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Scientific Basis of Innovation Activity

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# **GENERAL PROBLEMS OF THE MODERN RESEARCH AND INNOVATION POLICY**

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# STATISTICAL INDICATORS OF CYBERSECURITY DEVELOPMENT IN THE CONTEXT OF DIGITAL TRANSFORMATION OF ECONOMY AND SOCIETY

**Introduction.** The scale and destructive consequences of the unlawful impact on cyberspace is a key problem of modern geopolitics, and cyber reliability is recognized as one of the most important security priorities by the subjects of international relations.

**Problem Statement.** Monitoring of cyber incidents and anomalies in information and communication systems and prompt response to risks determined by cyber threats require the development of a system of indicators and criteria for cybersecurity assessment.

**Purpose.** Summarize the international experience of assessing the cybersecurity, to position countries by their level of development in the global space, to identify strengths and weaknesses in cybersecurity management, and to ensure effective protection of cyberspace at the national level.

**Materials and Methods.** Used the component indices of the international rankings characterizing the potential of the digital economy (ICT IDI, NRI, EGDI) and the participation of countries in the field of cybersecurity (GCI and NCSI).

**Results.** It has been argued that cybersecurity ratings play the role of a kind of identifier of the relative advantages and vulnerabilities of the national cyber strategies, and indicate the need for their review in order to strengthen protection against cyber-attacks and improve the cyber risk management system.

In countries with a high level of economic development, which is largely based on the contribution of IT technologies to the national production, the cybersecurity potential is significantly higher, regardless of geolocation. The discovered correlation between GCI, information society development indices (IDI, NRI, EGDI) and GDP per capita confirms that the digital transformation of the economy and society acts as a key driver of economic development if the information- and cyber-security are assured only. The best practices are highlighted, and critically weak segments of the national cybersecurity are identified.

**Conclusions.** Using the NCSI indicators, the preparedness of Georgia and Ukraine to prevent the implementation of fundamental cyber threats and to manage cyber incidents and large-scale cyber crises is assessed.

Keywords: cybersecurity, cyber threats, cybercrime, global cybersecurity index, national cybersecurity index, and security management.

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Information and communication technologies (ICT), having become an integral component of the modern world, contribute to the emergence and intensive dissemination of fundamentally new models of communication, social integration, lifestyle, education, etc. However, the technological advances in informatization of society have created not only progressive opportunities, but also new challenges and threats in the field of cyber security: (i) unauthorized access to information and telecommunication systems and networks; (ii) targeted cyber-attacks on infrastructure facilities that ensure the life of society; (iii) breach of confidentiality of information stored, transmitted and processed in the information and telecommunication systems (state, commercial, banking secrets, personal data, intellectual property objects). The illegal actions of subjects of informational legal relations that create a danger to the vital interests of a person, society and the state as a whole, are defined by the term "cyber threats" [1, 2]. The sources or initiators of cyber threats can be international criminal groups of hackers, certain specialized groups trained in the field of information technology that operate in the interests of foreign states, terrorist and extremist groups, transnational corporations and financial and industrial groups.

The current global landscape of cyber threats is rather complicated, as evidenced by Cisco and Cybersecurity Ventures' researches [3]. Cyberthreats have various forms, scales and are constantly evolving. From the point of view of legal regulation of the problems of protecting the cyberspace, the whole range of illegal cybernetic influences can conditionally be combined into the following blocks: "classic" crimes; crimes specific to geopolitical struggle and cyber-attacks as components of military operations [4].

*"Classic" cybercrimes* are types of fraudulent activities aimed at unlawful access to confidential user information and automated databases: *fishing*, carding, hacking, malware and piracy. The object of cybercrime is personal data, bank accounts, logins and passwords, other personal information of both individuals and business and the public sector. A type of cybercrime is content cyberthreats (child pornography, Internet violence, drug trafficking, the dissemination of information of extremist content, etc.).

