uniformity and quality. The two-dimensional and three-dimensional AFM images (Figures 1 and 2) revealed a fine-grained surface structure with no pronounced defects. The root-mean-square roughness (Sq) was about 3.5 nm, the average roughness (Sa) was 2.7 nm, and the maximum peak height (Sp) was 12.4 nm. The slight deviations of the topography from the average plane indicate the formation of a uniform layer.

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Исследование морфологии плёнки производной полиалинина на алюминиевой подложке методом атомно-силовой микроскопии

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Investigation of the nanostructure of the PANI-1.1 polymer film on an aluminium substrate by atomic force microscopy

Conductive polymers, particularly polyaniline (PANI), represent an important class of materials that combine the properties of polymers and electrically conductive substances. (PANI-1.1) is a modification of polyaniline that exhibits unique electrical,

optical, and structural properties, making it a promising material for applications in microelectronics, sensor devices, solar cells, and other nanotechnology fields. In recent years, there has been a growing interest in studying the nanostructure of polyaniline, as the morphology of the material at the nanoscale directly influences its functional characteristics. Atomic force microscopy (AFM) has become one of the key tools for studying the surface of films, allowing for the acquisition of high-resolution images [1, 2].

The study used substrates made of sitall [3, 4], on which an aluminum layer ~350 nm thick was applied by thermal evaporation in a vacuum using an UVP-250. A PANI-1.1 layer ~100 nm thick was applied to the aluminum substrate using the same method.

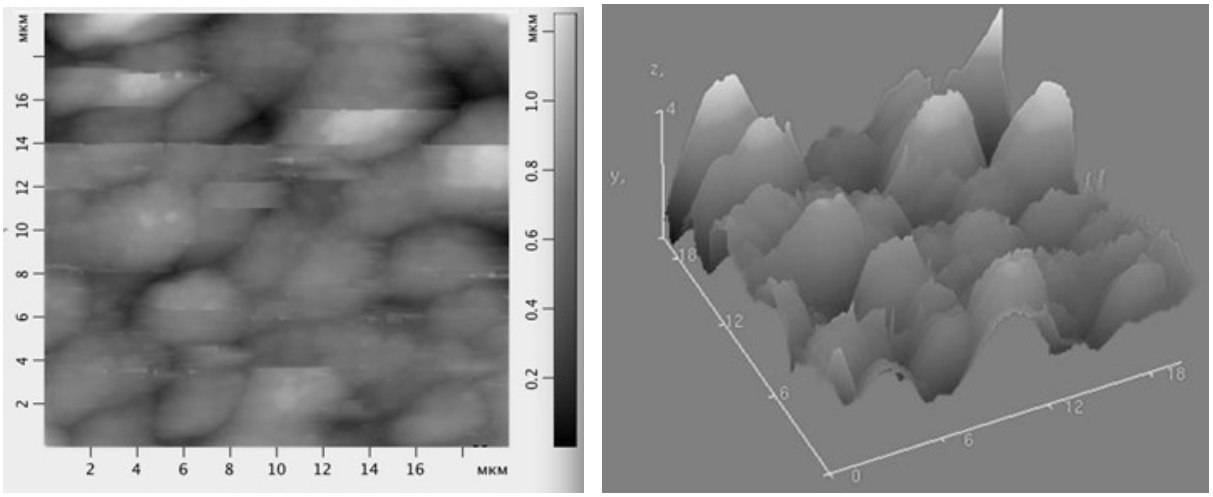

Fig. 1. Topography of the PANI-1.1 surface obtained by atomic force microscopy: a) 2D image (20x20 μm); b) 3D reconstruction of the surface

The surface morphology was studied using atomic force microscopy (AFM) in a semi-contact mode. The scanning was performed in a 20×20 μm area. The obtained 2D and 3D images (Fig. 1) allowed us to assess the surface topography and roughness parameters. The analysis of the AFM images revealed a nanostructured surface of PANI-1.1, consisting of fibrous aggregates and spherical particles with a size of ~5 μm. The structure is characterized by heterogeneity and the presence of local inhomogeneities, which is typical for conductive polymers obtained by vacuum deposition. Due to the fact that we have protrusions that exceed the average profile

height by 200 nm, we take the root-mean-square roughness (Sq), which is equal to 84 nm, while the average roughness (Sa) is equal to 63 nm.

The AFM study in the semi-contact mode revealed a nanostructured surface of the polymer layer, consisting of fibrous aggregates and spherical particles with a size of ~5 μm. The morphology's heterogeneity indicates that the structure is quite complex at the phase boundary. This is a disadvantage for electronics, as the 84 nm roughness makes the film unsuitable for creating reliable circuits. However, in sensorics, this roughness becomes an advantage. The increased contact area with the target agent enhances the sensor's sensitivity.

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Исследование наноструктуры полимерной пленки ПАНИ-1.1 на алюминиевой подложке методом атомно-силовой микроскопии

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Comparative analysis of modern digital training systems for training operators of technological installations

Technological processes are characterized by a high level of complexity and industrial incidents can have serious financial and environmental consequences including loss of life in the oil and gas industry. Effective management of these processes requires highly qualified operators who carried significant responsibility for production management [1].

The need has arisen to develop models of complex technological systems for training and professional development of specialists in various fields with the rapid development of information technology. Consequently, in many countries the use of computer simulators for training operators in the oil and gas production refining and petrochemical industries is becoming a mandatory requirement.

So, the use of training complexes allows us to improve the professional training of technological personnel in the industry, allowing them to obtain valuable practical experience – to develop fundamental skills in working with the control system and acting in emergency situations without putting the real technological process at risk [1].

Despite the spread of simulation systems, the scientific literature deficiency a systematic comparative analysis that would allow for the identification of key trends, advantages and disadvantages of various simulation platforms as well as recommendations for their selection for specific technological processes.

The actuality of this study conditioned by need to analyze existing technical solutions for training process personnel, minimizing the risks of process accidents and improving the quality of specialists in the oil refining industry.

This paper provides a systematic review of modern solutions in the field of training systems for the oil and gas industry. The focus is on solutions registered as patents and software demonstrating their technological innovation and practical implementation.

Table 1 presents the results of the comparative analysis of simulator systems.

Table 1

Comparative analysis of training complexes

№	Main purpose	Key functions	Unique features	Technological processes
1	training of oil refining specialists	- formation and visualization of the calculation scheme of the UCPN; - simulation modeling of technological objects [2].	the possibility of partial oil refining at the field	complex oil treatment unit
2	training on the ELOU-AVT unit	- modeling of typical technological processes of primary oil refining; - testing of starting, stopping and localization of emergency situations; - working in the RSU operator interface [3].	full compliance with the block structure of the ELOU-AVT installation	primary oil refining at the ELOU-AVT installation
3	design and modernization of existing production facilities	- database of pure substances; - material and heat balance of technological schemes; - dynamic calculation of hydraulic systems; - modeling of ejector systems and supersonic separation systems [4].	accounting for dynamic flow modes in pipelines	integrated modeling of complex process installations

A classification of training systems was proposed within which three main categories were identified who based on the comparative analysis:

1. Specialized simulators characterized by in-depth development of specific process installations.

2. Universal platforms capable of simulating various technological processes and integrating with control systems. Their key advantage is flexibility.

3. Simulators for solving applied engineering problems combine training functions with engineering calculations and design capabilities making them a

valuable tool not only for personnel training but also for optimizing technological processes.

So, the study confirms that modern simulator systems have become an integral part of operator training in the oil and gas industry. The analysis showed that these systems are rapidly evolving with solutions emerging for both highly specialized installations and universal platforms capable of simulating various technological processes. Further improvements to simulator systems will directly contribute to improved safety.

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Сравнительный анализ современных цифровых тренажеров для подготовки операторов технологических установок

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Investigation of the propeties of biological materials using a scanning probe microscope

Scanning probe microscopy (SPM) is a method for studying the morphology and local properties of a solid surface with high spatial resolution.

The study of biological objects using SPM is important for studying the structure and functions of living systems [1, pp. 391-392].

Before starting the study, it is important to choose the right method of biomolecule immobilization. Non-covalent immobilization is based on a set of weak intermolecular interactions [2, p. 113].

Covalent immobilization involves the formation of strong chemical bonds between molecules and the substrate surface. This method ensures the fixation of the sample and resistance to external influences [2, p. 114].Therefore, the object retainer for SPM should be atomically dense, hydrophilic, multifunctional and should not adversely affect the probe scanning. This set of requirements significantly limits the choice of materials.

The most important aspect for studying the structural and functional relationships of biological objects is obtaining high-resolution images with a high signal-to-noise ratio to determine the parameters of a molecule with sufficient accuracy.

The purpose of the work was to study the theory of properties of biological objects using SPM.

After studying the literature, it was decided to choose one of the types of oligonucleotides as the object of research. These are molecules that consist of sequences of nucleotides of only one type (adenine, thymine, guanine, or cytosine).

Oligonucleotides provide the flow of current through the sequences of compounds. Therefore the oligonucleotide dT_{12} was selected.

Before starting the practical part of the experiment, we have examined a fragment of the dT_{12} molecule and modeled in the MolView program.

Fig. 1. The model of the molecule dT_{12}

In the Fig. 1 we can see thymine – nitrogenous bases with a single-ring structure, disoxeriboses and phosphate groups.

After working with the theoretical materials, it is planned to use a scanning probe microscope for a practical experiment.

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Исследование электрических свойств биологических материалов с помощью сканирующего зондового микроскопа

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Features of helimagnon dynamics in a frustrated magnetoelectric model

The study of competing exchange mechanisms in spin systems is now among the key problems in condensed matter physics. When exchange interactions begin to compete with each other, the so-called frustration often arises, which dramatically alters the properties of the model [1]. Such frustrated systems behave quite differently from their non‑frustrated counterparts, and it is precisely this fact that makes their analysis especially valuable for understanding complex magnetic phenomena [2].

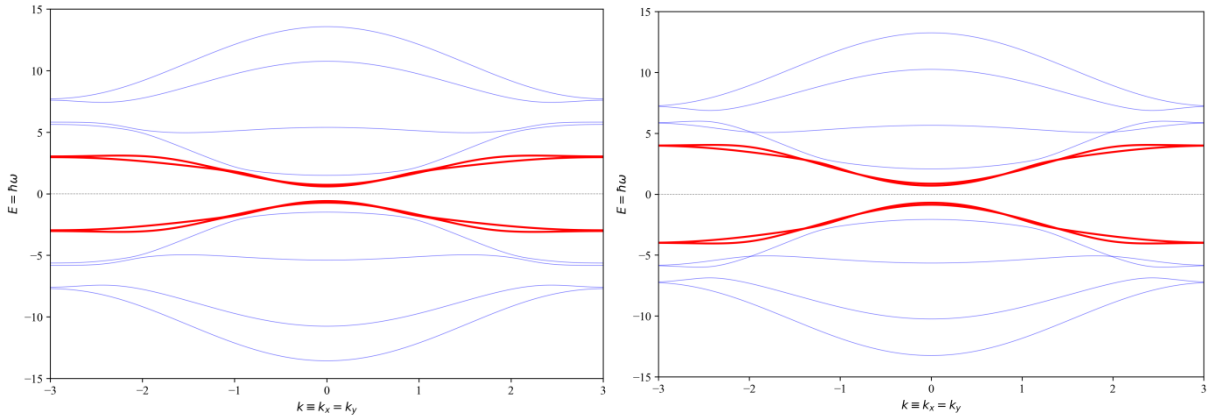
Among such systems, conducting helimagnets – characterized by a spiral ordering of magnetic moments – deserve special attention. Obtaining the spectrum of helimagnons in these systems is not straightforward because the periodic spiral structure acts as an effective potential and is precisely what governs the formation of the spectrum [3].

As for the Heisenberg model, where frustration originates from the competition between exchange channels, much still remains unclear. If, for example, one includes antiferromagnetic exchange between second‑nearest neighbours in the classical version, the ground state of the system becomes degenerate, which seriously complicates its description. Such degeneracy can lead to the formation of a variety of magnetic configurations. Further progress here requires new theoretical approaches – both numerical methods and analytical ones.

This work studies a model of thin films with a body-centred cubic (BCC) lattice, which consists of six magnetic layers and two ferroelectric layers (top and bottom). In this model, spiral order develops along the z-axis, which is directed perpendicular to the film surface.

For a helically ordered structure to exist in a BCC lattice, the condition $|J_2| \geq J_1$ must be satisfied. To determine the classical spin configuration of the ground state at the surface, we analysed the expression for the spin energy along the z-axis. The problem was solved iteratively.

Using the obtained ground-state configuration, we calculated the spin-wave spectrum by means of the two-time temperature Green's function method. The dispersion equation was derived after diagonalising the matrix, which made it possible to compute the frequencies of the spin modes for each pair of wave numbers (see Fig. 1).



(а) (б)

Fig. 1. Spin waves with the parameter $J_2/J_1 = -1.4$ *for: (a)* $J_{mf} = 0.0$*, (b)* $J_{mf} = -0.5$*. The surface spin-wave modes are highlighted in red.*

Comparing the first panel ($J_{mf} = 0.0$) with the last one ($J_{mf} = -0.5$) at a fixed ratio $J_2/J_1 = -1.4$, one observes a qualitative change in the spin dynamics. An increase in the magnetoelectric interaction leads to larger spin deviation angles inside the magnetic layer – the non-collinearity becomes more pronounced. At the same time, the spin-wave dispersion increases, indicating growing spatial inhomogeneity, and the critical temperature decreases.

The work was carried out within the framework of the state assignment agreement No. 075-03-2024-123/1 dated 02/15/2024 topic No. 324-21.

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Особенности динамики гелимагнонов в фрустрированной магнитоэлектрической модели

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Synthesis of quercetin complexes with apple pectin and their antioxidant activity

Low solubility of quercetin in liquids produced by the human body at the physiological pH level limits its bioavailability. Binding of flavonoids to polysaccharides allows you to overcome this limitation and increase the degree of absorption of the substance by the body.

The way in which flavonoids and polysaccharides are connected to each other in plant tissues (through ionic interactions, hydrogen bridges, or hydrophobic contacts) depends directly on their molecular structure. Once they enter the gastrointestinal tract, these substances dissociate from their original associations, making the antioxidants easier to absorb and improving the health of the intestinal microbiome.

The work had two main objectives: the first - to synthesize quercetin complexes with apple pectin, and the second - to study how these complexes exhibit antioxidant activity towards Fe^{2+}/Fe^{3+}.

The process of complex formation is implemented according to the methodology described in previous works. [1]. Equal volumes of an aqueous alcohol solution of quercetin with a concentration of 1.66 - 15.00 mmol/ml and an equal volume of a 1.5% suspension of polysaccharide were drained in a buffer solution with a pH of 6.86. Sorption was carried out at room temperature, stirring for half an hour under normal conditions or 10-15 minutes under ultrasound irradiation in an ultrasonic bath. Then the suspension was filtered or centrifuged and the residual concentration of quercetin was determined in the solution.

The value of adsorption (A, mmol/d) was calculated according to the formula and constructed an experimental isotherm (Fig.1):

$$\mathbf{A = (C_0 - C_P)V/m}$$, where

C_0 - the initial concentration of quercetin in solution, mmol/ml;

C_p - the concentration of quercetin in the studied solutions after adsorption, mmol/ml;

V- the volume of the flask for the test solution, ml;

m - the mass of the sorbent taken for analysis, g.

The shapes of the adsorption curves have the form of classical Langmuir isotherms, with access to a plateau characterizing the adsorption limit. This shows a monomolecular process that combines physical adsorption with chemisorption elements.

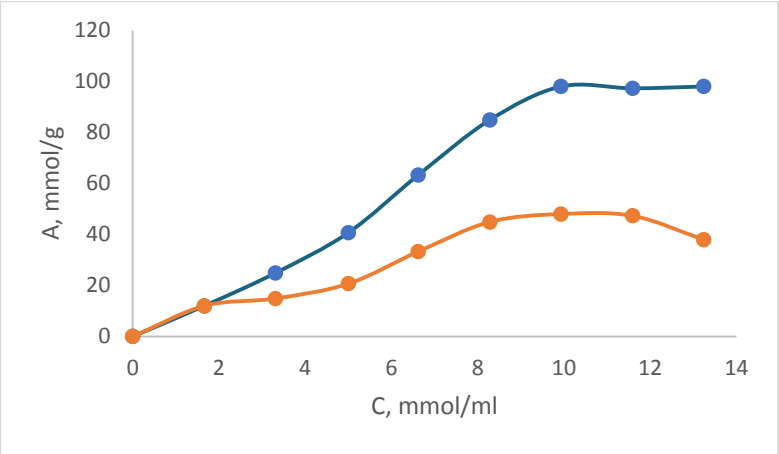

Fig. 1. Isotherms of quercetin adsorption on apple pectin at pH 6.86 under normal conditions and under ultrasound irradiation (blue - apple pectin +quercetin using ultrasound, red - apple pectin +quercetin without ultrasound)

The isolated complexes were studied using UV and IR spectroscopy. The presence of a bathochromic shift of the maximum absorption in UV spectra, shifting to the range of λ~380-400 nm for systems containing pectin, is reliable to experimental evidence of the formation of the corresponding complexes. Only quercetin has a λ max of 315 nm. In the IR spectra of the obtained complexes, a broad absorption band is observed in the range of 3500–3100 cm^{-1}, corresponding to the valence vibrations of hydroxyl groups (both polysaccharide and phenolic), with a main maximum at 3250–3260 cm^{-1}. In addition, the carbonyl group of ring A shifts to 1640 cm^{-1} in the quercetin spectrum, and a band at 1610 cm^{-1} characteristic of the chromone cycle appears.

The study of the reducing capacity of quercetin and its complexes was conducted using the ferricyanide method (Oyazu method) and by observing the interaction of Fe(III) salt with o-phenanthroline. (Table 1).

Table 1

Values of antioxidant activity of complexes with quercetin

	antioxidant activity according to the Oyazu method	antioxidant activity according to the FRAP method
Quercetin	0.125	0.003
Quercetin+pectin	0.429	0.006

As you see from the table, the quercetin-pectin complex has increased reducing activity. Given its good water solubility, it is also promising for use in pharmacology.

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Синтез комплексов кверцетина с яблочным пектином и их антиоксидантная активность

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The effect of ionotropic gelation on the sorption properties of wound-healing polysaccharide matrices

The polymer matrices of succynil-chitosan (SC) were prepared by freeze-drying aqueous solutions of polymers with various compositions. The samples were first frozen at -85°C for 3.5 hours, then freeze-dried at a pressure of 0.1 Pa for 40 hours, followed by drying to constant weight in an oven. The relative amount of water (m_t) absorbed by the matrix at specified time was determined by the gravimetric method, by keeping the samples in a desiccator in water vapor for a specified time (t), and calculated using the formula:

$$m_t = \frac{\Delta m_t}{m_0} * 100\%,$$

where m_0 is the initial mass of the polymer in the matrix, and Δm_t is the difference between the mass of the matrix at specified time and the initial mass of the polymer in the sample.

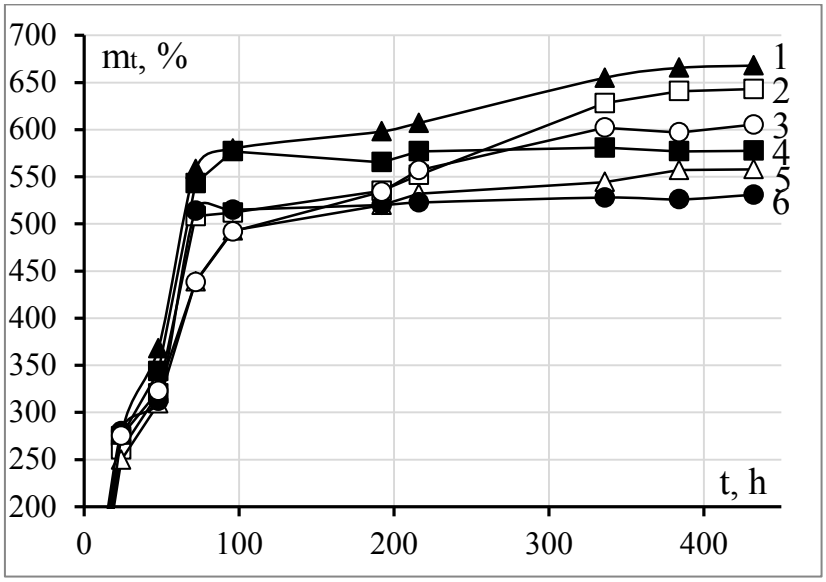

Fig. 1. Degree of sorption of polymer matrixes prepared from solutions of various compositions as a function of sorption time (wt%): 3% SC, 3% glycerin, 0.25% $ZnSO_4$ (1); 3% SC, 1% glycerin, 0.25% $ZnSO_4$ (2); 3% SC, 0.25% $ZnSO_4$ (3); 3% SC, 1% glycerin, (4); 3% SC, 3% glycerin, 0.5% $ZnSO_4$ (5); 3% SC (6)

Analysis of the effect of the composition of polymer blends on the sorption properties of the resulting materials (Fig. 1) shows that these materials are characterized by limited swelling and an ability to reach an equilibrium sorption degree. Glycerin increases the equilibrium sorption degree of the material (curves 4, 6), presumably due to its cryoprotective properties. At the same time, the addition of polyvalent metal salts ($ZnSO_4$) to the initial solution increases the time required to reach the equilibrium sorption degree (curves 1, 2, 3, 5) and increases the equilibrium sorption degree itself (curves 2 and 4; 3 and 6), which may indicate an increase in the material's porosity. This may be due to the onset of ionotropic gelation in the system: the strength of the intermolecular network of cross-links increases due to the formation of additional bonds, which reduces the intensity of pore collapse during the freeze-drying stage. It is noteworthy that a further increase in the $ZnSO_4$ content in

the solution greatly reduces the equilibrium sorption degree (curves 1, 5), which may be due to a deterioration in the thermodynamic quality of the solvent and a change in the conformational-supramolecular state of the polyelectrolyte in the presence of an excess of the foreign electrolyte.

Thus, we have demonstrated the possibility of controlling the sorption properties of materials based on the sodium salt of N-succinylchitosan by creating an ionotropic gelation effect and by varying the quantitative content of components in the mixture.

Влияние ионотропного гелеобразования на сорбционные свойства ранозаживляющих полисахаридных матриксов

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Physical and mechanical properties of polymer phosphor materials

Polymers with phosphors of various compositions are actively used in industry and science. Their value is in their ability to absorb ultraviolet light and emit narrow-band light. For practical use, such materials must be durable, resistant to UV radiation, oxidation, and retain their luminescent properties for a long time.

An urgent practical task is the development of luminescent materials characterized by a long and intense decay, as well as the ability to maintain

operational capability in atmospheric conditions for a long period. Polyvinyl chloride (PVC) was chosen by us as the polymer matrix. Special additives have been introduced to ensure the transparency of the material. In the working process samples of phosphor composites of various types based on plasticized strontium aluminate PVC doped with europium and dysprosium oxides were obtained. When producing PVC materials, the concentration of plasticizer in the composition and the brand of phosphor used was varied.

The mechanical properties of polymer materials under tension were determined using an AGS-10kNX universal testing machine (Shimadzu, Japan) in accordance with GOST 34370-2017. Type 1A samples obtained from plates were used.

According to the tests, the following physical and mechanical characteristics of PVC materials were determined: modulus of elasticity, tensile strength, elongation at tearing.

The test results showed that the values of the physical and mechanical parameters of the obtained PVC samples are in the following range: modulus of elasticity from 5 to 47 N/mm2; tensile strength from 9 to 13 N/mm2; elongation at tearing from 116 to 1000%. Thus, the properties of PVC compounds directly depend on the composition of the plasticizer. An increase in its concentration leads to a decrease in strength and modulus of elasticity, while increasing elongation at tearing.

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Физико-механические свойства полимерных люминофорных материалов

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Quantum chemical modeling of the structure of chelated multi-ligand phenyl-containing N,O transition metal complexes

Based on the data obtained using quantum chemical modeling, we analysed the structural of chelated amino acid different-ligand complexes of late 3d elements (Co(II), Cu(II), Ni(II), Zn(II)) with four amino acids [1-2] – S-AlaH, GlyH, S-PheH, and S-ValH with the general formula [M(S-Phe)(S-L)], where L is S-Ala(1), S-Phe (2), Gly (3), and S-Val (4).

Patterns have been established in the implementation of the structure of complexes between metals, as well as patterns in the appearance of the conformation "bathtub" or "chair" [2]. Such an implementation of the structure can be related to three main factors that arise in an optically active carbon atom: tetrahedral geometry, the absolute configuration of the chiral center (R,S) of the ligand, as well as the spatial arrangement of the ligands relative to the complex framework, which manifests itself in the axial or equatorial position of the substituent in the amino acid [2].

It is known that during the formation of chelated amino acid complexes of transition metals, metal ions bind to ligands by N,O chelation, forming two five-membered cycles [3-5].

It was found that metal ions exhibiting coordination numbers 4 (Cu(II)) or 6 (Co(II), Ni(II)) during complexation with N,O-ligands form a planar-square or octahedral structure, respectively. At the same time, the plane formed by the chelate rings has some distortions. This distortion is typical for both cis and trans isomers (Fig. 1-3).

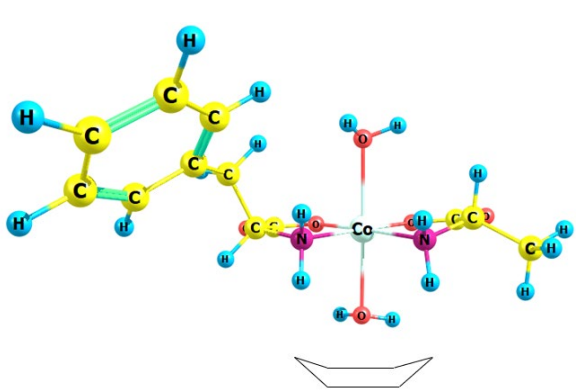

Fig. 1a
$CoC_{12}N_2H_{16}O_4{*}2H_2O$
cis-S-Phe(A)-S-Ala(E)
«bathtub»

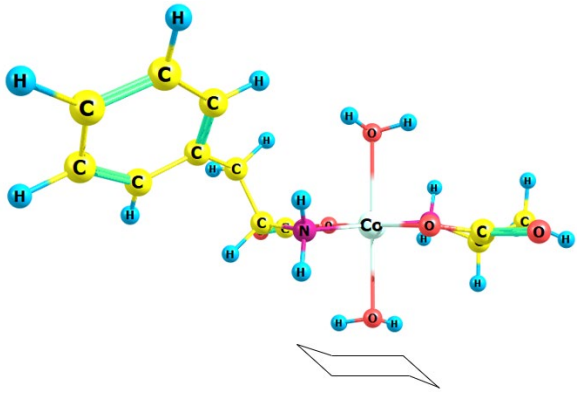

Fig. 1b
$CoC_{12}N_2H_{16}O_4{*}2H_2O$
Trans–S-Phe(A)-S-Ala(E)
«chair»

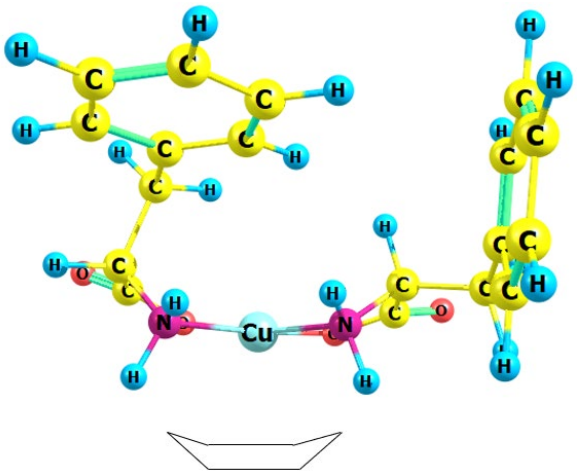

Fig. 2a
$CuC_{18}N_2H_{20}O_4$
cis-S-Phe(A)-*S*-Phe(E)
«bathtub»

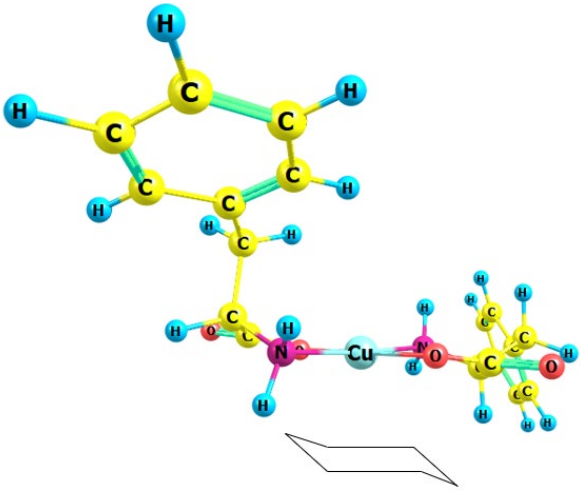

Fig. 2b
$CuC_{18}N_2H_{20}O_4$
trans-S-Phe(A)-*S*-Phe-(E)
«chair»

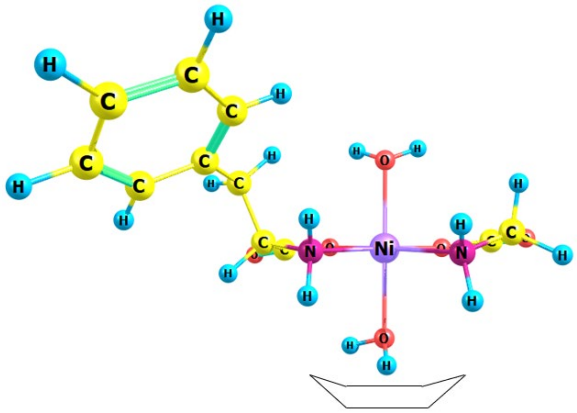

Fig. 3a
$NiC_{11}N_2H_{14}O_4{*}2H_2O$
cis-S-Phe(A)-Gly
«bathtub»

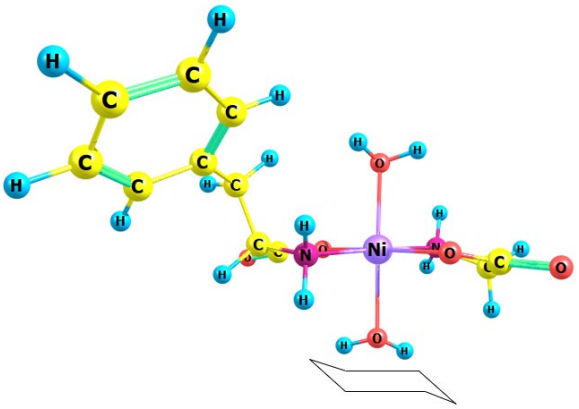

Fig. 3b
$NiC_{11}N_2H_{14}O_4{*}2H_2O$
trans-S-Phe(A)-Gly
«chair»

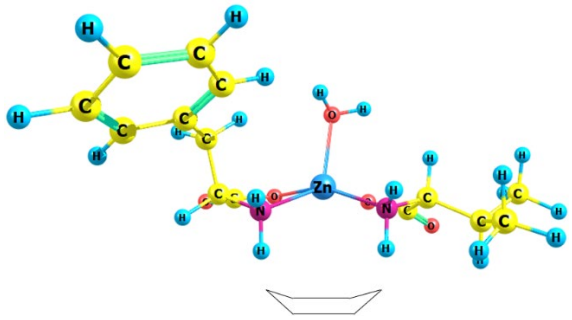

Fig. 4a
$ZnC_{14}N_2H_{20}O_4{*}H_2O$
cis-S-Phe(A)-(S)-Val(E)
«bathtub»

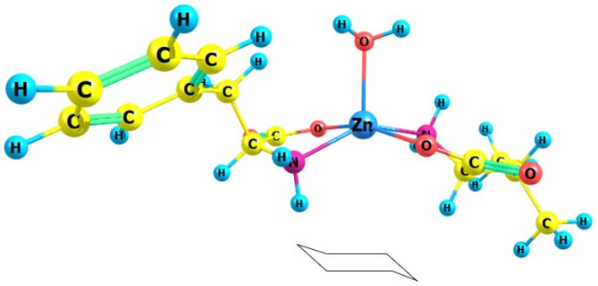

Fig. 4b
$ZnC_{14}N_2H_{20}O_4{*}H_2O$
trans–S-Phe(A)-S-Val(E)
«chair»

In the case when the coordination number of the metal is equal to 5 (Zn(II)), the framework of the molecule is quite strongly distorted. In this case, the degree of distortion of the structure is determined by both the cis- and trans-isomerism of the resulting complex (Fig. 4) and the absolute configuration of the chiral center of the ligand.

Thus, it can be seen from the figures that the distortion of the structure of the resulting complex by the general formula [M(S-Phe)(S-L)] is determined by the coordination number of the metal ion and the absolute confirmation of the chiral center of the ligand. In this regard, chelated S-S-amino acid complexes Ni(II) and Co(II) have a slight distortion of the structure from the ideal octahedron, which is caused by the influence of ligands in the axial position of the complex (water molecules). Cu(II) complexes are slightly distorted in the cis configuration, while in the trans configuration they tend to form a regular flat square; and the Zn(II) complexes, due to the odd coordination number and, consequently, the unequal influence of ligands, are strongly distorted and represent a pyramid, which is more strongly distorted for trans isomers than for cis isomers.

For complexes with the general formula [M(S-Phe)(R-L) the conformation of the resulting molecules will be opposite to the [M(S-Phe)(S-L)] complexes due to the inversion of the chiral center of the ligand.

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Квантовохимическое моделирование структуры хелатных разнолигандных фенилсодержащих N, O-комплексов переходных металлов

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Clarification of the parameters of HYSYS isomerization processes of the pentanehexane fraction by quantum chemical methods

The pentane-hexane isomerization process is a key process in the production of high-octane, environmentally friendly components of commercial gasoline. Effective

management of this process is impossible without the use of precise mathematical models. Aspen Hysys, an industry standard, is widely used for modeling and optimizing isomerization units. However, the accuracy of modeling in Hysys directly depends on the reliability of the input thermodynamic and kinetic parameters, which are often determined on the basis of empirical correlations and can have significant errors [1, 2]. Modern quantum chemistry methods, particularly density functional theory (DFT), provide tools for calculating molecular properties and reaction mechanisms at a fundamental level. This allows for independent and reliable data on the enthalpy of formation, entropy, activation energies, and pre-exponential factors for the isomerization reactions of n-pentane and n-hexane [3].

The aim of this study is to substantiate an approach to improving the adequacy of modeling the PHF isomerization process in Aspen Hysys by refining its key parameters based on the results of quantum chemical calculations. Fundamental aspects of PHF isomerization over bifunctional catalysts were analyzed, and key reactions and factors influencing the equilibrium and rate of the process were identified [4]. Shortcomings of existing modeling approaches in Aspen Hysys, related to simplified descriptions of reaction mechanisms and the lack of tools for automatic parameter calibration based on theoretical data, have been identified [5]. It has been shown that the use of quantum chemistry (DFT) methods allows for the highly accurate calculation of missing thermodynamic properties of isomers and reaction activation barriers, or the refinement of existing ones, thereby creating a basis for the verification and calibration of Hysys models.

Thus, integrating quantum chemical calculation data into the Aspen Hysys environment is a promising approach, enabling the transition from empirical parameter selection to modeling based on fundamental laws. Further research in this area, including the development of automated data transfer methods and the validation of refined models using experimental data, will contribute to improved forecasting accuracy, process optimization, and, consequently, increased economic efficiency of the isomerization process.

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Уточнение параметров HYSYS процессов изомеризации пентан-гексановой фракции методами квантовой химии

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Multisensory system based on composite sensors for identification of mineral water by brand

Electronic tongue [1] has found wide application in the field of pharmaceutical identification [2–4]. Identification accuracy is achieved by producing an image of the studied samples and comparing the obtained image with the analyzed object. This method allows for the consideration of both electroactive and non-electroactive components of a mixture, which opens up the opportunity for the wide application of such systems in different areas for product quality control. In the course of the current study, a multisensory system was developed for identifying mineral waters by brand.

Cross-sensitivity is a key property of the system, without which the analysis of multicomponent mixtures would be impossible. Therefore, to achieve cross-sensitivity, a multisensory system based on modified glassy carbon electrodes was used. The modifiers are composites consisting of a polyelectrolyte complex and gold and carbon nanoparticles [5]. Thus, the multisensory system consists of three working electrodes: GCE/PEC@SWCNT, GCE/PEC@rGO, and GCE/PEC@AuNPs.

The PCA model and SIMCA-classification were based on 11 mineral waters differing in total mineralization and chemical composition: Лысогорская, Donat, Ессентуки № 17, Ессентуки № 4, STELMAS, Borjomi, Gorji, Рычал-су, Мензелинская, Нарзан, Красноусольская. The obtained score plots of the MGK model are shown in Figure 1. A clear separation into clusters corresponding to the mineral waters is observed. Clusters of mineral waters with similar compositions were grouped into separate groups: waters with low mineralization and high sulfate ion concentrations were located in the lower right part of the plot (Menzelinskaya, Narzan, Krasnousolskaya). Also, it is important to note the pattern of clusters'

location: clusters of mineral waters with low mineralization are located on the right side of the score plots, and those with higher mineralization on the left; thus, PC1 is associated with overall mineralization; Clusters of mineral waters with higher concentrations of sulfate ions are located in the lower part of the score plot, while those with lower concentrations are in the upper part; thus, PC2 is associated with sulfate ion concentration; along the diagonal vectors, the clusters of mineral waters are positioned according to changes in the concentration of hydrocarbonate ions and sodium and potassium ions. The SIMCA-classification demonstrates effective identification of mineral water samples by brand – Type I and II errors do not exceed 13.3% (Table 1).

The effectiveness of mineral water sample identification is confirmed by the results of PCA modeling and SIMCA-classification. The location of clusters on the score plot corresponds to the compositions of the mineral waters under study and follows clear patterns, while the error rate in identification using the SIMCA method is minimal. Thus, the developed system is able to identify mineral waters by brand, thereby providing an opportunity for effective quality control.

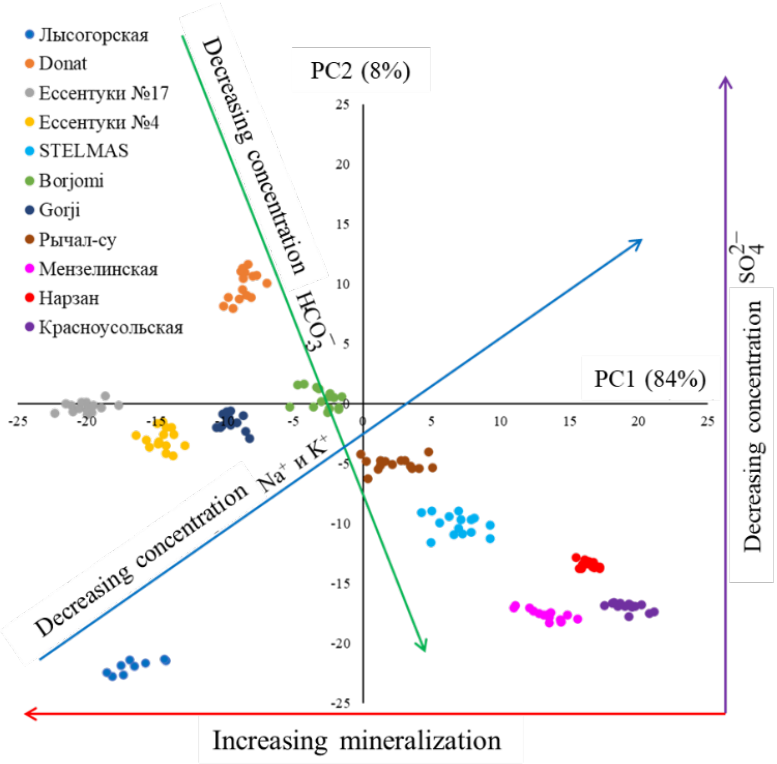

Fig. 1. Score plots of PCA model of mineral waters on a multisensory system

Table 1

Results of SIMCA-classification of mineral waters of various brands on a multisensory system

RS* / TS**	Лысогорская	Donat	Ессентуки №17	Ессентуки №4	Стэлмас	Боржоми	Gorji	Рычал-су	Мензелинская	Нарзан	Красноусольская
Лысогорская	100				13.3			13.3			
Donat		86.7									
Ессентуки №17			100	13.3							
Ессентуки №4				100							
Стэлмас	13.3				100		13.3				
Боржоми						100					
Gorji							100	13.3			
Рычал-су							13.3	100			
Мензелинская									86.7		13.3
Нарзан										100	
Красноусольская										13.3	86.7

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Мультисенсорная система на основе композитных сенсоров для идентификации минеральных вод по производителю

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Methods for Modification of Pectin Films

Currently, the development and refinement of innovative film dressings for the treatment of different wounds have received considerable attention in medicine. There are many reasons for the rising interest in wound dressings, including increasing global military activities, the rapid growth of antibiotic-resistant bacteria, the demand for biocompatible and environmentally friendly materials, and the fast progress of personalized medicine. An ideal modern wound dressing should meet all

of the following requirements at once: it must be fully biocompatible to avoid triggering immune responses, biodegradable so it doesn't need to be removed, bacteriostatic or antimicrobial to prevent infections, able to maintain appropriate moisture for optimal healing, and highly permeable to vapors and gases to ensure proper oxygenation of the wound.

Among the many materials used to create such dressings, natural biopolymers like pectin and chitosan succinate stand out for their unique properties First, like many other polymers, they are characterized by biological activity. Second, they contain functional groups that allow the immobilization of biologically active compounds. Such properties make it possible to create sophisticated formulations that can deliver targeted therapy and release drugs in a controlled way. In this regard, such films can be very helpful in the treatment of wounds by accelerating the healing process due to the constant presence of active components in the wound environment.

At the same time, however, there are several intrinsic limitations of the films made from pectin and chitosan succinate. They include low mechanical strength, sensitivity to moisture causing swelling or destruction, lack of accuracy in controlling the release rate of the embedded drugs, and inadequate properties that cannot provide an effective barrier to microorganisms while ensuring proper permeability to gases.

One of the effective ways to overcome the aforementioned problems is the use of copolymer matrices. In particular, they enable the following:

1. Increased mechanical stability is provided by the combination of the molecular structures of pectin and chitosan succinate, making it possible to produce films that do not tear, stretch, or otherwise break during application.
2. Moisture absorption is optimized to prevent overhydration that may interfere with the process of tissue regeneration and underhydration that can irritate the wound area or negatively affect the integrity of the film.
3. Controlled delivery and sustained release allow one to accurately regulate the dosage and timing of substance delivery, thus guaranteeing constant exposure of the

wound to therapeutic agents. As a result, the healing process can be accelerated and the dressing can be changed less frequently.