Cyber espionage. This is a criminal activity aimed at unauthorized access to information containing the state secrets in the field of defense, science and technology, economics, finance, foreign relations. Cyber espionage is most often an element of special information operations of special services of foreign states and an instrument of influence on the geopolitical environment.

Cyber diversions and cyber terrorism are politically motivated hacker attacks on critical infrastructure or any technological processes through a computer network, in particular, the Internet. Cyber diversions are mainly aimed at the destruction of industrial equipment, automated control systems, and military infrastructure facilities.

During unlawful interference in the work of information and telecommunication systems and networks, several interrelated threats can be realized at the same time, and radically different subjects of information legal relations, say, hacker groups and private IT companies controlled by special services, can be involved in their implementation. This indicates a rather complex nature of modern cyber incidents. In the political confrontation of countries, in order to achieve certain military and political goals, cyberspace is used as an arena of military operations — cyber warfare [5].

The steady increase in the number and power of cyber-attacks, motivated by the interests of individual states, groups and individuals, is one of the modern global trends [3; 6]. From year to year, cybercrimes are becoming more organized, technically advanced and psychologically elegant, and the consequences of using cyberspace for illegal purposes are becoming ever more widespread and destructive. According to the *Allianz* Risk Barometer yearbook, global losses from cybercrimes reach USD 600 billion per year, which is almost three times the average annual loss from natural disasters [7]. Large-scale targeted cyber-attacks and the associated risks to the national security have become a key problem of modern geopolitics, and the protection of the cyber environment is increasingly seen by the subjects of international relations as one of the most important security priorities. Under these circumstances, the development of effective nationwide cybersecurity systems that can timely identify real and potential threats, adequately respond to them and eliminate the consequences with minimal losses is of utmost importance.

Nowadays, almost all the leading countries experience cyber-attacks and form and constantly modernize the national cyber security systems to protect the national cyberspace. However, given the high technical capabilities of cybercriminals, the latent and transnational nature of cyber-attacks, no country is able to fight them on its own. Expert claims are true that cybersecurity should therefore become a collective responsibility [8]. It is possible to prevent and counteract all sorts of crimes with the use of information and communication technologies, subject to coordinated international cooperation in the field of cybersecurity. At the same time, it is important to combine the efforts and experience of various countries in the fight against cybercrime both at the state level and at the level of the commercial. public and private sectors. The creation of such a holistic international system of cooperation allows for the rapid exchange of the necessary information and to consolidate the efforts of countries to prevent the latest cyber threats.

# 1. INTERNATIONAL CYBERSECURITY RESEARCH EXPERIENCE

The Global Cybersecurity Agenda (GCA ITU) has become the basis for international cooperation and coordination of countries' confidencebuilding and security activities in the information society. According to GCA requirements, every ITU partner country must have a Computer Emergency Response Team (CERT), which is responsible for protecting state information resources and information and telecommunication systems from unauthorized access and misuse, as well as breaches of their privacy, integrity and accessibility.

At the global level, cybersecurity is the subject of consideration by the UN General Assembly, as well as a number of international organizations: G7 Group, Council of Europe, the European Union (EU), North Atlantic Treaty Organization (NATO), Organizations for Economic Cooperation and Development (OECD), Asia-Pacific Economic Cooperation (APEC), World Economic Forum (WEF), etc. They work in the following areas: creating a single database on cyberthreats and a system for the constant exchange of information, improvement of technical standards and rules, attention is paid to security issues on the Internet.

A single cybersecurity certification for IT products, services and processes is being introduced in the EU, which will undoubtedly enhance the security of online services and consumer devices and will facilitate the smooth functioning of the Digital Single Market. A key role in cybersecurity certification rests with the European Network and Information Security Agency (ENISA) [9].