4. Effective barriers to bacteria combined with permeability to gases provide excellent protection from infections while allowing cells in the wounded area to breathe.

In summary, the development of films based on copolymers of pectin and chitosan succinate is a promising direction in the biomedical industry. They combine such qualities as biocompatibility, increased stability, and improved functionality that allows addressing most of the issues related to wound dressings. Therefore, copolymer films can prove useful in the treatment of a wide range of wounds caused by various factors.

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Методы модификации пектиновых плёнок

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Molekulardynamische Bewertung der energetischen Stabilität des physikalischen Netzwerks in Polyvinylalkohol-Lösungen

Stabilität der Betriebs- und Transporteigenschaften von Polymermaterialien auf Polyvinylalkohol-Basis (PVA) wird durch die Architektur des Systems nicht-kovalenter Wechselwirkungen bestimmt. In wässrigen PVA-Lösungen wird die Bildung eines fluktuierenden Verhakungsnetzwerks durch die Konkurrenz zwischen Hydratationsprozessen der Makromoleküle und der Ausbildung intermolekularer Wasserstoffbrückenbindungen begleitet. Traditionelle Analysemethoden erlauben es nicht, den energetischen Beitrag einzelner Komponenten zur Stabilisierung der Knotenpunkte eines solchen Netzwerks vollständig zu bewerten [1-3]. In der vorliegenden Arbeit wurde mittels vollatomistischer Molekulardynamik-Simulation die Dichte der elektrostatischen Wechselwirkungen sowie das energetische Profil der Systeme im optimalen Konzentrationsbereich von 8–13 Gew.-% untersucht. Die Studie zielt darauf ab, thermodynamische Faktoren zu identifizieren, die die strukturelle Umordnung der Lösungen beim Übergang in den Zustand eines ausgebildeten Netzwerks physikalischer Knotenpunkte determinieren.

Die Analyse der energetischen Profile der Systeme im Gleichgewichtszustand ergab eine qualitative Transformation der Struktur nicht-kovalenter Wechselwirkungen. Es wurde festgestellt, dass mit steigender PVA-Konzentration von 8% auf 13% der Absolutwert der elektrostatischen Energie erwartungsgemäß von $-1{,}61 \cdot 10^4$ auf $-1{,}04 \cdot 10^4$ kcal/mol sinkt, was auf die verringerte Anzahl an Lösungsmittelmolekülen im Simulationsvolumen zurückzuführen ist. Die Berechnung der spezifischen Energiedichte pro Volumeneinheit der Zelle zeigte jedoch einen umgekehrten Trend: einen Anstieg des Wertes von 0,43 auf

0,47 kcal/mol $Å^{-3}$. Trotz der scheinbar geringen Differenz ist dieser Zuwachs um 9,3 % physikalisch signifikant, da er vor dem Hintergrund eines erheblichen Lösungsmitteldefizits im System (Verringerung der Wassermoleküle um 40%) erfolgt. Dies deutet darauf hin, dass die Abnahme der Hydratationsenergie vollständig durch die Bildung stärkerer intermolekularer PVA-PVA-Kontakte kompensiert wird. Die visuelle Analyse bestätigt die Ausbildung eines kontinuierlichen Gerüsts aus intermolekularen Kontakten (physikalischen Knotenpunkten) bei 13 Gew.-% (Abb. 1).

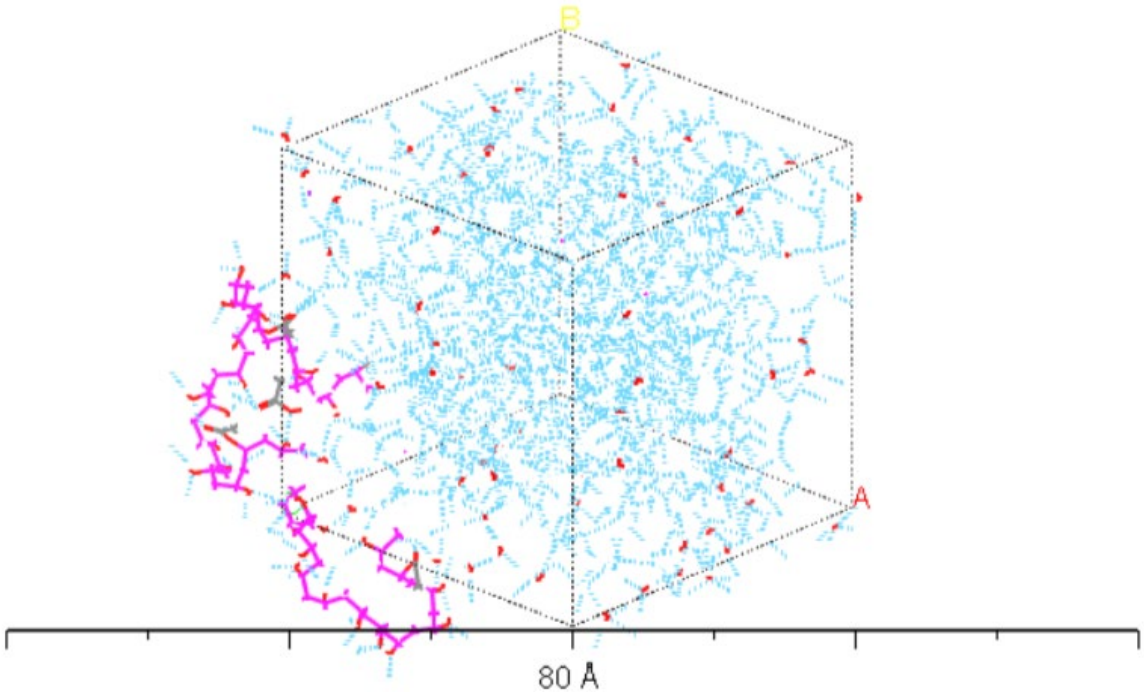

Abbildung 1. Visualisierung des Netzwerks physikalischer Knotenpunkte (Wasserstoffbrückenbindungen) im Modell einer 13 Gew.-%igen PVA-Lösung

Somit ist im 13% System ein Effekt der Energielokalisierung in den Netzwerkknoten zu beobachten, was zu einer qualitativen Strukturverfestigung führt und zusätzliche Energiebarrieren für die Ionenmigration schafft.

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Молекулярно-динамическая оценка энергетической стабильности физической сетки узлов в растворах поливинилового спирта

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Molekulardynamische Untersuchung zum Einfluss der Verhakungsnetzdichte auf die Topologie von Transportkanälen in Polyvinylalkohol-Spinnlösungen

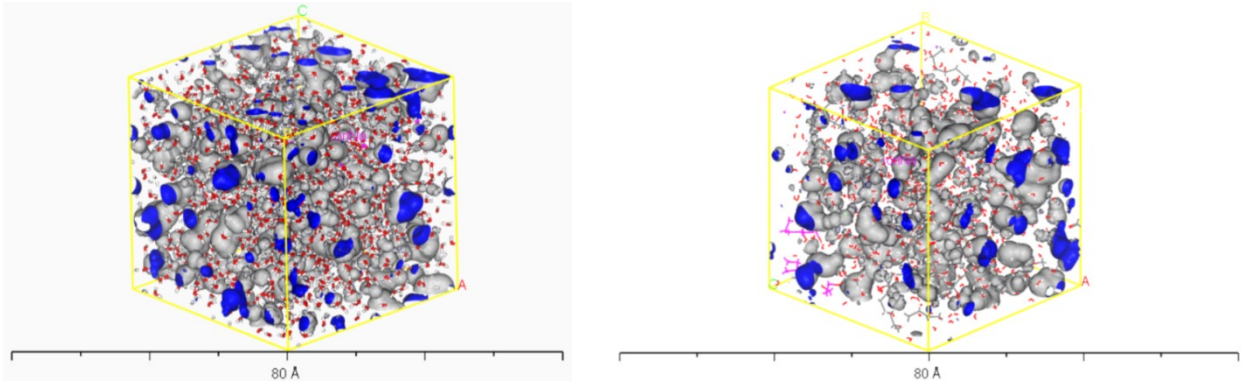
Die Entwicklung biomedizinischer Nanomaterialien mittels Elektrospinning erfordert eine präzise Kontrolle der rheologischen und elektrophysikalischen Parameter der Ausgangslösungen. Polyvinylalkohol (PVA) gehört zu den vielversprechendsten Polymeren für die Herstellung von Wundauflagen, jedoch wird die Transporteffizienz von Arzneistoffen und Ladungsträgern in seiner Matrix direkt

durch die Dichte des entstehenden Verhakungsnetzwerks limitiert. In der vorliegenden Arbeit wurde mittels atomistischer Modellierung eine systematische Untersuchung der Entwicklung des freien Volumens und der Topologie von Transportkanälen in PVA-Spinnlösungen im für das Elektrospinning optimalen Konzentrationsbereich von 8–13 Gew.-% durchgeführt. Der Einsatz von Computerdesign ermöglicht eine molekulare Interpretation makroskopischer Änderungen der Diffusionszugänglichkeit in den Systemen, was einen notwendigen Schritt zur Optimierung von Zusammensetzungen mit vorgegebenen therapeutischen Eigenschaften darstellt [1-2].

Die Erstellung der vollatomistischen Modelle der PVA-Lösungen erfolgte im Modul «Amorphous Cell» (Kraftfeld COMPASS II). Zur Gewährleistung der statistischen Zuverlässigkeit der Ergebnisse wurde eine Serie von Zellen im Konzentrationsbereich von 8 bis 13 Gew.-% mit einem Schritt von 1 % konstruiert. Die Gitterparameter variierten zwischen 33,4 und 28,0 Å in strikter Übereinstimmung mit den Referenzwerten der Systemdichten. Für jedes Modell wurde eine mehrstufige Geometrieoptimierung mit dem «Smart Minimizer»-Algorithmus bis zum Erreichen der Energiekonvergenz durchgeführt. Die Analyse des freien Volumens (FV) und der zugänglichen Oberfläche (SA) erfolgte mittels Connolly-Oberflächenmethode unter Verwendung einer Sonde mit einem Radius von 1,4 Å, was den geometrischen Dimensionen eines Lösungsmittelmoleküls sowie hydratisierter Ionen entspricht.

Die Analyse der gewonnenen Daten ergab eine stetige Tendenz zur Verengung der Transportwege mit steigender PVA-Konzentration. Es wurde festgestellt, dass die Erhöhung des Polymer-Massenanteils von 8 % auf 13 % zu einer Verringerung des freien Volumens (FV) von 13,03 % auf 10,80 % führt. Dabei zeigt der Parameter der zugänglichen Oberfläche (SA) einen deutlich stärkeren Rückgang um 45 %, was nicht nur auf eine geometrische Kompression des Systems, sondern auch auf eine qualitative Umordnung seiner Topologie hindeutet. Die Visualisierung der Transportkanäle (Abb. 1) bestätigt den Prozess der Fragmentierung des freien Raums. Dieser Effekt ist auf die Bildung eines dichten Verhakungsnetzwerks zurückzuführen,

das als sterische Barriere für die Diffusion fungiert.



(а) (б)

Abbildung 1. Modelle des freien Volumens in den PVA-Zellen: a – 8 Gew.-%, b – 13 Gew.-%.

Die Modellierung ergab, dass bei einer Erhöhung der PVA-Konzentration auf bis zu 13 % das freie Volumen des Systems auf einem ausreichenden Niveau erhalten bleibt. Trotz der Verengung der Transportkanäle bleibt das System für Ladungsträger permeabel. Die Zunahme der Dichte des Polymernetzwerks trägt zu einer geordneteren Ionenmigration bei, was den stabilen Anstieg der elektrischen Leitfähigkeit der Lösungen in diesem Bereich erklärt.

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Исследование влияния плотности сетки зацеплений на топологию транспортных каналов в формовочных растворах поливинилового спирта методом молекулярной динамики

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Methodische Aspekte des atomistischen Designs und der Optimierung amorpher Zellen zur Vorhersage der Eigenschaften von Polyvinylalkohol-Systemen

Die Effizienz molekulardynamischer (MD) Untersuchungen im Bereich von Polymersystemen unterschiedlicher Konzentration hängt entscheidend von der Qualität der Anfangskonfiguration des atomistischen Modells ab. Bei der Modellierung von Polyvinylalkohol-Lösungen (PVA) im Bereich der Verhakungsnetzbildung besteht das Hauptproblem darin, ein thermodynamisches Gleichgewicht unter den Bedingungen eines begrenzten freien Volumens und einer hohen Packungsdichte zu erreichen. Eine fehlerhafte Wahl der linearen Zellenparameter oder der Geometrieoptimierungsstrategie führt zu Artefakten bei der Berechnung von Transport- und Energiecharakteristika. In der vorliegenden Arbeit werden methodische Aspekte der präzisen Konstruktion amorpher PVA-Zellen betrachtet, einschließlich Algorithmen zur Dichteverifizierung, der Auswahl von Kraftfeldparametern und der mehrstufigen Minimierung der potenziellen Energie. Die Entwicklung eines zuverlässigen Designprotokolls für solche Modelle ist notwendig, um die Vorhersagekraft der atomistischen Modellierung bei der Entwicklung neuer biomedizinischer Materialien zu erhöhen [1-2].

Ein entscheidender Schritt des Algorithmus ist die Korrelation der linearen Abmessungen der periodischen Zelle mit experimentellen Werten bzw. Referenzwerten der Lösungsdichte. Um Artefakte der „Selbstüberschneidung“ von Polymerketten über die Zellgrenzen hinweg auszuschließen, wurde eine optimale Kantenlänge im Bereich von 28,0–33,4 Å bestimmt. Als strukturelles Basiselement wurde ein PVA-Makromolekül mit einem Polymerisationsgrad von n=40 verwendet, was eine repräsentative Auswahl an Konformationszuständen bei gleichzeitiger

Aufrechterhaltung der Recheneffizienz gewährleistet. Besonderes Augenmerk wurde im Protokoll auf das Verfahren zur Relaxation von Spannungen gelegt, die beim Aufbau ausreichend dichter Systeme entstehen. Die vorgeschlagene Strategie der mehrstufigen Optimierung der potenziellen Energie umfasst die Verwendung des „Smart Minimizer“ Algorithmus mit schrittweiser Erhöhung der Konvergenzgenauigkeit. Dies ermöglichte es, lokale Energieminima zu vermeiden und das System auf die Dynamikberechnung mit einem Integrationszeitschritt von 0,5 fs vorzubereiten. Durch den Einsatz des Kraftfelds COMPASS II konnte das System der Wasserstoffbrückenbindungen zwischen den Hydroxylgruppen des PVA und den Lösungsmittelmolekülen am adäquatesten beschrieben werden, was durch die Stabilität der Gesamtenergieverläufe über die gesamte Simulationsdauer bestätigt wird. Die Effizienz des vorgeschlagenen methodischen Ansatzes wurde an einer Serie von sechs unabhängigen Modellen im PVA-Konzentrationsbereich von 8–13 Gew.-% bestätigt. Es wurde festgestellt, dass die Verwendung des optimierten Aufbaualgorithmus eine hohe Konvergenz der Ergebnisse gewährleistet: Die Fluktuationen der potenziellen Energie nach Abschluss der Relaxation überschritten 0,01 % nicht. Das entwickelte Protokoll ermöglichte es, einen monotonen Charakter der Änderung des freien Volumens (FFV) ohne anomale statistische Ausreißer nachzuweisen, was bezeichnend für korrekt ausbalancierte Systeme ist. Die Verifizierung anhand des Parameters „Surface Area“ zeigte, dass die gewählte Zellgröße ausreicht, um die Topologie der Transportkanäle adäquat zu beschreiben.

Zusammenfassend lässt sich festhalten, dass die vorgeschlagene Methodik ein universelles Werkzeug für das operative Screening der Strukturmerkmale von Polymersystemen unterschiedlicher Konzentration darstellt.

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Методические аспекты атомистического дизайна и оптимизации аморфных ячеек для прогнозирования свойств систем поливинилового спирта

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Rheological profiling of bacterial cellulose produced by various acetic acid bacterial strains: an experimental comparison

1. Why bacterial cellulose matters in biomedicine

The search for biocompatible and biodegradable materials for medical applications has recently focused on microbial polymers. One prominent example is bacterial cellulose (BC), which is secreted by acetic acid bacteria. Unlike its plant counterpart, BC offers an unusual combination of physical and biological properties. Specifically, it possesses high tensile strength, substantial elasticity, a highly developed porous structure, and excellent compatibility with living tissues. These

attributes make BC a strong candidate for use in clinical settings, particularly in wound management.

To illustrate, when compared with chitosan – another well-studied biopolymer [1] – BC meets nearly all specifications required for effective wound dressings. Such specifications include:

- preservation of adequate moisture at the wound site;
- provision of proper thermal insulation;
- unimpeded oxygen transport to injured tissues;
- creation of a protective barrier against bacterial pathogens;
- absence of allergenic or irritant effects.

Additionally, because the human body does not produce cellulolytic enzymes, BC undergoes only negligible biodegradation over short time frames. This physiological stability allows BC-based materials to function reliably over extended implantation or application periods.

2. Origin and preparation of the samples

The BC specimens examined in this study were generated at the Department of Biochemistry and Technology of Microbiological Productions, Ufa State Petroleum Technological University (UGNTU). Three distinct producer strains of acetic acid bacteria were employed, namely:

- *Komagataeibacter raeticus*,
- *Komagataeibacter sucrofermentans*,
- *Novoacetomonas hansenii*.

For the biosynthesis step, a static cultivation protocol was adopted. Each strain was grown separately in 250 mL Erlenmeyer flasks filled with 50 mL of Hestrin–Schramm growth medium. The exact composition of this nutrient solution is summarized in Table 1.

Table 1

Composition of the Hestrin–Schramm culture medium

Component	Concentration (% w/w)
Glucose	2.0
Yeast extract	0.5
Peptone	0.5
Disodium hydrogen phosphate	0.27
Citric acid	0.15

Ethanol was additionally supplied as a supplementary carbon source at a final concentration of 1% (v/v).

3. Rheological measurements: equipment and protocol

The central question addressed in this work was whether BC gels derived from different bacterial strains exhibit distinguishable rheological responses. To answer this, viscosity measurements were conducted using a commercially available modular rotational rheometer (Thermo Scientific HAAKE MARS III). All tests were run under oscillatory conditions.

Key measurement parameters were as follows:

- Oscillation frequency range: from 0.01 Hz to 10 Hz (swept continuously);
- Measuring geometry: cone–plate configuration;
- Cone diameter: 35 mm.

No additional pre-shearing or temperature variation was applied; all measurements were performed under identical ambient conditions to ensure comparability.

4. Experimental outcomes

The collected data revealed that the viscosity characteristics of BC samples are not uniform across different producer strains. On the contrary, each bacterial strain yielded a BC gel with a distinct rheological signature. In simple terms, the choice of

microbial producer directly influences the flow behavior of the resulting cellulosic material.

These findings suggest that strain selection can be used as a tool for tailoring the mechanical properties of bacterial cellulose for specific biomedical applications – an aspect that warrants further investigation.

5. Conclusion (brief summary)

- BC is a microbially synthesized polymer with properties superior to plant cellulose for certain medical uses.
- Three different acetic acid bacterial strains were successfully used to produce BC gels.
- Rheological testing clearly demonstrated strain-dependent differences in viscosity profiles.
- The observed variability opens possibilities for targeted strain selection in BC production.

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Реологическое профилирование бактериальной целлюлозы, полученной различными штаммами уксуснокислых бактерий: экспериментальное сравнение

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Assessing the rheology of bacterial cellulose: a comparative study of samples obtained from different acetobacter strains

1. General context

Among naturally occurring polymers, bacterial cellulose (BC) occupies a special position. It is synthesized by bacteria belonging to the acetic acid group and exhibits a combination of properties not typically found together in plant-derived cellulose. Specifically, BC demonstrates high mechanical strength, good flexibility, a well-developed porous network, and outstanding biocompatibility. Such a property profile has drawn attention to BC as a potential material for biomedical engineering. One promising direction involves wound care. As previously shown for chitosan [1], BC fulfills virtually all requirements for modern wound dressings. These include: maintaining a moist environment around the injury, providing sufficient thermal insulation, allowing oxygen diffusion to the wound bed, acting as a physical barrier against invading microorganisms, and showing no signs of allergenic activity. Furthermore, because humans do not possess enzymes that can hydrolyze cellulose, BC degrades very slowly inside the body. This slow breakdown makes long-term application of BC-based products feasible.

2. Materials and experimental approach

The BC samples analyzed in this work were produced at the Department of Biochemistry and Technology of Microbiological Productions (UGNTU, Ufa). Three different producer strains were used, all belonging to the group of acetic acid bacteria: *Komagataeibacter raeticus*, *Komagataeibacter sucrofermentans*, and *Novoacetomonas hansenii*. For biosynthesis, static cultivation was chosen. Each culture was grown in a 250 mL Erlenmeyer flask containing 50 mL of Hestrin–

Schramm nutrient broth. The composition of the growth medium (in weight percent) was as follows:

- glucose – 2.0%;
- yeast extract – 0.5%;
- peptone – 0.5%;
- disodium hydrogen phosphate – 0.27%;
- citric acid – 0.15%.

To supply additional carbon, ethanol was introduced at a level of 1% (v/v). The primary research question was to characterize how the resulting BC gels behave under mechanical stress, i.e., their rheological response. For this purpose, a modular rotational rheometer (Thermo Scientific HAAKE MARS III) was employed. Measurements were performed in oscillatory mode. The oscillation frequency was swept from 0.01 Hz up to 10 Hz. A cone–plate measuring head with a cone diameter of 35 mm was used throughout all experiments.