NATO plays an important role in developing a unified approach to cybersecurity as a component of the national security. Within the organization, there are several specialized units that focus on the development of strategies and mechanisms for cyber-threat detection and counteraction to cyberattacks, as well as offering a wide range of educational, training and training opportunities. The EU-NATO interaction is the cornerstone of Euro-Atlantic cybersecurity in the military field, and cyber defense is one of NATO's priorities [10; 11]. The role of NATO in providing cybersecurity not only to Allies but also to Partner countries is increasing.

Cybersecurity is not just a set of strategies and principles for protecting cyberspace from threats. It is an ongoing process, the active component of which is monitoring incidents and anomalies in network systems and responding promptly to the risks caused by cyber threats. The balanced use of forces and means of ensuring cybersecurity requires appropriate methodological tools, first of all, the formation of a system of indicators and criteria for assessing the development of cybersecurity at the global and local levels.

At present, the main developers of theoretical and methodological foundations and applied aspects of statistical assessment of cybersecurity are mainly information and analytical teams of experts in international organizations specializing in information- and cyber-security: International Telecommunication Union (ITU), Centre for European Policy Studies (CEPS), e-Governance Academy (eGA) of Estonia, Potomac Institute for Policy Studies, EY Global Information Security Survey (GISS), world leaders in the field of network technologies and the cybersecurity industry Cisco Security and Cybersecurity Ventures, etc. Analytical reviews and reports from these organizations have been published by, among others, Kerry Nelson, Lorenzo Pupillo, Raul Rikk, Melissa Hathaway, Paul van Kessel, Andra Zaharia, Steve Morgan, Martin Lee and others. Among domestic scientists, V. Buryachok, A. Voytsikhovkyy, I. Voronenko, Yu. Danyk, I. Diorditsa, D. Dubov, V. Lipkan, R. Lukianchuk, G. Piskorska, V. Petrov and others devoted their scientific works to the issue of cybersecurity.

## 2. METHODOLOGY FOR ASSESSING THE CYBERSECURITY AS A COMPLEX MULTIDIMENSIONAL PHENOMENON

The purpose of this research is to summarize the international experience of assessing the cybersecurity, to position countries by their level of development in the global space, to identify strengths and weaknesses in cybersecurity management, and to ensure effective protection of cyberspace at the national level.

The subject of research is the current state of the global cybersecurity and specifics of cybersecurity in the NATO Member States and Aspirant countries Ukraine and Georgia.

In accordance with the ISO/IEC 27032 – SIS international standard, cybersecurity integrates

network security, security of critical information infrastructure and Internet security [12]. Like any complex phenomenon, cybersecurity cannot be directly measured as it turns out to be a certain set of various signs and symptoms. Therefore, it is possible to measure/evaluate such phenomena only indirectly by aggregating the sets of these signs into one integral assessment. It is the integrated estimates (composite indices), formed on the basis of a unique data set, that are the basis for positioning countries in the world coordinate system.

The study uses international rating systems that characterize the level of the digital economy development and the country's involvement in cybersecurity: ICT Development index (IDI), Networked Readiness Index (NRI) [13], the UN Global E-Government Development Index (EGDI), Global Cybersecurity Index (GCI), National Cyber Security Index (NCSI). Each rating, in addition to the function of a comparative analysis of the potential of individual countries in the field of digital transformations or cybersecurity, serves as a kind of identifier of the relative advantages and vulnerabilities of national cyber strategies, indicates the need for their review in order to strengthen protection against cyber-attacks and improve the cyber crisis management system.

# 3. INDICATORS OF DIGITAL ECONOMY DEVELOPMENT

The ICT Development Index is used to measure the level of development and to monitor changes in information and communication technologies. Its calculation is based on 11 indicators, which are combined into three sub-indices: access to ICT, ICT usage intensity and ICT level of practical skills [14].