3. Observed differences

The experiments clearly showed that the viscosity profiles of BC samples depend significantly on which bacterial strain was used for synthesis. In other words, different producer organisms yield BC with different rheological characteristics.

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Оценка реологии бактериальной целлюлозы: сравнительное исследование образцов, полученных из различных штаммов Acetobacter

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Development of a web-based platform for urban air quality monitoring

Urban air pollution poses a significant threat to public health and the environment. In many cities, including Ufa, air quality data is collected by various agencies (e.g., Roshydromet, Ministry of Ecology of Bashkortostan) but is often published on separate, non-uniform websites, making holistic analysis difficult for both experts and the public. This fragmentation hinders effective environmental monitoring and informed decision-making [2].

Modern web technologies and geoinformation systems (GIS) offer powerful tools to aggregate, visualize, and analyze such heterogeneous data. This paper describes the development of a functional prototype for a unified urban air quality monitoring platform for the city of Ufa. The primary goal is to create an intuitive, interactive dashboard that integrates data from different sources, visualizes key pollutants and the Air Quality Index (AQI) on a map, and provides tools for temporal analysis. The prototype establishes the architectural foundation for a future digital twin of the urban air environment [1,3].

Data Model and Technology Stack

The platform's data model is built around monitoring stations and pollutants. It includes 18 stations from two real-world agencies in Ufa: Roshydromet and the Ministry of Ecology of Bashkortostan. A comprehensive dictionary of 37 pollutants was created, storing for each its name, unit, Russian Maximum Allowable Concentration (MAC), and a health description. For the prototype phase, realistic

pollutant values are generated client-side based on these MACs to simulate real-time data feeds.

The platform is developed as a single-page application (SPA) using a modern frontend ecosystem. At its core, the application leverages React with TypeScript, which provides robust type checking and component-based architecture. Vite serves as the build tool, enabling rapid development with optimized production builds. For geospatial visualization, the project uses Leaflet and its React wrapper react-leaflet, providing an interactive mapping experience with custom markers. All data visualization components are built with Chart.js and react-chartjs-2 [5].

System Functionality

The interactive map serves as the primary navigation interface, displaying all 18 monitoring stations across Ufa with precise geographic coordinates. Each station marker is visually encoded with two distinct characteristics: its color reflects the current AQI value following a standard color scale from green (good) to red (hazardous), while its shape indicates the governing organization. This dual visual encoding allows users to immediately assess both the air quality status and data source for any location.

The platform implements a custom AQI calculation algorithm based on Russian MACs. For each station, the system computes the ratio of each pollutant's current value to its respective MAC, then aggregates these ratios into a unified index value, categorized into descriptors ranging from "Good" to "Very Unhealthy." A dedicated sidebar panel displays current concentrations for all monitored pollutants, each accompanied by a visual progress bar showing the percentage relative to the MAC, with exceedances highlighted in distinctive colors [4].

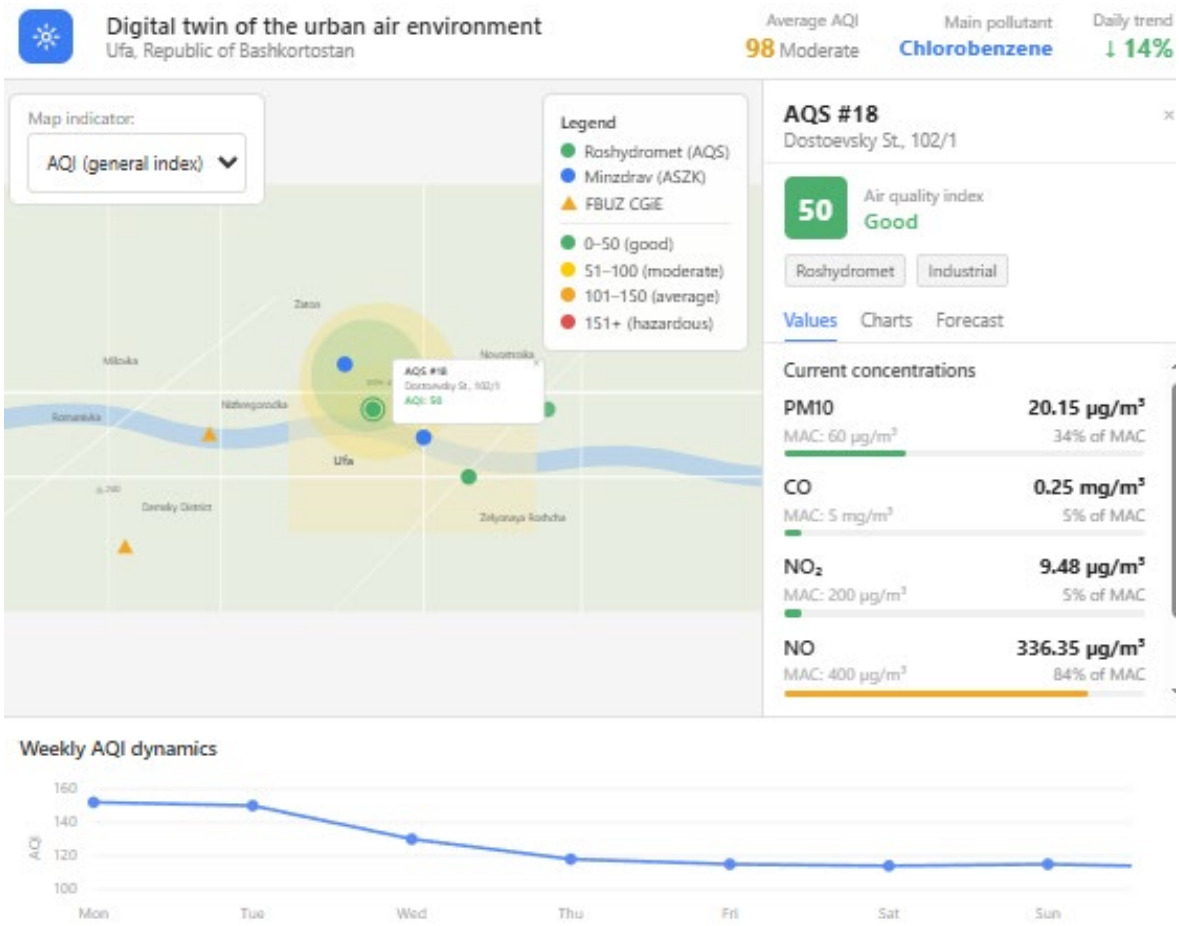

Fig. 1. Overview of the prototype platform: interactive map of Ufa with monitoring station markers, station detail panel, and weekly AQI dynamics chart

Beyond individual station analysis, the platform offers aggregated views of urban air quality. The main header displays the city-wide average AQI, identifies the primary pollutant, and shows a trend indicator with percentage change (Fig. 1). A dedicated chart panel presents weekly AQI trends for a user-selected station, allowing for comparative analysis across different monitoring locations. A comprehensive pollutant reference guide provides educational information about all 37 monitored substances, including their health effects and regulatory limits.

AQI Forecasting Feature

A notable feature of the platform is the 72-hour AQI forecast module. When a user opens any monitoring station, the "Forecast" tab displays an interactive Chart.js graph showing projected AQI values for the next 72 hours, generated through trend simulation algorithms based on the current pollutant dynamics (Fig. 2). The chart

provides a visual forecast summary indicating whether air quality is expected to improve or deteriorate. This functionality serves as a prototype for future integration with real meteorological and dispersion models.

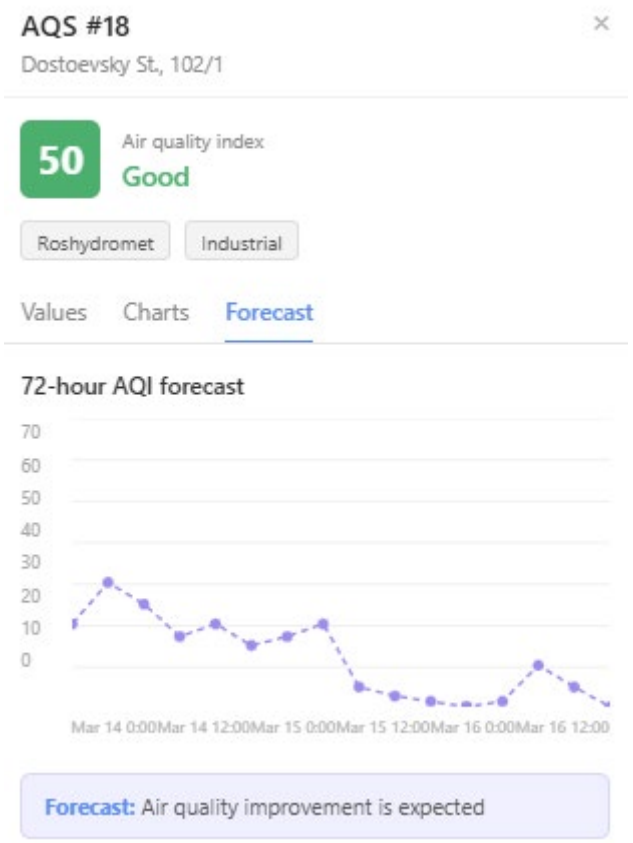

Fig. 2. 72-hour AQI forecast displayed as an interactive chart in the station detail panel

Conclusion

The developed prototype successfully demonstrates the concept of a unified urban air quality dashboard. It effectively integrates spatial and temporal data visualization, allowing a user to quickly assess the overall air quality situation in Ufa, identify potentially problematic stations via map colors, and drill down into detailed pollutant data. The use of different icon shapes for agencies provides immediate visual context about the data source; the integration of MAC-based assessment directly into the pollutant cards makes the information meaningful for users familiar with Russian environmental standards.

The primary limitation of the current version is its reliance on simulated data. However, this approach was intentional to validate the user interface and user

experience (UI/UX) and to establish a robust data pipeline structure. The next phase of development will focus on replacing the data generator with real API calls to open data sources of the included agencies, transforming the prototype into a live monitoring and decision-support platform for urban ecology and public health.

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Разработка веб-платформы для мониторинга качества воздуха в городе

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Fire safety of oil products storage in tank farms: accident rate analysis and the main causes of fires

Fire safety of petroleum product storage is one of the most important tasks in the operation of tank farms and warehouses. Petroleum products belong to the category of flammable and combustible liquids, which causes a high probability of fires in case of violation of the rules of storage and operation of equipment. Fire safety includes a set of technical, organizational and engineering measures aimed at preventing emergencies, minimizing fire risks and protecting people, property and the environment.

Tanks store a wide range of toxic, flammable, and explosive products, depending on the specific production requirements. The most common petroleum products are:

– Gasoline: Flammable liquid (FL), with a flash point of 27-39°C, auto-ignition temperature of 246°C, explosive concentration of vapor-air mixture from 1% to 6% by volume. Fire class caused by its combustion is B, subclass B1 (combustion of liquid materials that are insoluble in water);

– Acetone: Flammable liquid (FL), with a flash point of -18°C, concentration limits of flame propagation by volume: lower – 2.7%, upper – 13%;

– Propane: Flammable gas, explosive concentration of vapor-air mixture from 1.7% to 10.9%, auto-ignition temperature of 500°C;

– Propylene: Flammable gas, miscible with water, auto-ignition temperature of 455°C;

– Ethylene: Flammable gas, partially miscible with water, auto-ignition temperature of 475.6°C.

Most accidents are caused by fuel spills, fires, and explosions. Among the cases presented, the most significant are considered to be: a fuel spill at the CHPP-3 in Norilsk, which led to major contamination of soil and water bodies, an explosion and a fire at the Kirishi oil refinery with the fatal outcome of five people.

In Russia, more than ten large fires are recorded annually at storage facilities [1]. According to the analysis, emergencies are most dangerous on oil pipelines, accounting for 55% of the total number of incidents, as well as on reservoirs (14%) and pumping stations (10%) (Figure 1.1).

It is worth noting that these fires are often accompanied by explosions, which account for 45% of the total number of fires (Figure 1.2).

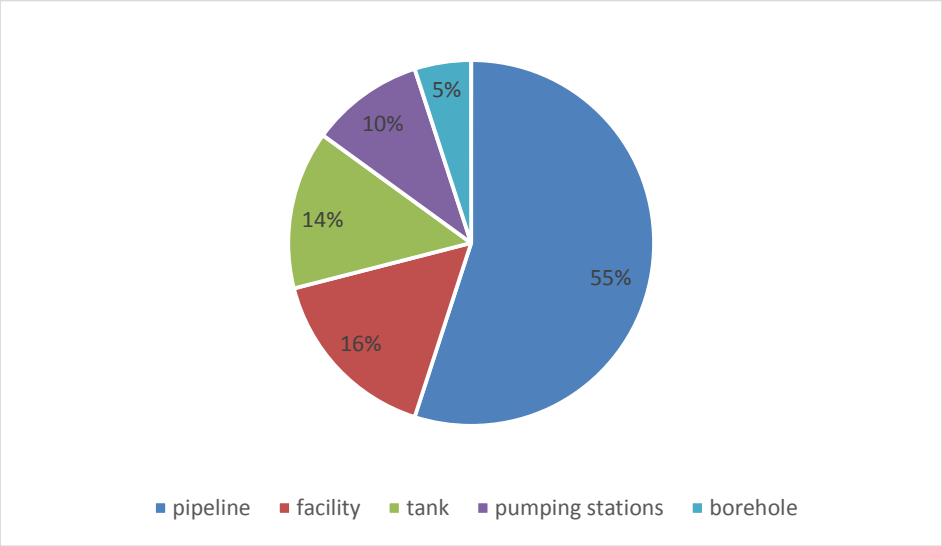

Fig. 1.1. Distribution of accidents by type of facilities

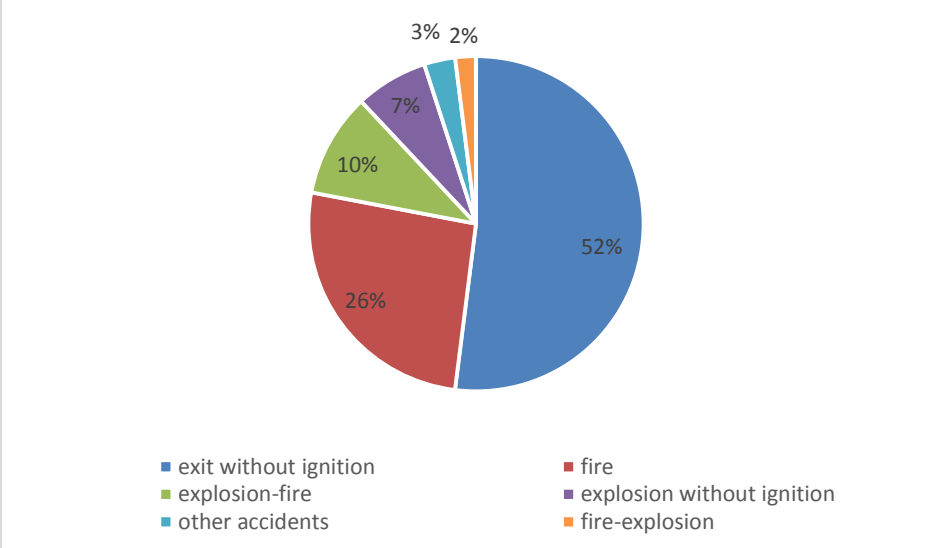

Fig. 1.2. Distribution of types of accidents at facilities

The main factors leading to accidents are the inadequate technical condition of the tanks, their long service life, as well as erroneous engineering decisions made during construction. Based on the analysis of accidents at similar facilities in the oil and gas industry, the most common causes of fires can be identified:

– exposure to atmospheric electricity;
– spontaneous combustion of pyrophoric deposits;
– explosion of combined - cycle gas mixtures during sampling;
– carrying out repair and fire work in violation of fire safety standards and requirements [2].

The occurrence of emergencies in the territory of the reservoir park leads to a deterioration of the environment, since the leakage of petroleum products leads to contamination of soil and rivers, causing toxic pollution, which causes serious damage to ecosystems and disrupts water quality, threatening flora and fauna, as well as increasing risks to human health.

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Пожарная безопасность хранения нефтепродуктов в резервуарных парках: анализ аварийности и основные причины возникновения пожаров

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Geographic Information Mapping of Soil Cover

In modern agriculture, operational access to reliable and comprehensive data on land resources held by agro-industrial enterprises is essential.

Effective farm management and the sustainable utilization of soil fertility depend on detailed knowledge of soil conditions across individual fields and plots. One of the methods for studying soils is mapping and the compilation of soil maps and cartograms. [2]

The aim of this work is to develop a standard geographic information system in the format of a web map to present the results of an agrochemical survey.

The object of this study is the soils of the agricultural enterprise JSC Poultry Farm "Komsomolskaya" located within the boundaries of the Kungur Municipal District of Perm Krai (Figure 1).

The soil cover is represented by the predominant soil types: soddy-podzolic soils – 822.2 ha, light gray forest soils – 2,023.8 ha, and gray forest soils – 271.3 ha. According to the particle size distribution, the soils are heavy loamy.

The spatial data source is an agrochemical cartogram of JSC Poultry Farm "Komsomolskaya" at a scale of 1:17,000.

The source of attribute information is the "Materials of the agrochemical survey of agricultural lands of JSC Poultry Farm 'Komsomolskaya', Kungur District, Perm Krai", prepared by the Federal State Budgetary Institution "Perm State Center for Agrochemical Service" in 2022.

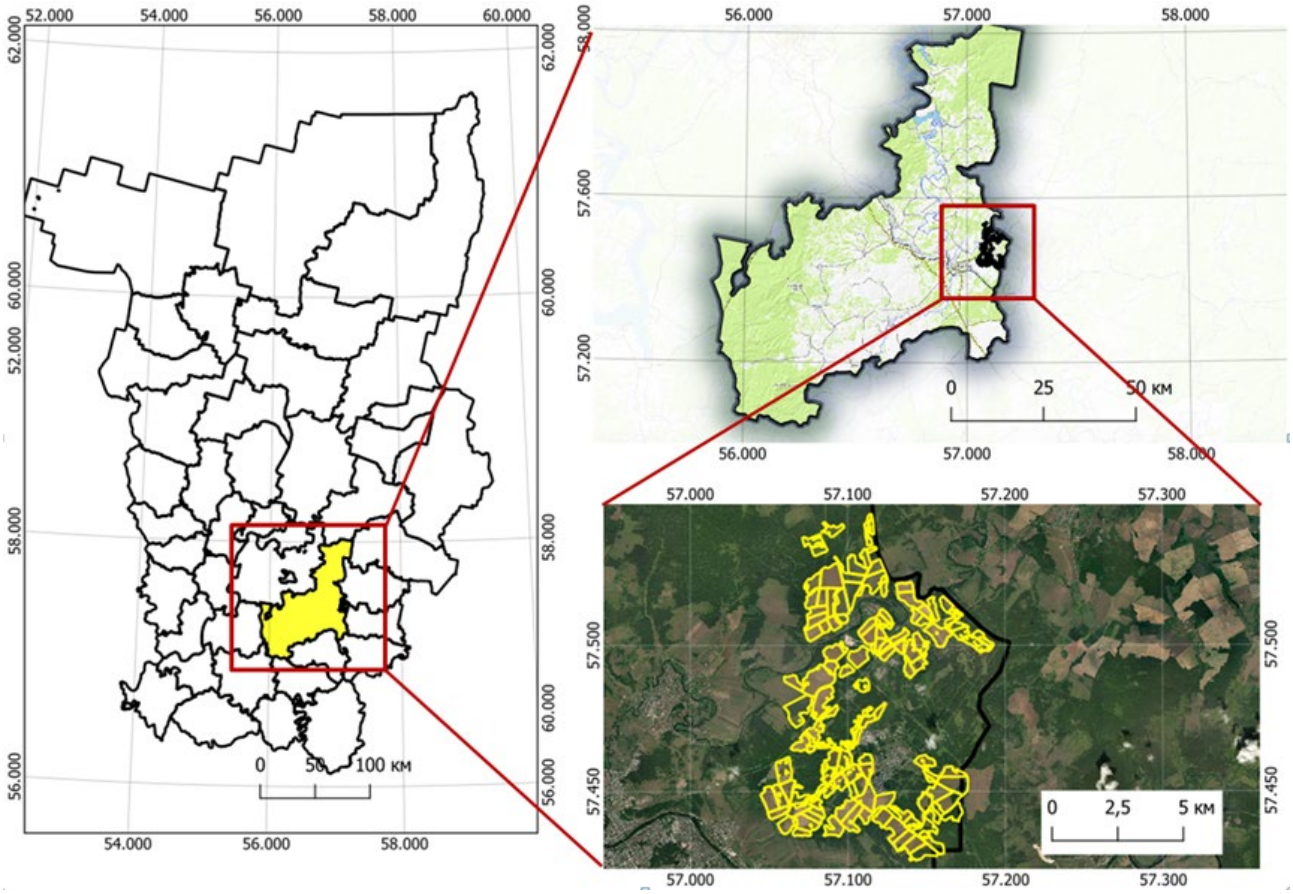

Fig. 1. Location of the territory of the Komsomolskaya Poultry Farm JSC on the cartogram background

The methodology included the following steps. First, the scanned cartogram was georeferenced to a projected coordinate system.