The Network Readiness Index NRI measures the propensity of countries to leverage ICT capabilities. The index aggregates 53 indicators combined into four basic sub-indices. Three of them characterize the role of government, business and society in shaping the prerequisites for the development of ICT, and the fourth one describes the socio-economic effects of using the ICT: availability of conditions for the development of ICT (regulatory, business and innovation environment); readiness of citizens, business and government to use ICT (infrastructure and digital content, accessibility of ICTs, population skills); the level of use of ICT at public, business and private levels; the impact of ICT on the economy and society [15]. The NRI is considered to be the most comprehensive source for assessing the quality of the internal environment of ICT development and the ability of society and its institutions to make effective use of existing and new knowledge. The index identifies drivers and barriers to network readiness and widespread adoption of ICT in the country. This assumes the equal role and responsibility of all the "players" of the society: government, business, and citizens.

The rapid spread of the Internet and the global network has become the basis for the transformation of public administration in the direction of its adaptation to the requirements of the information society. The level of willingness and ability of the national government agencies to provide online government services using the ICT is indicated by the rating of countries based on the Electronic Government Development Index (EGDI). The index aggregates 13 indicators, which, from the point of view of international experts, embody the country's ability to participate in the information society [16]. These indicators are combined into three sub-indices: the Online Service Index (OSI), the Telecommunication Infrastructure Index (TII), and the Human Capital Index (HCI).

# 4. CYBERSECURITY INDICATORS 4.1. Global Cybersecurity Index (GCI)

The monitoring of the status of the global network space of the UN member countries is carried out by ITU. To assess the countries' involvement in cybersecurity, ITU experts annually determine the Global Cybersecurity Index (GCI), which relies on the country's legal, technical, managerial institutions, their educational and research capabilities, the availability of cooperation mechanisms and information exchange sys-



Fig. 1. The pillars of the Global Cybersecurity Index

tems in networks. Accordingly, the level of development of cybersecurity at the national level is analyzed by five pillars: legislative framework, technical implementation, organizational measures, capacity building, national and international cooperation. Each pillar is represented by a certain number of indicators based on binary answer options that confirm the presence or absence of certain, predefined solutions for cybersecurity (24 indicators in total). The structure of the GCI by pillars is illustrated in Fig. 1, the number of indicators is indicated in parentheses.

According to GCI data, in 2018, 9 out of 10 countries had cybersecurity legislation: the vast majority of countries had a national cybersecurity strategy (58%) and an active national CERT (56%) that helped detect attacks on government computer systems and databases, as well as critical infrastructure facilities [17].

The purpose of the GCI is to enable the UN member states to identify potential ways to strengthen the protection of the global network space against cyber threats. The results of the 2018 global cybersecurity survey at a planetary level indicate a significant digital divide between countries in the context of awareness of cyber threats and their ability to prevent them. Based on the GCI, countries are divided into three classes by their level of commitment: the high class has the highest level of global cybersecurity commitments (GCI  $\geq$  0.670); the medium one has developed complex commitments and is involved in cybersecurity programs and initiatives ( $0.340 \leq$  $\leq$  GCI  $\leq$  0.669); and the low one has initiated a cybersecurity commitment (GCI  $\leq 0.339$ ). 53 countries are assigned to the high class, 54 ones to the medium class, and 87 ones to the low class. The shares of these classes by the world regions are





shown in Fig. 2. The largest number of countries with a high cybersecurity development is concentrated in Europe (30): 20 countries are NATO members; their GCI ranges from 0.931 (the United Kingdom) to 0.527 (Greece). Georgia takes the  $18^{th}$  place (GCI = 0.857, high class), and Ukraine is ranked  $54^{th}$  (GCI = 0.661, medium class).

Most often, cyberattacks are experienced by countries with high levels of economic development, which are largely based on the contribution of IT technologies to national production (mainly OECD member countries, which account for more than two-thirds of global GDP). In terms of the volume and scale of IT technology, the level of cybersecurity in all highly developed countries, regardless of geolocation, is much higher. Table 1 shows the ratings for all five pillars of cybersecurity among the leading countries of the world's regions: the United Kingdom, in Europe; the USA, in the American continent; Singapore, in the AsiaPacific region; Saudi Arabia, in the Middle East; Mauritius, in Africa; and Russia, in the Central Eurasia.

Almost all of the leading countries have reached peak values (0.200) in the Legal, Technical and Organization areas. Much lower values in the Cooperation area (interagency and international cooperation, public-private partnership). In Russia, the GCI values are the lowest in all cybersecurity areas compared to other regional leaders.

The sample of NATO member countries in terms of cybersecurity development should be recognized as statistically homogeneous, which with probability of 0.95 confirms the Grubbs' test (G = 2.26 < G1 - 0.05 = 2.73). In this sample, one can also trace the relationship between the Global Cybersecurity Index (GCI), the information society development indexes (IDI, NRI, EGDI) and the indicator of economic development of countries (GDP per capita). All coefficients of the cor-

| Table 1. Global Cybersecurity In | ex (GCI) of the Regiona | l Leaders in Terms of the | GCI Pillars in 2018 |
|----------------------------------|-------------------------|---------------------------|---------------------|
|----------------------------------|-------------------------|---------------------------|---------------------|

| Index pillars     | United Kingdom | USA   | Singapore | Saudi Arabia | Mauritius | Russia |
|-------------------|----------------|-------|-----------|--------------|-----------|--------|
| Legal             | 0.200          | 0.200 | 0.200     | 0.187        | 0.182     | 0.197  |
| Technical         | 0.191          | 0.184 | 0.186     | 0.179        | 0.168     | 0.162  |
| Organizational    | 0.200          | 0.200 | 0.192     | 0.158        | 0.200     | 0.177  |
| Capacity building | 0.189          | 0.191 | 0.195     | 0.198        | 0.186     | 0.166  |
| Cooperation       | 0.151          | 0.151 | 0.125     | 0.160        | 0.144     | 0.135  |
| Global Index      | 0.931          | 0.926 | 0.898     | 0.881        | 0.880     | 0.836  |

Source: created by the authors on the basis of [17].

relation matrix (Table 2) are significant with a probability of 0.95: that is, the digital transformation of the economy and society depends on the economic development of the country and, in turn, plays the role of a key driver of economic development only if information- and cyber security are ensured.

Thus, GCI is a unique and easy-to-use tool for assessing the countries' preparedness for a particular type of cyber threats, forcing them to identify areas where cybersecurity can be strengthened and protect the economic interests of the country: by improving legislation, standards, market leverage or other initiatives.

# 4.2. National Cyber Security Index (NCSI)

The preparedness of countries to prevent the realization of fundamental cyber threats, manage cyber incidents and large-scale cyber crises is measured by the National Cyber Security Index (NCSI). Considering the principles of cybersecurity developed by the European Union, this index includes the most important aspects of network and information security, electronic identification, trust services, protection of personal data and many other aspects [18]. By statistical nature, the NCSI is a relative value that, as a percentage, indicates the degree to which a country meets cybersecurity criteria.

#### Table 2. Relationship of the Global Cybersecurity Index (GCI) with the Information Society Development Indices (IDI, NRI, EGDI) and the Level of Economic Development (GDP per capita) of NATO Members

| Variable | Correlation matrix<br>Number of observations N = 28<br>(Casewise deletion of missing data) |       |       |       |                   |  |  |  |
|----------|--|-------|-------|-------|-------------------|--|--|--|
|          | GCI  | IDI   | NRI   | EGDI  | GDP per<br>capita |  |  |  |
| GCI      | 1.000  | 0.583 | 0.691 | 0.598 | 0.564             |  |  |  |
| IDI      | 0.583  | 1.000 | 0.878 | 0.814 | 0.847             |  |  |  |
| NRI      | 0.691  | 0.878 | 1.000 | 0.815 | 0.877             |  |  |  |
| EGDI     | 0.598  | 0.814 | 0.815 | 1.000 | 0.787             |  |  |  |
| GDP per  |  |       |       |       |                   |  |  |  |
| capita   | 0.564  | 0.847 | 0.877 | 0.787 | 1.000             |  |  |  |

Source: created by the authors on the basis of [17].