Vectorization and attribute data integration were performed in QGIS 3.34.6, an open-source GIS platform. The client-side web application was developed using Leaflet interfaces, implemented with the qgis2web plugin and Visual Studio Code. The resulting web application was deployed on GitHub, demonstrating the feasibility of using freely available tools for creating and publishing interactive maps.

As a result of the vectorization of soil polygons, a geoinformation layer of soils was created, containing attribute information characterizing the agrochemical parameters of the soils.

The development scheme of the GIS project includes two blocks: the cartographic block – the GIS project, and the web mapping block, which is based on the operation of the qgis2web module and HTML code editing. [1]

As a result of vectorization, the total number of polygons was 126. After filling in the attributes characterizing the agrochemical polygon number, humus content, pH level, phosphorus and potassium content, area, and soil type for each polygon, the GIS project structure was established.

It includes 4 blocks: general data, soil properties – which is the main block, soil erosion model, and base maps.

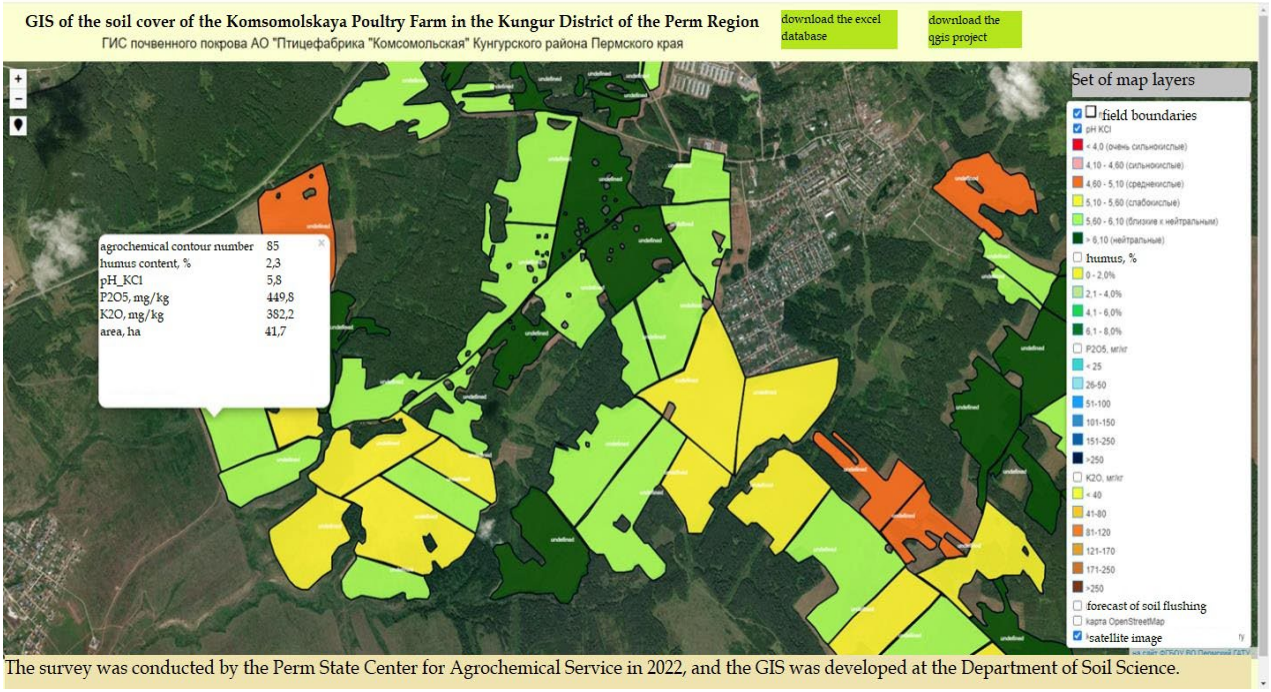

Fig. 2. The final version of the soil cover geoinformation system hosted on GitHub

A key benefit of GIS-based mapping is the capacity to generate thematic maps from vector layers and their corresponding attribute data.

Four maps were created: humus content, pH level, content of mobile forms of phosphorus and potassium.

These maps show that the predominant areas are soils with low humus content (3.6), pH levels close to neutral (5.7; range 5.6–6.0), and very high content of mobile forms of phosphorus (345) and potassium (391).

This indicates that while soil acidity is optimal for most crops, the low humus content suggests the need for organic matter management, despite the sufficient availability of phosphorus and potassium.

The assessment of erosion hazard for the farm's land plots was carried out

using the Universal Soil Loss Equation model - RUSLE (Wishmeier-Smith equation), developed in the USA.

The model was solved using the QGIS raster calculator. [3]

This study resulted in a functional web-based GIS that consolidates agrochemical and erosion data for the farm's 126 soil polygons. The agrochemical analysis indicates optimal pH and high phosphorus and potassium levels across most of the territory, but highlights low humus content as a limiting factor requiring organic matter management. Erosion hazard modeling identified 13 polygons (30% of the agricultural land) that require priority anti-erosion measures. The web map developed with the use of open-source platforms provides farm managers with an accessible tool for data-driven decision-making and demonstrates a cost-effective approach for digital soil mapping in agricultural enterprises.

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Геоинформационное картографирование почвенного покрова

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Reagent methods for heavy metal removal from galvanic wastewater

The treatment of galvanic (electroplating) wastewater remains a critical environmental challenge due to the presence of toxic heavy metals such as Cr, Ni, Cu, and Zn. Among the available technologies, chemical precipitation is the most widely used in industrial practice due to its simplicity and cost-effectiveness. This work provides a comparative analysis of reagent-based methods for heavy metal removal, focusing on their efficiency, limitations, and operational safety [3].

Hydroxide precipitation using NaOH or Ca $(OH)_2$ is the most common approach. By raising the pH to 8-11, dissolved metals are converted into insoluble hydroxides. While this method is low-cost and well-established, it has significant drawbacks: different metals precipitate optimally at different pH levels, making complete removal difficult in mixed-metal wastewater. Additionally, the process generates large volumes of gelatinous sludge that is hard to dewater, and some metal hydroxides may redissolve under alkaline conditions [3].

Sulfide precipitation (Na_2S, NaHS) offers superior removal efficiency due to the extremely low solubility of metal sulfides [4]. Studies show >99% removal of Cd, Zn, and Cu, even in the presence of chelating agents [4]. However, its industrial adoption is limited by operational risks: excess sulfide is toxic and corrosive, and there is a danger of H_2S gas emission [4].

To address these limitations, hybrid hydroxide-sulfide systems have been developed. A two-step process using NaOH followed by a small dose of Na_2S can effectively remove all metals while minimizing sulfide usage and reducing the risk of

H_2S release. This approach combines the low cost of hydroxide precipitation with the high efficiency of sulfides.

Newer organosulfide reagents such as TMT (trimercaptotriazine) and DTC (dithiocarbamates) have emerged as safer alternatives. They operate effectively across a wide pH range (3-9), achieve >99.9% removal of metals like Pb, Cd, Cu, and Hg, and produce no H_2S. Although more expensive, they overcome the pH sensitivity of hydroxide methods and the safety concerns of inorganic sulfides [4].

Coagulation-flocculation with aluminum or iron salts ($Al_2(SO_4)_3$, $FeCl_3$) is often used as a polishing step (a typical process flow diagram is shown in Figure 1) [1, 3]. Experimental studies demonstrate that using NaOH and $Ca(OH)_2$ in combination with a flocculant can achieve up to 91% removal of total iron and 94.6% removal of suspended solids from galvanic wastewater [1]. Recent studies (2026) confirm that iron-based coagulants are most effective for Cr removal, while polyaluminum chloride works best for Ni and Zn, achieving overall efficiencies above 90% [2].

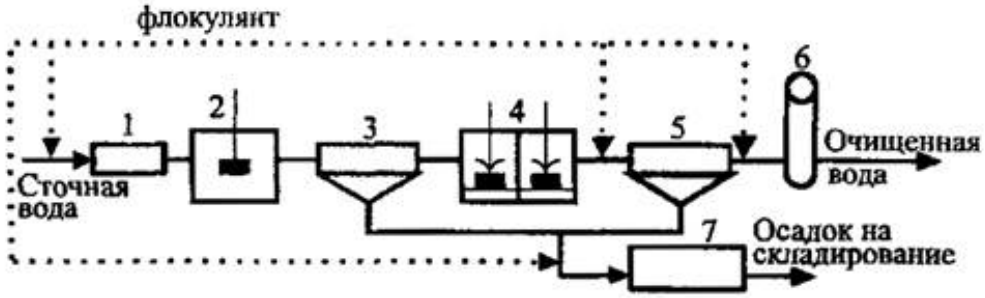

Fig. 1. Schematic diagram of the coagulation-flocculation and sedimentation unit (1 – wastewater inlet, 2 – flocculant dosing, 3-6 – treatment stages (mixing, flocculation, settling), 7 – sludge disposal)

The choice of reagent method depends on wastewater composition, regulatory requirements, and operational priorities. For facilities handling mixed metals, a two-step approach combining hydroxide precipitation with organosulfide polishing offers the best balance of cost, safety, and compliance. For simpler waste streams, hydroxide precipitation with coagulation remains practical if sludge management is addressed.

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Реагентные методы удаления тяжелых металлов из гальванических сточных вод

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The effect of complex treatment on the enzymatic activity of oil-contaminated soil during phytoremediation

Oil pollution is a severe and serious environmental threat. Oil is toxic to most living organisms, including plants and microorganisms. It disrupts the balance of

ecosystems, reduces their productivity, and decreases biodiversity. The problem is exacerbated by the widespread use of hydrocarbons in the global economy, which increases the risk of accidents and spills during oil extraction, transportation, and storage. Therefore, it is necessary to develop and implement effective measures to mitigate their consequences and restore ecosystems.

The aim of the study is to develop and optimize a comprehensive bioremediation technology aimed at maintaining the enzymatic activity of the soil and ensuring the effective removal of petroleum products from contaminated soils.

The object of the study was the common chernozem, contaminated with commercial oil at a concentration of 4% of the dry weight of the soil. After the soil was contaminated, the biopreparation Lenoil was added, based on the hydrocarbon-oxidizing bacteria Psevdomonas turukhanskensis IB 1.1. Mineral fertilizers were added to various samples: phosphorus-potassium (PK), an aqueous solution of the complex fertilizer Fertico (Fв), the granular complex fertilizer Fertico (Fc), and humic acids (HA). A month later, the Azolen preparation containing the nitrogen-fixing bacteria Azotobacter vinelandii IB 4 was added to some of the samples, after which seeds of phytoremediant plants were sown – peas of the Elite variety and mung bean of the Durdona variety. The seeds were previously treated with an Agrobiologist biopreparation based on Pseudomonas protegens DA 1.2. During plant growth, their seedlings were treated with the Agrobiologist preparation once a week by spraying. After 60 days, soil samples were taken to analyze their enzymatic activity. Catalase activity was determined using the gasometric method, while lipase activity was measured using the titrimetric method.

The results of the catalase study showed that oil pollution doubled the metabolic activity of the soil microbiota, indicating that natural self-purification processes were activated under stress conditions. The use of the biopreparation "Lenoil" in combination with various fertilizers resulted in a decrease in enzymatic activity. The application of PK fertilizer proved to be the most effective for stimulating enzymatic activity in combination with this biopreparation. The addition

of Fc had the least stimulating effect on the activity of catalase.

When using the Agrobiolog preparation, there was no effect on the activity of soil enzymes as a result of the specific method of using this biopreparation, as its effect was directed at plants and did not affect soil microorganisms. The complex of Lenoil and Agrobiolog preparations did not affect lipase activity, while the activity decreased slightly when Azolen was added compared to the same test without it.

Soil contamination also led to a 2-fold increase in lipase activity. The effectiveness of Lenoil in activating lipases was significantly influenced by the use of mineral fertilizers. Fertilizers Fb and GK contributed to the most effective increase in enzymatic activity, while RK and Fc slightly reduced the activity of lipases compared to untreated contamination. This suggests that the correct selection of mineral fertilizers can improve microbiological activity and enhance the biodegradation of oil.

Therefore, to effectively phytoremediate and restore oil-contaminated soils, it is recommended to use a combination of biological products, mineral fertilizers, and phytoremediation plants, taking into account the specific characteristics of each component and environmental conditions.

Влияние комплексной обработки на ферментную активность нефтезагрязненной почвы при фиторемедиации

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Секция 2

ПРОБЛЕМЫ ПРОФЕССИОНАЛЬНОЙ КОММУНИКАЦИИ

ЕСТЕСТВЕННЫЕ НАУКИ

УДК 502/504:656.2

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Analysis of the effectiveness of measures to protect wild animals from collisions with trains in Russia

The length of the Russian railway network, a significant part of which passes through forest and taiga zones, creates a constant risk of train collisions with wild and agricultural animals. These incidents result in animal deaths, economic losses, traffic safety hazards and damage to rolling stock. Minimizing the anthropogenic impact on the fauna is not only an environmental, but also a technological task, which is reflected in the sustainable development policy of Russian Railways.

In the first nine months of 2025, 178 cases of collisions and collisions of trains with animals occurred in Russia, including more than 1.5 thousand incidents of animals on the way in January. Most often, cattle, moose, wild boars and Red Book dzerens in Transbaikalia fall under trains. In the Astrakhan region in 2023, the number of collisions with livestock increased by 48%, reaching 120 cases. In Dagestan, 167 such incidents were recorded in 2024. The lack of centralized accounting makes it difficult to assess the situation.

To reduce the number of collisions of trains with animals, engineering fences, eco-ducts and signal systems are being introduced. Fencing effectively protects against large animals, but requires regular maintenance and cannot always stop more jumping species. Ecoducts help preserve ecosystems and animal migration routes. By

2024, 257 eco-ducts were built, most of which are located on roads. The largest project on the railways is the Moscow-St. Petersburg high-speed highway, which includes eco-ducts, noise screens and systems that prevent animals from getting on the way.

Signaling and repelling systems are designed to prevent animals from getting out of the way by affecting their senses. Russian Railways is testing the Sirena-5 speaker system, which makes sounds that scare away predators and large ungulates. Tests of systems based on neural networks for recognizing wild animals from video recordings are also underway for the purpose of operational notification. In remote areas, employees use ultrasonic devices, stun lights and gas canisters.

During the construction of the Moscow-St. Petersburg high-speed highway, measures are being taken to minimize the negative impact on the environment.

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The project bypasses specially protected natural areas (SPNA), includes the construction of eco-ducts for safe crossing of paths by animals, as well as the installation of noise barriers and systems to prevent animals from entering the path.

Ten eco-ducts were erected in Tatarstan, both eco-ducts and noise screens appeared in the Tver region, and the first Russian eco-duct was opened in the Kaluga region in 2016.

Анализ эффективности мер защиты диких животных от столкновений с поездами в России

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Der Nobelpreis für Physiologie oder Medizin 2025: Entdeckung der regulatorischen T-Zellen und des Gens Foxp3

Am 6. Oktober 2025 wurde der Nobelpreis für Physiologie oder Medizin an drei Wissenschaftlern verliehen: Shimon Sakaguchi von der Universität Osaka, Mary Brunkow und Fred Ramsdell. Sie wurden für die Entdeckung des Mechanismus der peripheren immunologischen Toleranz ausgezeichnet, insbesondere für die Identifizierung regulatorischer T-Zellen (Treg) und des Schlüsselgens Foxp3 [1]. Diese Entdeckung hat das Verständnis der Immunregulation revolutioniert.

Die Geschichte dieser Entdeckung begann 1995, als Shimon Sakaguchi und seine Kollegen zeigten, dass eine bestimmte Population von $CD4^+$-T-Zellen, die den Oberflächenmarker CD25 exprimieren, die Fähigkeit besitzt, Autoimmunreaktionen bei Mäusen zu unterdrücken [2]. Sakaguchi wies nach, dass die Entfernung dieser Zellen zur Entwicklung verschiedener Autoimmunerkrankungen führt, während ihre Rückübertragung die Krankheit verhindert. Diese Arbeit zeigte erstmals, dass die Immunsuppression kein passiver, sondern ein aktiv regulierter Prozess ist.

Parallel dazu untersuchten Mary Brunkow und Fred Ramsdell die genetische Ursache der scurfy-Maus, einer Mutante, die eine tödliche lymphoproliferative Erkrankung entwickelt. Im Jahr 2001 identifizierten sie das defekte Gen als Foxp3, das für ein Transkriptionsfaktor-Protein aus der Forkhead/Winged-Helix-Familie kodiert. Die Forscher zeigten, dass eine Mutation in diesem Gen zum Verlust der regulatorischen T-Zellen führt und die Tiere an einer schweren Autoimmunerkrankung sterben [4, S. 68]. Kurz darauf wurde bestätigt, dass Mutationen im humanen FOXP3-Gen das IPEX-Syndrom (Immune Dysregulation, Polyendocrinopathy, Enteropathy, X-linked) verursachen, eine schwere Autoimmunerkrankung bei Kindern [1, S. 18].

Die Bedeutung dieser Entdeckungen liegt in der Aufklärung des zentralen Mechanismus der peripheren Immuntoleranz. Regulatorische T-Zellen fungieren als „Bremsen“ des Immunsystems und verhindern, dass dieses körpereigene Gewebe angreift [3]. Das Foxp3-Gen erweist sich als der „Master-Regulator“, der die Entwicklung und Funktion dieser Zellen steuert. Ohne Foxp3 können keine funktionsfähigen Treg-Zellen gebildet werden, was zu unkontrollierten Autoimmunreaktionen führt.

Die klinischen Anwendungen dieser Forschung sind vielfältig. Bei Autoimmunerkrankungen wie Multipler Sklerose oder Typ-1-Diabetes besteht das Ziel darin, die Funktion der Treg-Zellen zu stärken oder wiederherzustellen. Aktuelle Forschungen konzentrieren sich auf die Entwicklung von Therapien, die die Anzahl der Treg-Zellen im Körper erhöhen oder ihre suppressive Funktion verbessern. In der Onkologie hingegen versucht man, die Treg-Zellen im Tumorgewebe gezielt zu schwächen, da diese die Immunantwort gegen Krebszellen unterdrücken [4].

Die Identifizierung von Oberflächenmarkern wie CCR8 ermöglicht es, Treg-Zellen selektiv im Tumor zu eliminieren, ohne die systemische Immuntoleranz zu gefährden. Die Auszeichnung mit dem Nobelpreis würdigt eine Entdeckung, die nicht nur grundlegende Prinzipien der Immunologie aufklärte, sondern auch konkrete therapeutische Perspektiven für Millionen von Patienten mit Autoimmunerkrankungen und Krebs eröffnet hat.

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Нобелевская премия по физиологии и медицине 2025: открытие регуляторных Т-клеток и гена Foxp3

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Cooperative Birth and Vocal Plasticity of Sperm Whales: A Synthesis of Social Synchrony and Acoustic Culture

Observing births in wild cetaceans remains a challenging task in marine biology. Documented births have been observed in less than 10% of cetacean species [1, p. 215]. A recent study by Aluma and colleagues (2026) represents a paradigm shift in this field. It uses a multimodal approach that includes drone video footage, underwater acoustic monitoring, and ship-based photography. This allowed researchers to document the birth of a baby sperm whale (*Physeter macrocephalus*) off the coast of Dominica in a well-studied social group known as "Group A" [2, p. 3].

The most striking aspect of this study is that all 11 members of Group A exhibited cooperative behavior by physically supporting the newborn baby and

bringing it to the surface for its first breath. This behavior goes beyond previously documented cases of "midwifery" observed in captive bottlenose dolphins [3, p. 1298] and demonstrates the coordinated teamwork of wild deep-sea species. The evolutionary analysis conducted by Aluma and colleagues suggests that the practice of lifting cargo together originated before the last common ancestor of toothed whales (*Odontoceti*) and baleen whales (*Mysticeti*), approximately 36 million years ago. However, researchers note that the cooperative raising of calves appears to be a unique feature of toothed whales [2, p. 12].

Acoustic analysis has shown that, in addition to visual contact, these animals have a well-developed social coordination. Orcas communicate through a series of clicks known as "codes," which serve as social signatures that allow them to identify cultural clans and groups [4, p. 312]. During the study, numerous vocalizations were recorded during the 34-minute birthing process. Statistically significant changes in the style of code vocalizations were identified in relation to two key events: the onset of active delivery and the subsequent interaction with a group of short-finned pilot whales (*Globicephala macrorhynchus*) [2, p. 7]. The shift at the onset of delivery indicates a transition from normal vocalizations to a "cohesion" mode, which is consistent with the hypothesis that vocalization variability increases during periods of vulnerability to maintain group cohesion [5, p. 822]. The shift in behavior during an interspecies encounter may represent a kind of vocal "code switching" – a change in the structure of the signal to express aggression or coordinated defense.

The detailed description provided by Aluma et al. is of great importance for conservation. The fact that all 11 individuals in Group A participated in the breeding process highlights the critical role of social structure integrity for successful reproduction. It has been proven that underwater noise from shipping or seismic exploration masks the vocalization of cetaceans and disrupts their behavioral patterns [1, p. 220]. If vocal coordination is necessary for successful parturition, acoustic pollution in calving areas may have direct consequences for the animals' fitness. This

study not only sheds light on a previously unknown aspect of whale life, but also sets a new methodological standard for studying rare behavioral phenomena in the wild.

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Совместные роды и вокальная пластичность кашалотов: синтез социальной синхронии и акустической культуры

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Mitochondrial dysfunction as a factor of aging

Mitochondria are important organelles in eukaryotic cells responsible for adenosine triphosphate synthesis, calcium balance regulation, apoptosis, and a variety

of metabolic processes. Modern research shows that mitochondrial dysfunction is not just a concomitant of aging, but is one of its key mechanisms. This concept, first proposed by D. Harman within the framework of the free-radical theory, has been significantly developed due to recent discoveries related to mitochondrial deoxyribonucleic acid (hereinafter referred to as DNA), organelle dynamics, and qualitative control mechanisms [1].

Mitochondrial DNA is represented in cells in the form of many copies. With age, there is an accumulation of somatic mutations, including both point substitutions and large deletions. A critical point is that mitochondria with deletion mt DNA have a selective advantage: they replicate faster than full-fledged organelles. This leads to an increase in the proportion of functionally defective mitochondria, which in turn reduces energy production and increases oxidative stress. Studies in yeast models show that in senescent cells there is a loss of transmembrane potential and impaired protein import.

The key event is the excessive formation of reactive oxygen species (ROS). The greatest damage is caused by the perhydroxyl radical, which triggers the peroxidation of polyunsaturated fatty acids in the inner membrane of the mitochondria. Especially important is the oxidation of cardiolipin and phosphatidylethanolamine, lipids necessary for the formation of supramolecular complexes of the respiratory chain. Damage to these lipids further enhances the formation of ROS, creating a vicious circle [2]. Toxic peroxidation products modify proteins, including mitochondrial DNA polymerase, resulting in an increased mutation rate.

Mitophagy is a selective autophagy process that is responsible for the utilization of damaged mitochondria using the PINK1/Parkin system. With age, mitophagy activity decreases, leading to the accumulation of defective organelles, especially in cells that do not divide (such as neurons and cardiomyocytes). This, in turn, exacerbates energy shortages.

Modern methods are aimed at maintaining mitochondrial homeostasis. Mitochondrial-oriented antioxidants (such as MitoQ and SkQ1) accumulate in the mitochondria and reduce oxidative stress. Physical activity promotes mitochondrial biogenesis through activation of PGC-1α and improves mitophagy. Transplantation of healthy mitochondria is an innovative approach: preclinical studies show an improvement in cognitive function in old mice after the introduction of "young" mitochondria. In 2025, the first clinical trials of this technology for the treatment of mitochondrial diseases and slowing down the aging process will begin [3].

Thus, mitochondrial dysfunction is an integral mechanism of aging that combines genetic damage, oxidative stress, and proteostasis disruption. Understanding these processes opens up prospects for therapeutic interventions aimed at prolonging active longevity.

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Митохондриальная дисфункция как фактор старения

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Why is it reasonable for humankind to count sparrows nowadays?

On February 7-15, 2026, Russia will host the All-Russian Census of Sparrows, which is organized annually during the winter and summer seasons. This was announced by Anna Mostovaya, a member of the Union for the Protection of Birds of Russia and the Russian Network for the Study and Protection of Feathered Predators, in an interview with RIA Novosti.

Recently, in many countries of the world, particular in Europe, there has been a decrease in the number of sparrows. The real reason or causes are still not clear to experts.

The census is conducted annually in two seasons: from the second to the third weekend of February and August. Mostovaya said that it is convenient to count birds in February, as they gather on bushes, actively chirp and have not yet started the breeding season.

A brownie and a field sparrow participate in the census. According to Mostovaya, a sharp decline in the number of house sparrows is recorded in many countries of the world, but in Russia the scale of the decline cannot yet be accurately estimated – monitoring data for 10-15 years is needed for this.

The expert also stressed the importance of human assistance. It is necessary to preserve the habitats and feeding of birds, especially in winter. The sparrows' diet is based on millet and millet, and in the cold season they also willingly eat sunflower seeds and lard, Mostovaya said. The census website says that it is conducted in two seasons – winter and summer. Specialists need data on the number of sparrows from the same points at the same time of the annual cycle in the largest possible area. Anyone can take part in the events.

The population of the house sparrow is particularly affected, the number of

which has decreased catastrophically in many of the surveyed regions. In contrast, the field sparrow can live in natural areas far from humans, but it is increasingly settling nearby and even mixed flocks with brownies are found. This trend is of interest to experts. Sparrows need care and support from people, the expert reminds. For example, people can organize bird feeding. The main food for sparrows is millet and millet (without shell). In the cold season, sparrows prefer unroasted unsalted sunflower seeds, and in severe frosts they will not give up fat, like many other birds that huddle to human habitations in winter.

• The house sparrow constantly lives next to a person, strongly depends on him. Any change in human economic activity affects this species.

• The field sparrow lives outdoors in the summer, but only winters in the city. At the same time, in the south, the field sparrow can nest far from habitation, although in the north it also clings to people.

Next to a person, sparrows have nothing to eat, no place to hide and hatch their chicks. The house sparrow is a pronounced synanthropic species. Thousands of years ago, it began to settle near humans and, as urbanization increased, it successfully expanded its range. The proximity to humans turned out to be mutually beneficial: sparrows feed their chicks with insects, helping to protect crops from pests, and it is easy for sparrows to find shelter, warmth and food next to humans.

But in recent years, something has gone wrong.

Some of the possible reasons for the decline in sparrow numbers:

• In the new houses, there are practically no niches in which birds used to shelter from the weather and safely hatch their chicks.

• Farming and park landscaping methods, including lawn mowing, prevent seeds from ripening to feed adult birds.

• Treatment of plants with pesticides against pests reduces the chances of successfully breeding chicks due to lack of food.

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field sparrow can live in natural areas far from humans, but it is increasingly settling nearby and even mixed flocks with brownies are found. This trend is of interest to experts. Sparrows need care and support from people, the expert reminds. For example, people can organize bird feeding. The main food for sparrows is millet and millet (without shell). In the cold season, sparrows prefer unroasted unsalted sunflower seeds, and in severe frosts they will not give up fat, like many other birds that huddle to human habitations in winter.

Почему сегодня для человечества так важно считать воробьев?

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Die Rolle langer nichtkodierender RNAs für die Rezeptivität von Endometrium und Perspektiven der Diagnostik von Implantationsstörungen

Die Embryonenimplantation ist ein hochkomplexer, mehrstufiger biologischer Prozess, der eine präzise synchronisierte molekulare Interaktion zwischen der Blastozyste und dem Endometrium erfordert. Die Qualität des Embryos und die Rezeptivität des Endometriums gelten als Schlüsselfaktoren für eine erfolgreiche Implantation. Das Endometrium ist die innere Schleimhaut der Gebärmutter, es besteht aus zwei Schichten: dem konstanten Stratum – diese Schicht ist basal und dem hormonsensitiven Stratum – diese Schicht ist funktional. Unter dem Einfluss der Steroidhormone (Östrogen, Progesteron) wird das Endometrium zyklisch umgebaut.

Die Rezeptivität des Endometriums bezeichnet dessen Fähigkeit, den Embryo

aufzunehmen und seine weitere Entwicklung zu ermöglichen. Das „Implantationsfenster“ beim Menschen öffnet sich etwa am 19. Tag eines normalen Menstruationszyklus und schließt am 23. Tag (Dauer: 4-5 Tage). Innerhalb dieses Zeitraums durchläuft die Implantation drei aufeinanderfolgende Phasen:

1. **Apposition** – Der Embryo orientiert sich in der Uterushöhle. Progesteron induziert die Entfernung von Mucinen von der Epitheloberfläche, wodurch Adhäsionsmoleküle (z. B. Integrine αVβ3) freigelegt werden. Diese dienen als Signale für die Lokalisation des Embryos.

2**. Adhäsion** – Es entsteht eine stabile Verbindung zwischen dem Trophoblasten und den Epithelzellen über Ligand-Rezeptor-Interaktionen. Zu den Schlüsselmolekülen gehören LIF (Leukämie-Hemmfaktor), Osteopontin und verschiedene Integrine. Diese Phase ist irreversibel und stellt den eigentlichen Beginn der Implantation dar.

3. **Invasion** – Trophoblastzellen dringen in die Stromazellen des Endometriums ein. Es kommt zum Umbau der mütterlichen Gefäße und zur Bildung der Plazenta. Dieser Prozess ist abhängig von der Dezidualisierung der Stromazellen (Umwandlung in deziduale Zellen) und der lokalen Immuntoleranz. Eine gestörte Dezidualisierung führt häufig zu Implantationsversagen oder Fehlgeburten. Eine Störung einer dieser drei Phasen kann selbst bei Vorhandensein eines hochwertigen Embryos zum Implantationsversagen führen.

Lange Zeit galt die histologische Datierung nach Noyes als Goldstandard zur Beurteilung der Endometriumrezeptivität. Diese Methode ist jedoch hochgradig subjektiv, weist eine geringe Reproduzierbarkeit auf und erfasst nicht das funktionelle molekulare Profil des Endometriums. Der moderne ERA-Test (Endometrial Receptivity Array) analysiert die Expression von 238 protein-kodierenden Genen und kann eine Verschiebung des Implantationsfensters erkennen. Allerdings ignoriert dieser Test die große Gruppe der nichtkodierenden RNAs, die etwa 98 % des menschlichen Transkripts ausmachen.

Lange nichtkodierende RNAs (lncRNAs) sind Moleküle mit einer Länge von

mehr als 200 Nukleotiden, die nicht in Proteine übersetzt werden. Sie zeichnen sich durch drei Eigenschaften aus: *hohe Gewebespezifität* – viele lncRNAs werden nur in bestimmten Zelltypen exprimiert. *Regulatorisches Potenzial* – sie wirken als molekulare „Schwämme“ (ceRNA-Mechanismus), modulieren die Chromatinstruktur oder beeinflussen die mRNA-Stabilität. *Dynamische Expression im Zyklus* – im menschlichen Endometrium wurden bis zu 742 lncRNAs identifiziert, die sich zwischen rezeptiven und nichtrezeptiven Phasen signifikant unterscheiden.

Ergebnisse aktueller Studien: Bei Patientinnen mit wiederholten Implantationsversagen (RIF) ist die Expression der lncRNA **H19** signifikant reduziert (Zeng et al.). H19 ist an der Zellproliferation und an dem genomischen Imprinting beteiligt. In Tiermodellen (Zhang et al., 2019) konnte gezeigt werden, dass **lncRNA 882** als kompetitive endogene RNA (ceRNA) für miR-15b fungiert und dadurch die Expression von LIF erhöht – einem Zytokin, das für die Adhäsion des Embryos essenziell ist.

In einer Studie von Obukhova et al. (2022) wurden 44 Frauen untersucht (Altersgruppen: 23–27 Jahre vs. 47–50 Jahre). Bei Patientinnen über 45 Jahren fanden sich 144 signifikant differenziell exprimierte Transkripte, die mit zellulärer Seneszenz, gestörter Dezidualisierung und verminderter Rezeptivität assoziiert sind. Xu et al. (2019) analysierten Endometriumbiopsien von 5 Frauen mit RIF und 5 fertilen Kontrollpersonen (Alter 18–37 Jahre) mittels RNA-Seq. Sie identifizierten lncRNAs wie H19, NEAT1 und TRG-AS1 als zentrale Knoten in ceRNA-Netzwerken, die mehrere tausend Gene regulieren. Zusätzlich wurden 13 verschiedene microRNAs nur in der Endometriumgruppe von RIF-Patientinnen nachgewiesen, die die Expression von etwa 3800 Genen potenziell beeinflussen.

Zusammenfassend können von uns solche Stichpunkte unterstrichen werden:

1. LncRNAs spielen eine wesentliche Rolle bei der Regulation der Rezeptivität von Endometrium, insbesondere über den ceRNA-Mechanismus (z. B. Regulation von LIF und HOXA10). Ihre hohe Gewebespezifität und zyklusabhängige Expression machen sie zu vielversprechenden Biomarkern für die personalisierte

Reproduktionsmedizin.

2. Die Integration von lncRNA-Panels in die präimplantative Diagnostik könnte den optimalen Zeitpunkt des Embryotransfers präzise bestimmen und die Erfolgsraten der IVF deutlich verbessern.

3. Einschränkend fehlen derzeit große prospektive Studien am humanen Endometrium unter Berücksichtigung des Alters der Patientinnen.

Роль длинных некодирующих РНК в рецептивности эндометрия

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Large Language Models (LLM): training and their applications in automation

Large Language Models (LLMs) are neural networks based on transformers, trained on a massive corpus of text. They possess a wide variety of skills including natural language understanding, code generation, and complex reasoning [1]. So widely used now are models like GPT-4, LLaMA and Claude that they are being employed directly in engineering and industry. By linking human language and machine-executable logic, they mark a turn in the way we can build and operate automated systems.

The training pipeline of an LLM has two phases. During pre-training, the model reads more than several trillion tokens of corpora and learns to predict the next

token autoregressively, learning grammar, facts, and reasoning. Running on distributed clusters of thousands of GPUs/TPUs, the computational costs for these frontier models are in the hundreds of million dollars. During the fine-tuning stage, the pre-trained model is adjusted with human preferences by Reinforcement Learning from Human Feedback (RLHF): human annotators are asked to rank model outputs, a reward model is trained on these rankings and the LLM is optimized through proximal policy optimization (PPO). Direct Preference Optimization or DPO is a more computationally efficient alternative and is a recent practical alternative to the full RLHF pipeline [2].

In industrial automation, LLMs are reshaping the interaction between engineers and control systems. Traditional programmable logic controller (PLC) programming requires specialized expertise and extensive manual effort for each reconfiguration. LLM-based agents can now generate IEC 61131-3 structured text programs from natural language task descriptions, interpret SCADA interface data, and perform root cause analysis on industrial alarm logs. In robotics, LLMs function as high-level reasoning engines: they decompose ambiguous instructions into executable subtasks, coordinate multi-agent systems, and interface with external tools and APIs through agentic frameworks such as LangChain and AutoGen [3].

Despite their transformative potential, LLMs present challenges in safety-critical deployments, including hallucination, context limitations, and adversarial prompt sensitivity. Hybrid architectures combining LLMs with formal verification and physics-based models are being developed to ensure reliability. As these challenges are addressed, LLMs are positioned to become foundational components of the next generation of intelligent, adaptive, and human-centered automated systems.

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Большие языковые модели (LLM):
обучение и применение в автоматизации

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Graphene oxide: how selective protection against bacteria works

The cleanliness of things that we come into contact with every day – whether it's clothes, masks or toothbrushes – is not only a matter of comfort, but also of health. Classical antibiotics, for all their effectiveness, have played a cruel joke on us: the bacteria have learned to defend themselves, and now we are dealing with resistant strains. This explains the interest in new materials that can inhibit the growth of microbes without harming humans and without provoking another round of evolution of superbugs.

Graphene oxide (GO) became the focus of the presented study. Scientists

wondered: how does this substance deliver a pinpoint blow to a bacterial cell, completely without touching the cells of the human body?

Graphene oxide is structurally a carbon plane with a thickness of one atom (graphene itself), dotted with oxygen–containing groups. This "chemical edge" gives the material the ability to easily mix with water and interact with other molecules. A curious detail has emerged: these oxygen groups act like a lock that only one key fits, a lipid called POPG (phosphatidylglycerol). And POPG is a part of the membranes exclusively of bacteria. Mammalian cells have membranes arranged differently, and there is no such "password" there. For graphene oxide, the human cell remains simply invisible and uninteresting.

The process can be compared to the operation of a magnet, which attracts only a certain type of metal, ignoring the rest. GO finds a unique label in the bacterium, attaches to it, and disrupts the integrity of the shell. Bottom line: the microorganism dies, and neighboring human cells continue to work as if nothing had happened. The work provided a clear molecular rationale for what had previously been a hunch.

It is curious that technology has already left the walls of scientific institutes and gone to the people. The toothbrush with antibacterial graphene coating, created on the basis of university patents, has sold more than 10 million copies worldwide. The same principle is embedded in the GrapheneTectile material, from which uniforms were sewn for the demonstration performances of the taekwondo team at the 2024 Olympics in Paris. Fibers with this additive do not lose their bactericidal properties even after dozens of washing cycles, which opens the way for them to manufacture sportswear, medical textiles and other household items in contact with the skin.

These applied things are based on a fundamental physical discovery. Recall that graphene itself was isolated in 2004 by Konstantin Novoselov and Andrey Geim, natives of Russia, who worked at the University of Manchester. The 2010 Nobel Prize in Physics was a recognition of the significance of their work, and this paved the way for biomedical experiments with graphene derivatives.

Professor Sang Wook Kim, who led the research team, emphasizes: it was possible to scientifically prove why graphene oxide is able to distinguish a pathogen from healthy tissues. Relying on this mechanism, it is possible to create not only safe "chemically clean" clothes. The horizon is much wider: wearable gadgets, smart dressings, and fundamentally different approaches to fighting infections where conventional drugs are already powerless in the face of microbial resistance.

Оксид графена: как работает избирательная защита от бактерий

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УДК 615.47:616-08

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Electronics can save lives

It is hard to imagine modern medicine without electronics. Over the past few decades, electronic devices have moved far beyond simple convenience tools – today they are directly responsible for keeping people alive. Whether it is a tiny chip implanted near someone's heart or a gas sensor mounted on a factory wall, electronics has become a core part of how we protect human life.

The invention of implantable and wearable biomedical devices is among the most important contributions of electronic devices to medicine. ICDs and pacemakers are implantable devices that ensure the heart rhythm creates impulse to not have sudden cardiac arrest. Modern pacemakers have ultra-low-power microcontrollers, wireless telemetry modules, and lithium-ion batteries that last more than ten years, showing the top level of miniaturized electronic engineering. In the same way,

biosensor arrays and real-time signal processing algorithms are used in continuous glucose monitoring systems for diabetic patients to obtain life-saving metabolic information without blood sampling [1].

The implementation of electronic systems that can be networked is being used in EMS operations to carry out assessments and provide care. Automated External Defibrillators (AEDs) are now found in many public places. They contain intelligent signal analysis circuits. These circuits can differentiate shockable rhythms, like ventricular fibrillation, from non-shockable rhythms. Thus, a first responder without any medical training can deliver effective cardiac therapy. The utilization of AEDs in IoT-enabled emergency response networks allows for real-time monitoring of AED locations and fast dispatching to users, which reduces the time taken to reach the patient and applies a shock-defibrillation. This is a critical factor in improving survival chances during a cardiac arrest [2, 3].

In industrial facilities, electronic protection systems avert disasters. Gas leak detection sensors made from metal-oxide semiconductor (MOS) provide continuous monitoring of the atmosphere in hazardous facilities. In conclusion, electronics represents an indispensable pillar of modern life-safety infrastructure. The convergence of microelectronics, sensor technology and wireless communication has produced systems capable of monitoring, diagnosing, and responding to life-threatening conditions with unprecedented speed and precision. Continued investment in biomedical electronics research and cross-disciplinary collaboration between engineers and medical professionals will be essential to further expand the boundaries of what technology can do to protect human life.

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Электроника спасает жизни

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Main Directions and Problems of Theoretical Physics: A Historical Path to the Quantization of Gravity

Twentieth-century theoretical physics gave science two fundamental concepts: general relativity, which treats gravity as the geometry of spacetime, and quantum mechanics, which describes the laws of the microcosm. Each of these theories has been brilliantly confirmed in its own domain – from cosmological scales to the physics of elementary particles – yet their synthesis faces insurmountable difficulties today.

The problem of quantizing gravity became the main challenge for theoretical physics in the second half of the twentieth century, and attempts to solve it led to the formation of two competing programs: string theory and its variations (for example – M-theory), and loop quantum gravity (LQG).

String theory which emerged in the 1970s proposed replacing point-like particles with one-dimensional objects strings – which naturally allowed gravity to be incorporated into a unified quantum framework.

Throughout the 1980s and 1990s this approach was regarded as the leading candidate for a “theory of everything”; however, the lack of experimentally testable predictions and the reliance on unobservable extra dimensions gave rise to widespread criticism. A key problem of string theory is the so-called landscape – the existence of about 10^{500} different vacuum states which deprives the theory of predictive power.

A separate heated debate concerns the potential fundamental unverifiability of the string approach. The energies required for the direct observation of strings (the Planck scale, $\sim 10^{19}$ GeV) are orders of magnitude beyond the reach of any conceivable accelerator, shifting the question of the theory’s truth from the experimental realm to that of mathematical elegance and philosophical preference.

The alternative approach – loop quantum gravity – rejected the introduction of extra dimensions and focused instead on directly quantizing the fabric of spacetime itself. Despite its mathematical elegance and absence of redundant degrees of freedom, loop quantum gravity faces difficulties in recovering classical geometry in the large-scale limit. Remarkably, both programs exhibit a similar methodological crisis: they generate highly sophisticated mathematical machinery but remain empirically unverifiable given current technological capabilities.

This has led part of the scientific community to doubt that the problem is purely technical; perhaps a reconsideration of the very foundations of physical knowledge is required. A historical analogy with the crisis of classical physics at the turn of the 19th and 20th centuries suggests that the way forward may lie not in further complicating existing theories, but in a radical shift of conceptual paradigm.

Thus, the current stage of development of theoretical physics can be characterized as a transition from the search for a single “theory of everything” towards an awareness of the limits of existing methods and the need to develop new epistemological approaches.

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Основные направления и проблематика теоретической физики: исторический путь к квантизации гравитации

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Research of the optical properties of polyanilin by spectroscopy methods

Currently, significant interest focuses on the photoconductive properties of organic semiconductors, particularly polyaniline-based thin films. Their photoconductivity depends heavily on the solvent, dopant type, and concentration. Optical spectroscopy is a key characterization tool, allowing band gap determination from absorption spectra; a narrower band gap correlates with higher conductivity. Furthermore, maintaining the supramolecular structure during heat treatment up to 350 °C is critical for ensuring reproducible electrophysical properties [1-2].

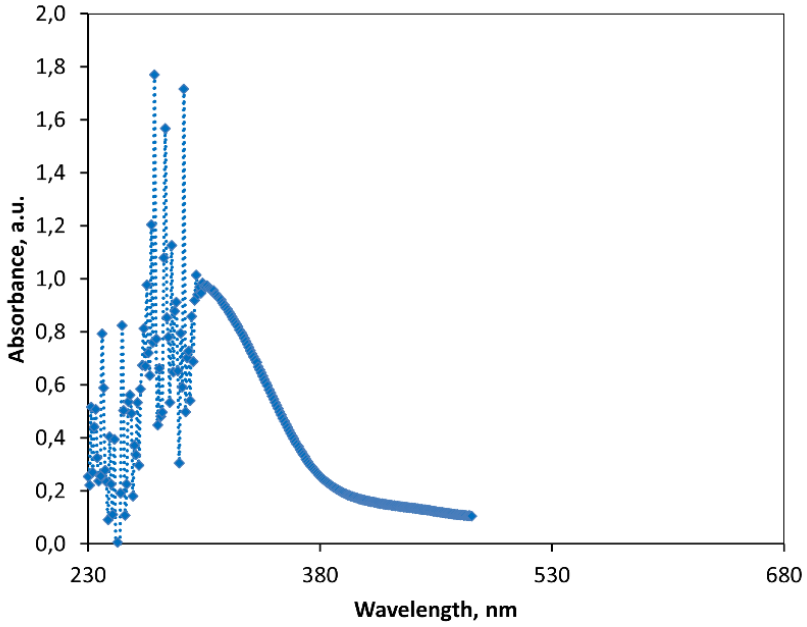

Fig. 1. Polyaniline absorption spectrum

Fig. 1 shows a curve describing the absorption spectrum of a polyaniline sample. The spectrum demonstrates an intense band in the ultraviolet region with a maximum around 300-320 nanometers and an optical density of approximately 1.0 a.u. After 350 nanometers, there is a gradual decrease in absorption, and in the 400-500 nanometer region, there is a small shoulder characteristic of polyaniline quinoid structures.

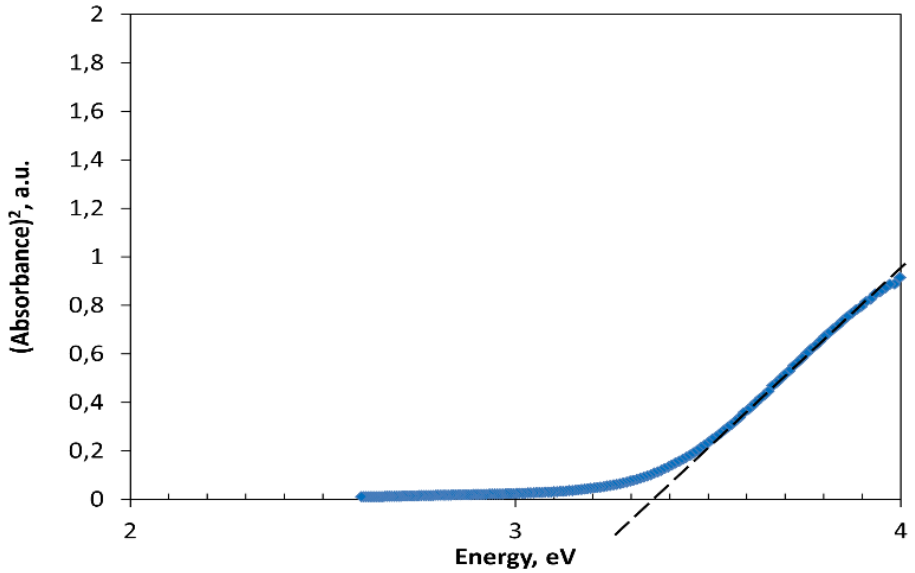

Fig. 2. Dependence of the optical density square on photon energy

Fig. 2 shows the dependence of the square of the optical density on the photon energy, which was used to determine the band gap width using the Tauc method.

There is almost no absorption at energies below 3 eV, while there is a sharp increase in the curve above 3.3 eV. By extrapolating the linear portion to the x-axis, the band gap of the polyaniline sample was estimated to be between 3.30 and 3.35 eV.

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Исследование оптических свойств полианилина методами спектроскопии

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Graphen: physics of two-dimensional carbon and its properties

What is graphene?

Carbon has several forms such as three-dimensional, one-dimensional and zero-dimensional. Graphene is a two-dimensional allotropic form of carbon, the most

studied from a theoretical point of view [1, p. 12]. It is a monatomic layer of carbon that has incredible properties. Graphene was discovered in 2004 by scientists Andrey Geim and Konstantin Novoselov and in 2010 they were awarded the Nobel Prize in Physics for their work with graphene [2, p. 3].

Unique properties of graphene

Graphene being pure carbon, has a unique structure thar allows each of its particles to enter into mixing reactions from different sides. The particles on the edges of the graphene sheet exhibit a special chemical activity. This is due to the fact that this region contains the largest number of edge atoms. The impurities inside the graphene sheet increase the reactivity. Graphene can be modified with various chemical groups, which makes is possible to create a variety of materials, including graphene oxide and fluorinated graphene. The modification of graphene with hydrogen is called graphene.

Where is graphene used?

Graphene, due to its outstanding characteristics, is widely used in various fields.

In electronics, graphene is used to create ultrafast transistors and flexible displays. It transmits 97.7% of light and conducts current well, which allows it to replace fragile and expensive materials in transparent electrodes. Graphene is also used in photodetectors operating in a wide optical range.

In the energy industry, graphene is used in supercapacitors and lithium-ion batteries due to its high specific surface area and conductivity, which increases their capacity and charging speed. Due to its strength, graphene is added to polymers, concrete and other materials to create heavy-duty and lightweight composites for automotive, aviation and sports equipment.

Graphene is used in medicine for targeted drug delivery, cancer therapy (photothermal cell destruction), as well as in biosensors and tissue engineering. Graphene's high sensitivity makes it possible to create glucose, gas, and biomarker sensors based on it for medical diagnostics.

Due to the high thermal conductivity of graphene, it is used to remove heat in smartphones (Huawei, Xiaomi) and laptops. It is also used in audio technology to improve sound quality, in membranes for water filtration and in smart window coverings that reduce noise and prevent icing.

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Графен: физика двумерного углерода и его свойства

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The Pik Reactor In Neutron Studies

PIK is a high-flux research nuclear reactor being developed in Gatchina by the B. P. Konstantinov Petersburg Nuclear Physics Institute (NRC Kurchatov Institute – PNPI) [1].

PIK, originally developed on the basis of water-moderated reactors, is a research complex distinct from a power reactor, the purpose of which is to produce the maximum neutron flux density. These neutrons are subsequently used for structural neutron diffraction. Its enormous success is attributed to the neutron facility to built within the reactor. The PIK reactor is the most powerful neutron scattering

reactor in the world; however, to date, no new ideas or proposals exist that could increase the neutron flux while maintaining the energy release (2 MW per L^3), which requires continued decommissioning [2-4].

Virtual modeling and computer simulation methods are used to solve and optimize such problems. Existing programs and mathematical models make it possible to completely disrupt and simulate the behavior of physicochemical systems and the processes occurring within them. The usage of such programs requires extensive knowledge in computer science and cheminformatics, chemistry and physics, as well as an understanding of instability and weak-solid flux. Specialists with knowledge of these phenomena are in incredible demand in today's rapidly evolving scientific field.

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Physics and mathematics in nature: three secrets

In our daily life, we often meet interesting phenomena. They catch our attention, and we want to understand how they work. To help us with that, we use the laws of physics and mathematics.

Today I want to show you three phenomena and explain how they happen. We will learn:

– Why a cat always lands on its paws.

– How a chameleon changes its color.

– Why a snowflake always has the shape of a hexagon (six sides).

1. The Cat That Always Lands on Its Paws

You have probably seen that cats can land on their paws, even if you drop them upside down. This ability is natural for them.

It may seem amazing to us. We think an animal needs something to push off from. But a cat turns in the air without anything to push against.

The secret: The cat uses the law of conservation of angular momentum. It changes its moment of inertia to control its spin. A classic mathematical explanation of this phenomenon was first proposed by Kane and Scher in 1969, who described the cat as a system of two cylinders connected by a flexible axis [1, p. 663-665].

How does this work? Let's look at a figure skater first.

A figure skater changes her spin speed by changing her moment of inertia:

– When she puts her arms close to her body, she spins faster.

– When she stretches her arms out, she spins slower.

We can understand this with a simple formula: $L = I \times \omega$.

Where:

– L = angular momentum (stays the same)

– I = moment of inertia (changes when she moves her arms)

– ω = spin speed (changes in the opposite way to keep L the same)

Now, how does the cat do it?

A figure skater spins as one whole body. But a cat can do this trick two times — first with its front part, then with its back part. Why? Because the cat has a very flexible spine.

The cat's L (angular momentum) stays the same, just like the skater's. But the cat changes its moment of inertia in two steps:

Step 1: The cat tucks its front paws in (small moment of inertia). The front part turns quickly toward the ground. At the same time, the cat stretches its back paws out (large moment of inertia). The back part stays in place.

Step 2: Now the front part is already facing down. The cat stretches its front paws out (large moment of inertia). The front part stops turning. Then the cat tucks its back paws in (small moment of inertia). The back part turns quickly to face down.

Result: All four paws point down, and the cat lands safely.

The cat uses the laws of physics to land on its paws. In a very short time, it follows an instinct – a gift from nature.

2. How a Chameleon Changes Color

A chameleon can change the color of its skin. It uses this ability for:

– Communicating with other chameleons

– Showing its mood (anger, fear, calm)

– Controlling its body temperature

To change color, the chameleon uses the physics of light.

How do we see color?

When light hits an object, the object absorbs some waves and reflects others. The reflected waves go into our eyes, and we see a certain color. Which color we see depends on the wavelength:

– Short waves → blue, green

– Long waves → orange, red

What is under the chameleon's skin?

The chameleon's skin has several layers.

Upper layer: Tiny, transparent crystals arranged in neat rows – like a grid or a net.

Lower layer: Cells with a dark pigment. This layer works as a background. It absorbs extra light to make colors look bright.

For a long time, scientists believed that chameleons changed color using pigments. However, in 2015, a research team led by Teyssier proved that chameleons actually change color by changing the distance between guanine crystals in their skin [2, p. 1].

How does the color change?

When the chameleon is calm: The skin is relaxed. The crystals are packed close together. This grid reflects short waves – blue and green. Under the crystals there is also a yellow pigment. So we see green.

When the chameleon is excited (angry, scared, or wants to warm up): Muscles stretch the skin. The crystals move apart. The distance between them increases. This grid reflects long waves – yellow, orange, red.

The chameleon uses its natural body structure to communicate with the world. And it does this using physical laws.

3. Why a Snowflake Always Has Six Sides

We know that all snowflakes are unique. Temperature and humidity affect their shape. But all snowflakes share one thing: they always have six sides or six rays.

You will never find a snowflake with five or eight rays. Why?

It starts with the water molecule. A water molecule has one oxygen atom and two hydrogen atoms. When water freezes and turns into ice, the molecules connect to each other at a specific angle. They form a grid where the angle between bonds becomes 120 degrees. In his famous lectures, Feynman discussed how the bond angle of water molecules (about 105°) leads to the hexagonal symmetry of snowflakes[3, Vol. II, Chapter 7].

Why does nature choose a hexagon?

Nature always chooses the most stable and energy-efficient shape. For frozen water, the hexagon is the best choice. Why?

The hexagon is the only shape that:

– Fills a flat surface without gaps

– Matches the natural bond angle of water molecules (120°)

– Gives the maximum packing density

A real-life analogy: Cans in a box. Imagine you need to pack round cans in a box.

– If you put them in straight rows (square packing), there is empty space in the middle between four cans. This space is wasted.

– But if you shift every second row by half a can, the cans fall into those empty spaces. When you look from above, you see hexagons.

This hexagon packing gives you more cans in the same box. It is denser and more efficient.

The same thing happens with water molecules in a snowflake.

A snowflake always takes the shape of a hexagon because math tells nature to do so. The angles, the distances, the packing – everything follows numbers.

We have looked at three fascinating phenomena:

1. The cat – uses the physics of spin to land on its paws.

2. The chameleon – uses the physics of light to change color.

3. The snowflake – follows the math of angles to form a hexagon.

What unites all three? In each case, nature chooses the most effective solution. And to do this, nature uses two sciences that we find so interesting to study: physics and mathematics.

Nature does not guess. Nature calculates. Physics and math are its tools.

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Физика и математика в природе: три секрета

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Terminological Precision in Intercultural Communication of Medicinal Chemists

Work in the field of medicinal chemistry, especially that related to the computational assessment of protein–ligand interactions, constantly encounters a situation where English-language terms lack unambiguous Russian-language equivalents. Concepts established in international standards, when translated literally, lose part of their instrumental meaning, which complicates professional

communication between computational chemists, synthetic chemists, and pharmacologists.

One of the most illustrative examples is *docking*. According to the IUPAC definition, this is a set of methods that optimize the placement of a ligand in the binding site of a macromolecule and evaluate the quality of this placement using scoring functions [1]. In Russian-language literature, the calque “molecular docking” (молекулярный докинг) has become established, but the understanding that the procedure includes not only “docking” but also the subsequent analysis of the predictive power of the model is often lost behind it. For experimental colleagues, such incompleteness of the term can be critical.

A similar problem arises with the term *scaffold*. In the context of drug design, this is not merely a “skeleton” or “framework” of a molecule, but a structural core that determines the arrangement of pharmacophoric groups. Translating it as “framework” (каркас) neutralizes an important aspect – the ability of this core to undergo modifications while maintaining the key binding characteristics to the target. Without an understanding of this distinction, the meaning of strategies such as *scaffold hopping*, which have become a routine tool for searching for new chemical types of compounds, is lost.

The translation of *binding site* is no less challenging. Although Russian-language texts most often use “binding center” (центр связывания) or “binding region” (участок связывания), in modern structural biology this concept includes not only the static geometry of the pocket but also its conformational mobility [2]. The functionally significant region represents a dynamic ensemble of states that adapts to the ligand. A literal translation does not convey this lability, and therefore does not reflect modern approaches that take receptor flexibility into account.

The term *simulation* in Russian-language practice is often rendered as “modeling” (моделирование), whereas in the English-language methodological tradition it more often refers to molecular dynamics, that is, to accounting for the time evolution of the system. Without specifying the type of modeling, the listener or

reader may misjudge the level of accuracy and the time scale of the computations performed.

The way out of these terminological contradictions lies not in the search for an ideal translation, but in the development of a metalanguage for professional communication. Instead of mechanically using the calque “docking,” it is more productive to describe the procedure by indicating its purpose and method: for example, “computational screening of ligand orientation in the binding cavity with ranking by calculated binding affinity.” This approach eliminates ambiguity and corresponds to the standards for describing computational experiments adopted in international peer-reviewed journals.

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Терминологическая точность в межкультурной коммуникации медицинских химиков

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Potassium hexacyanoferrate (III): a comparative analysis of electronic structure within the framework of valence bond theory and crystal field theory

This article examines potassium hexacyanoferrate(III), commonly known as "red blood salt", and analyses its structure from two theoretical perspectives: valence bond theory (VBT) and crystal field theory (CFT). VBT explains the geometry and hybridization of the complex, whereas CFT reveals the origin of its colour through the splitting of d-orbitals. Thus, these theories not only describe the geometric structure and hybridization of molecules, but also elucidate the mechanisms underlying the unique physical and chemical properties of the substance.

According to Werner's coordination theory, a complex compound consists of an inner and an outer sphere. The central atom (coordination number = 6) together with its surrounding ligands form the inner sphere of the complex, which is conventionally enclosed in square brackets. All components written outside the brackets constitute the outer sphere [2, p. 7].

The valence bond method *(Fig. 1)* allows determination of the geometry of potassium hexacyanoferrate(III). Chemical bonds are formed using one s-orbital, three p-orbitals of the outermost energy level, and two d-orbitals of the penultimate level. This indicates that the complex adopts an octahedron configuration (hybridization type: d^2sp^3). Based on the structure of $K_3[Fe(CN)_6]$, it is noted that the complex is attracted to a magnetic field and is classified as an inner-orbital complex.

Crystal field theory *(Fig. 2)* describes the electrostatic interaction between the positively charged Fe^{3+} ion and the negatively charged ligands, modeled as point charges generating an electrostatic field. As a result of this interaction, the d-orbitals of the iron ion undergo splitting: electrons located closer to the ligands occupy higher

energy levels compared to those on more distant orbitals. CFT enables calculation of the crystal field stabilization energy (CFSE) and the magnetic moment (μ) [1, p. 192].

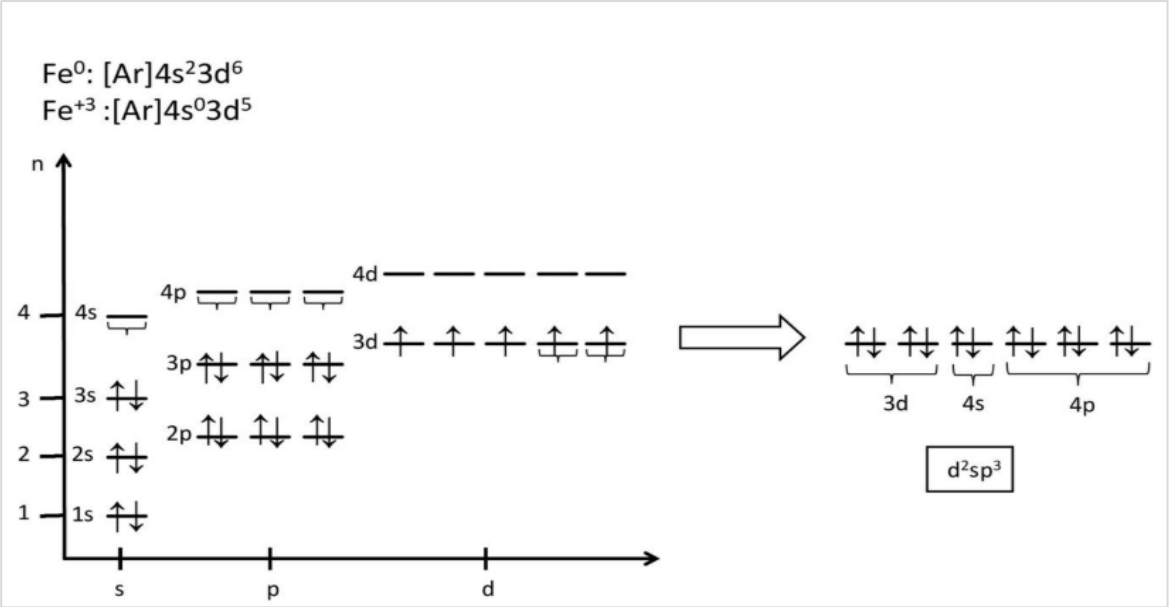

Fig. 1. Structure of $K_3[Fe(CN)_6]$ according to Valence Bond Theory

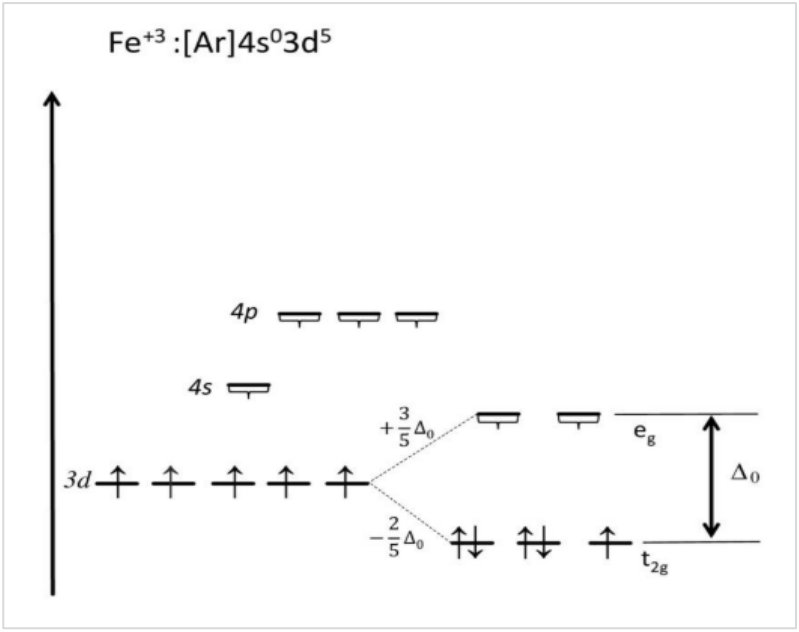

Fig. 2. Application of Crystal Field Theory to octahedron complexes

$$CFSE = -\frac{2}{5}\Delta_o \cdot 5 + \frac{3}{5}\Delta_o \cdot 0 = -\frac{10}{5}\Delta_o = -2\Delta_o$$

$$\mu = \sqrt{(n+2)\cdot n} = \sqrt{(1+2)\cdot 1} = \sqrt{3}\text{ мБ}$$

Consequently, the complex is colored due to the presence of free d orbitals and is low-spin due to the strong field of ligands.

Below is a summary table comparing theoretical approaches to the description of a coordination compound.

Table 1

Comparative characteristics of VBT and CFT for describing the structure of potassium hexacyanoferrate(III)

Criterion of comparison:	***VBT:***	***CFT:***
Explanation of complex geometry	+	+
Determination of hybridization type	+	–
Explanation of colour (d–d transitions)	–	+
Prediction of magnetic properties	+	+
Calculation of stabilization energy (CFSE)	–	+
Consideration of ligand field strength	–	+
Quantitative estimation of Δ_0	–	+
Explanation of low-spin/high-spin configurations	–	+
Explanation of para-magnetism in $[Fe(CN)_6]^{3-}$	+	+
Description of inner/outer sphere (Werner)	+	+

Thus, the complex of potassium hexacyanoferrate(III) can be characterized from the standpoint of two theoretical approaches. According to the valence bond method, the compound is formed by d2sp3 hybridization of the central Fe3+ ion, where the surrounding ligands provide electron pairs, forming an octahedron geometric structure. Within the framework of the crystal field theory, the complex is stabilized due to the low level of orbital filling. The presence of one unpaired electron determines the para-magnetic properties of a substance

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Красная кровяная соль: сравнительный анализ электронной структуры в рамках МВС и ТКП

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Synthesis and characterization of high-purity copper (II) sulfate for use as a micronutrient fertilizer and fungicide

Copper(II) sulfate ($CuSO_4 \cdot 5H_2O$) is an essential source of the micronutrient copper in agrochemistry. Copper is a component of key enzymes involved in plant photosynthesis and respiration, and it also increases resistance to fungal and bacterial diseases. However, the effectiveness and safety of copper-containing preparations directly depend on the purity of the compound. The presence of heavy metal impurities can lead to their accumulation in soil and plants, exerting a toxic effect. Therefore, the development of accessible methods for producing high-purity copper sulfate is an urgent task. The aim of this work is to develop a method for the synthesis of high-purity CuSO with subsequent verification of its composition by X-ray phase analysis (XRD).

The synthesis was carried out by dissolving 8.0 g of high-purity copper(II) oxide (CuO) in 100 ml of dilute sulfuric acid (H_2SO_4) with heating to 60–70°C and constant stirring. The hot solution was filtered to remove insoluble impurities. The filtrate was evaporated to one-third of its volume and left for slow cooling to room temperature. The precipitated intense-blue crystals of $CuSO_4 \cdot 5H_2O$ were separated

by filtration, washed with chilled distilled water, and dried. The product yield was 90%. XRD analysis of the obtained powder sample was performed on a diffractometer in the angle range 2θ = 5–100°. The synthesis of copper(II) sulfate with a 90% yield was successfully carried out using simple laboratory equipment. XRD analysis confirmed that the obtained compound is phase-pure copper(II) sulfate pentahydrate ($CuSO_4 \cdot 5H_2O$). The absence of impurity peaks proves the effectiveness of recrystallization. The proposed method is reproducible, safe, and optimal for obtaining copper(II) sulfate suitable for agricultural use as a micronutrient fertilizer and fungicide. High purity (>99.9%) guarantees no toxic effects on plants, stable solutions, and effective pathogen control.

Синтез и характеристика высокочистого сульфата меди (II) для применения в качестве микроудобрения и фунгицида

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Regulation of chemical safety in different countries

Chemicals are the foundation of modern civilization, without which it is impossible to exist. Unfortunately, many chemicals can be dangerous to human health and the environment. To make everything safe, there are rules all over the world that clearly prescribe how to handle chemicals: from production to disposal.

The problem is that chemical safety regulations vary greatly from country to country. In some places they are very strict, in others they are more lenient. In some cultures, people are more inclined to take risks, and the state relies on self–regulation,

while in others they prefer maximum caution and active regulation of everything related to chemistry. This creates a lot of difficulties.

To begin solving the problems, it is necessary to consider the peculiarities of the relations of different countries to possible hazards in the course of chemical activities of the state, their level of trust in scientific data and in government agencies. After a successful analysis, technical requirements should be agreed upon, strategies and plans should be developed that take into account possible disagreements, as well as the style and channels of communication.

Effective and beneficial international cooperation based on open dialogue, mutual respect and understanding of cultural aspects is the golden key to achieving unanimity and creating effective nationwide and acceptable systems for regulating chemical safety. This path contributes to the protection of human health and the environment, the development of the global economy and the building of friendly relations between countries.

Регулирование химической безопасности в разных странах

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Structural features of nanocrystalline lead sulfide (PbS) synthesized by precipitation

Lead sulfide (PbS) is a narrow-band semiconductor (band gap ~0.41 eV for bulk material) with unique optical and electrical properties that make it promising for use in infrared photodetectors, next-generation solar cells, and thermoelectric converters. The key factor that determines the functional characteristics of PbS is the

size of its crystallites: when it reaches a nanoscale, quantum confinement effects emerge, allowing for precise control of the material's optical properties. However, obtaining nanostructured PbS with reproducible parameters and minimal defects remains a challenging technological task. The aim of this work is to investigate the microstructural characteristics of a PbS sample synthesized in the laboratory of the Department of Inorganic and Technical Chemistry at the University of Science and Technology, and to assess the particle size and level of crystal lattice defects.

The lead sulfide sample was obtained by precipitation from aqueous solutions using a lead polysulfide complex. X-ray diffraction studies were conducted over a wide range of 2θ angles, from 26° to 95°. The phase composition was identified, and structural parameters were calculated using software for analyzing diffraction data. The size of the coherent scattering regions (D) was estimated using the Scherrer formula based on the physical broadening of the diffraction maxima, and the magnitude of microstrains (ε) was calculated based on the angular dependence of the peak broadening.

The analysis of the diffraction pattern confirmed the formation of a pure PbS phase with cubic symmetry (galena structure type, space group Fm-3m). The diffraction pattern showed 12 well-resolved reflections corresponding to the planes (111), (200), (220), (311), (222), (400), (331), (420), (422), (511), (333), and (440). The most intense peak at 2θ = 30.444°, corresponding to the (200) reflection, was taken as 100%.

The calculation of crystallite size based on individual reflections revealed a high degree of uniformity in the microstructure of the synthesized material. The D values vary in a narrow range from 13.2 nm (for reflection at 2θ = 69.225°) to 14.5 nm (for reflection at 2θ = 62.848°). The weighted average crystallite size is 13.8 nm. It is important to note that the particle size variation coefficient is extremely low, indicating that there is no pronounced growth anisotropy: the crystallites develop uniformly in all crystallographic directions, forming particles that are close to spherical or cubic in shape.

The assessment of the crystal lattice microstrains also demonstrated the high structural quality of the sample. The average relative strain value was 0.27%. The spread of values at different diffraction angles is insignificant (from 0.25% to 0.28%), indicating that there are no localized areas of high internal stress. The full width at half maximum (FWHM) for the main reflections is stable and ranges from 0.57° to 0.63°, which is consistent with the calculated nanoscale particle sizes and the low level of lattice distortions. The absence of significant broadening of peaks at high 2θ angles confirms the good crystallinity of the material and the absence of significant amounts of point defects or dislocations accumulated during the synthesis process.

The obtained results indicate that the chosen synthesis mode (deposition from polysulfide solutions under specified conditions) allows for the production of nanocrystalline lead sulfide with high structural characteristics. The small variation in crystallite sizes and the low level of microstrains create the prerequisites for the manifestation of clear quantum confinement effects and high carrier mobility in materials based on this powder. Further research will focus on studying the optical properties of the obtained nanoparticles and their application in composite materials for infrared optics and sensing.

Структурные особенности нанокристаллического сульфида свинца (PbS), синтезированного методом осаждения

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Synthesis and X-ray phase analysis of barium carbonate for medical purposes

Barium carbonate ($BaCO_3$) is a key precursor for the synthesis of barium sulfate, the main component of radiopaque agents used in medical diagnostics. The growing demands for the purity of pharmaceutical substances drive the development of effective synthesis methods. The precipitation method from aqueous solutions offers an optimal combination of cost-effectiveness, process control, and the ability to manage particle morphology.

The aim of this work is the synthesis of barium carbonate by precipitation from aqueous solutions followed by characterization of the product using X-ray phase analysis (XRD). The synthesis was carried out at room temperature by slowly adding an equimolar solution of Na_2CO_3 (analytical grade) to a solution of $BaCl_2 \cdot 2H_2O$ (analytical grade) with constant stirring (300 rpm). The resulting precipitate was filtered, washed with distilled water until a negative reaction for chloride ions, and dried at 80°C. XRD analysis was performed on a DRON-3 diffractometer (CuKα radiation) in the range 2θ = 20–100°. XRD analysis revealed the formation of a highly crystalline phase. The diffraction pattern corresponds to witherite (orthorhombic $BaCO_3$, space group Pmcn), fully matching reference data (PDF 00-005-0378). Intense reflexes were observed at 2θ ≈ 24.0°, 34.2°, 42.1°, and 44.9°, corresponding to the (111), (002), (221), and (132) planes. The crystallite size calculated for the (111) peak using the Scherrer formula was 45 ± 2 nm. The absence of extraneous peaks on the diffractogram confirms the phase purity of the product (>98%) and the selectivity of the synthesis method. A comparison with literature data shows that the obtained product is not inferior in purity and crystallinity to samples synthesized by more complex methods. The method is reproducible (confirmed by

three synthesis cycles) and energy-efficient.

Barium carbonate was successfully synthesized by the precipitation method. XRD confirmed the product as phase-pure witherite ($BaCO_3$) with >98% purity. The method is simple, reproducible, and cost-effective, making it suitable for the laboratory synthesis of standardized $BaCO_3$ for use as a pharmaceutical precursor.

Синтез и рентгенофазовый анализ карбоната бария медицинского назначения

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The luminescent method of blood detection using luminol solution

The investigation of violent crimes against individuals is impossible without a thorough examination of the crime scene. One of the key pieces of physical evidence in such cases is blood traces, which can not only confirm the fact that a crime has been committed but also help identify the perpetrator. However, perpetrators often attempt to destroy such traces by washing or concealing them, which significantly complicates the work of investigators.

Modern forensic science offers a number of methods for detecting blood traces – visual, chemical, and biological. Among these, a special place is occupied by the luminescent method using a luminol solution, which makes it possible to detect even minimal and thoroughly washed-away bloodstains that are invisible to the naked eye.

The purpose of this paper is to examine the mechanism of action of luminol, the process of chemiluminescence, the methods of preparing the solution, and to

analyze the advantages and disadvantages of this method in the context of its practical application in forensic science.

When luminol interacts with blood, blue chemiluminescence is observed. The glow occurs because luminol is a substance capable of blue chemiluminescence when it reacts with certain oxidizing agents. The exact mechanism of luminol chemiluminescence is a complex multi-step reaction, especially under aqueous conditions. In this case, it reacts with the iron present in blood and helps reveal traces invisible to the naked eye, even those that a perpetrator has attempted to conceal or wash away. When it is necessary to examine large areas or to search for old, washed-out bloodstains, the use of a luminol solution is the most optimal solution. This test has high sensitivity and sufficiently high specificity. A positive result is observed when a luminol solution interacts with blood diluted to a ratio of 1:500,000.

When treating surfaces with a luminol solution, another positive quality is that the characteristic glow of blood material after treatment is observed across the entire surface of the stain and fully replicates its shape. The use of a luminol solution requires additional preparation - examination with its use is conducted in a darkened room. In the case of incomplete darkening, a faint glow may go unnoticed. The luminol solution is prepared in two stages: the first involves dissolving weighed amounts of luminol and soda ash in distilled water (this solution can be stored for up to one month in a dark container); the second involves adding a 30% or 3% hydrogen peroxide solution immediately before use (a luminol solution combined with hydrogen peroxide cannot be stored).

Luminol is sold in pharmacies or chemical reagent stores in the form of a yellow powder. It can also be obtained in various forms — for example, it is an active ingredient in "Galavit" tablets, as well as in their analogues in the form of suppositories or ampoules (though this option will be very costly). Each tablet contains approximately 25 mg of the sodium derivative of luminol, and half a gram of this substance is sufficient to prepare 50 ml of a one-percent luminol solution. If plain dry luminol is used, it must first be dissolved in water before the reaction can take place.

The advantages of the luminescence method include high sensitivity and selectivity. The disadvantages include the existence of an upper limit on detectable concentrations, the irreversibility of most procedures, the sensitivity of analytical results to the presence of uncontrolled impurities, the need for temperature control, and the complexity of the instrumentation involved.

However, every method has its drawbacks. The luminol test does not distinguish between human blood and animal blood. The role that hemoglobin plays in human blood is performed in cold-blooded animals by hemocyanin, which contains copper rather than iron. Copper, in turn, also effectively catalyzes the oxidation and luminescence of luminol.

Another significant disadvantage of this method is that, beyond hemoglobin, there are other substances that sharply accelerate the oxidation of luminol - for example, sodium hypochlorite, which is a component of bleaching agents. This can in turn lead to false positive results, where luminescence occurs not due to the presence of blood but due to other substances. Nevertheless, the luminol test is very useful and is genuinely employed by forensic specialists, though its results are rarely relied upon exclusively.

The use of luminol makes any subsequent examination of the blood impossible, and therefore only a small portion of a bloodstain is subjected to preliminary testing, while micro-traces are not tested at all and are sent directly to the laboratory.

Blood stains can be used to identify a perpetrator, aided by the application of "biometric technologies" within the framework of personal data processing. Various chemical traps are also used in the fight against crime. For example, to prevent theft, devices are installed in locations where valuables are stored that, upon unauthorized entry, apply difficult-to-remove dye substances to the skin and clothing, or invisible markers that can prove a person's involvement in a crime. Certain medicinal substances can serve the same purpose - for instance, salicylic alcohol, which, upon

interaction with a three-percent solution of iron (III) chloride, changes its colorless appearance to violet.

Люминесцентный метод обнаружения крови с раствором люминола

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Application of potassium nitrate as a de-icing agent

Potassium nitrate (KNO_3) obtained by conversion synthesis has been studied. It does not corrode metals and does not damage concrete. X-ray phase analysis confirmed its high purity (no impurities). Due to its low aggressiveness and environmental friendliness, it is promising as a de-icing agent for airfields and roads. Potassium nitrate (KNO_3) is traditionally used as a mineral fertilizer, an oxidizer in pyrotechnics, and a preservative in the food industry. Recently, interest in its application in the road maintenance sector has grown due to properties such as minimal corrosive impact and the absence of degradation of road surfaces.

The study by Kistanova N. S. et al. describes a method for the conversion synthesis of KNO_3 from $Ca(NO_3)_2$ and KCl, ensuring a high product yield over a wide temperature range (from +20 to –20 °C).

The aim of this work is to evaluate the potential of phase-pure potassium nitrate, obtained via conversion synthesis, as an effective and safe de-icing agent, as well as to verify its purity by X-ray phase analysis (XRD). The synthesis of KNO_3 was carried out under laboratory conditions via a double displacement reaction:

$$Ca(NO_3)_2 + 2KCl \rightleftharpoons CaCl_2 + 2KNO_3.$$

The developed method for KNO_3 synthesis is simple to implement, reproducible, and does not require specialized equipment. X-ray phase analysis confirmed the high purity of the product, which is a necessary condition for its use as a de-icing agent. Due to its low corrosive activity, compatibility with concrete and asphalt concrete, as well as its environmental safety, potassium nitrate can be recommended for use at airfields, bridges, and in urban areas, especially in locations with strict environmental regulations.

Применение нитрата калия в качестве противогололедного реагента

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Theoretical and applied research problems of nanostructured semiconductors

Modern requirements for photovoltaic converters, sensors, and optoelectronic devices dictate the need to produce semiconductor materials with a controlled grain size and a minimum number of structural defects. In this context, cadmium sulfide (CdS) is one of the most promising materials due to its direct band gap and high photoactive properties. However, the performance characteristics of nanostructured CdS critically depend on the synthesis method, which determines the degree of crystallinity, particle size, and the level of internal stresses in the lattice. The purpose of this work is to perform a semi-quantitative X-ray phase analysis of a sample of nanocrystalline CdS, to estimate the size of crystallites and the level of

microdeformations based on diffraction data.

A sample of cadmium sulfide (batch identifier: 2026 03 02 CdS) obtained by precipitation was studied. X-ray examinations were performed in the range of sliding angles of 2θ from 25° to 82°. The diffractograms were deciphered with the identification of reflexes corresponding to the hexagonal modification (wurtzite). The Scherrer formula was used to calculate the crystallite size (*D*), and the microdeformations (ε) were estimated based on the analysis of the dependence of peak broadening on the diffraction angle (the Williamson–Hall approach).

Analysis of the diffraction pattern revealed the presence of seven main reflections characteristic of the CdS phase. The intensity of the peaks ranged from 14.4% to 100% (relative to the main peak at 2θ = 27.041°, plane (102)). The calculation of the crystallite sizes based on individual reflexes showed a significant heterogeneity in the microstructure of the material. The minimum CRO size (6.3 nm) is fixed for reflection (110) at 2θ = 44.629°, which indicates severe grinding or high defects in this direction. The maximum crystallite size (17.8 nm) is observed for the (101) plane at 2θ = 28.957°, where the minimum value of microdeformations (0.21%) is also recorded.

The average crystallite size over the entire data set was 11.6 nm, but the coefficient of variation of this parameter indicates a wide range of values (from 6.3 to 17.8 nm). Microdeformation analysis showed an average level of lattice distortion at 0.38%. The highest values of deformations (ε > 0.58%) were found for peaks at 2θ = 44.629° and 52.58°, which correlates with the zones of maximum peak broadening (FWHM up to 1.344°). This suggests that significant internal stresses accumulate in the structure of the material during synthesis, probably due to the rapid growth of nuclei or the presence of point defects.

The data obtained demonstrate that the sample under study is a nanostructured material with a developed surface and a high level of internal energy due to microdeformations. The presence of pronounced anisotropy in the size of crystallites requires consideration when further using the material in composites or thin films, as

this may affect the charge transfer pathways and optical properties. Further research will be aimed at optimizing synthesis conditions to reduce the level of micro-deformations and equalize the particle size in all crystallographic directions.

Теоретические и прикладные проблемы исследования наноструктурированных полупроводников

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Problems of intercultural communication in international chemical research

In modern science, which is becoming more and more global, chemistry is one of the most international fields. Working with scientists from other countries is not just helpful – it is necessary. Chemists often take part in joint research, publish in international journals, attend global conferences, and join shared programs. Because of this, they need not only strong professional knowledge but also good intercultural communication skills. However, such cooperation also brings challenges that can reduce its effectiveness.

One major problem is the difference in scientific terminology and naming systems. Even though there are international standards, different countries may still use their own notations or traditional ways to describe chemical compounds. This becomes especially difficult when translating scientific texts or analyzing results. Young researchers and students often struggle when reading foreign sources or writing their own papers.

Another key issue is the language barrier. English is the main language of international science, but not all specialists speak it at the same level. Chemists must learn not only general English but also specific scientific terms and how to clearly describe experiments and results. Small mistakes in wording can change the meaning, which is very important in chemistry where accuracy is critical.

Cultural and ethical differences also affect teamwork. Each country has its own traditions in how scientists communicate, write papers, share authorship, and work together. In some cultures, strict hierarchy is important, while in others open discussion is encouraged. These differences can lead to misunderstandings or conflicts. That is why it is important to understand and respect different scientific cultures.

There are also differences in research methods. Scientists from different countries may use different equipment, techniques, measurement systems, or ways of analyzing data. This can lead to different results or make experiments hard to repeat. To solve this, researchers need clear standards and detailed descriptions of their methods.

Today, chemists actively use online tools, databases, and digital platforms to work together. This creates new opportunities, but also requires good digital skills. Online communication also reduces non-verbal signals, which can sometimes cause misunderstandings between people from different cultures. Because of this, future chemists need to develop both digital and intercultural communication skills.

The progress of science depends greatly on effective international communication. Chemists need not only to improve their language skills but also to be flexible, understand cultural differences, and follow international standards. Education plays an important role here – through interdisciplinary courses, international projects, exchange programs, and conferences.

A modern chemist must be able to work successfully with people from different cultures. These skills are essential for career growth and success. They also help improve research quality, strengthen international cooperation, and prepare specialists who can compete in the global scientific community.

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Проблемы межкультурной коммуникации в международных химических исследованиях

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С О Д Е Р Ж А Н И Е

Секция 1

НАУЧНО-ТЕОРЕТИЧЕСКИЕ И ПРИКЛАДНЫЕ ПРОБЛЕМЫ ИССЛЕДОВАНИЙ

ГУМАНИТАРНЫЕ НАУКИ
(КУЛЬТУРОЛОГИЯ, ПЕДАГОГИКА, ФИЛОЛОГИЯ)

ЕСТЕСТВЕННЫЕ НАУКИ

ИНФОРМАЦИОННЫЕ НАУКИ

СОВРЕМЕННЫЕ ТЕХНОЛОГИИ ПИЩЕВОЙ ПРОМЫШЛЕННОСТИ И БИОИНЖЕНЕРИИ

ФИЗИКО-МАТЕМАТИЧЕСКИЕ НАУКИ

ХИМИЧЕСКИЕ НАУКИ

ЭКОЛОГИЯ И ЗАЩИТА В ЧС

Секция 2

ПРОБЛЕМЫ ПРОФЕССИОНАЛЬНОЙ КОММУНИКАЦИИ

ЕСТЕСТВЕННЫЕ НАУКИ

ИНФОРМАЦИОННЫЕ НАУКИ

ФИЗИКО-МАТЕМАТИЧЕСКИЕ НАУКИ

ХИМИЧЕСКИЕ НАУКИ

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