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In recent years, **Estonia** has become one of the world centers in the field of protecting the national information cyberspace and preparedness to confront online threats (the NATO Cyber Defense Center operates in the capital of Estonia). In 2019, Estonia met 91% of the cybersecurity criteria and was in the TOP-3 of the NCSI rating [18]. Fig. 3 shows the positions of Estonia, Georgia, and Ukraine in the NCSI's international digital development and national cybersecurity rankings. In Georgia, the share of fulfilled criteria is 65%, in Ukraine, it accounts for 64%. At the same time, in each of these countries, the development of the national cybersecurity and information and communication technologies is approximately at the same level, that is, the development of cybersecurity to a certain extent corresponds to the digital development of society.

The NCSI structure includes 3 components, 12 segments and 46 indicators. When drawing up the scale, the NCSI project analysts considered the existence of a national strategy in the field of ensuring measures to protect systems, networks and applications from digital attacks, their practical implementation, as well as legal responsibility. The value of each indicator depends on its weight in the structure of the index: for the presence of a legal act that regulates a particular area, experts score one point; 2-3 points for specialized unit; 2 points for official format of cooperation; 1-3 points for result/product. The total number of points for a certain segment ranges from 5 to 9 points, the maximum possible score (points) for all segments is 77. The NCSI index is determined by comparing the amount of points scored by the j-th country with the maximum possible score (points):

$$NCSI = \frac{Country \ Points \times 100}{Maximum \ Points}.$$
 (1)

In Estonia in 2019, the total number of points scored was 70, hence NCSI = 70 : 77 = 0.9091.

Similarly, the level of fulfillment of cybersecurity criteria for any NCSI segment is evaluated by comparing the score provided by experts with



*Fig. 3.* The level of development of information and communication technologies and cybersecurity (NCSI version) in Estonia, Georgia, and Ukraine in 2019, point

Source: created by the authors on the basis of [18].

the maximum possible one. The shares of the criteria met by the national cybersecurity segments of Ukraine, Georgia, and Estonia are presented in Table 3. Their values give grounds to identify the strengths and weaknesses of national cyberstrategies, in particular, regarding the country's ability to manage cyber incidents and large-scale cyber crisis.

When analyzing the development of national cybersecurity, NCSI values are also compared with the Digital Development Level indicator (DDL). The latter is calculated as the arithmetic average percentage the country received from the maximum value of the ICT Development Index (IDI) and the Networked Readiness Index (NRI):

$$DDL = \frac{IDI\% + NRI\%}{2}.$$
 (2)

The difference (NCSI - DDL) indicates the coherence (inconsistency) of the development of the national cybersecurity and digital technology. A positive result shows that the development of cybersecurity in the country is in line with digital development or is ahead of it; a negative one gives grounds to conclude that the digital society in the country is more developed than the scope of national cybersecurity.

In Ukraine, IDI = 56%, NRI = 60%, hence DDL = 0.5 (56 + 60) = 58%, so NCSI > DDL. In Estonia and Georgia, the development of national cybersecurity is also in line with the digital development of the information society.

The analysis of compliance with the criteria of individual segments of the national cybersecurity of Ukraine and Georgia gives grounds to draw the following conclusions.

Ukraine. In Ukraine, the positive segments of the cybersecurity sphere include: development of a cybersecurity concept; education and professional development in the field of cybersecurity; protection of personal data and the fight against cybercrime. In these segments, Ukraine received 80–100% of the maximum level. Less developed segments of cybersecurity are: protection of basic e-services; electronic identification and trust services; reaction to computer incidents. The most problematic cybersecurity segments in Ukraine should be recognized as an analysis of cyber threats, international cooperation in the field of cybersecurity; protection of digital services; ability to manage large-scale cyber crisis and military cyber operations.

**Georgia.** In Georgia, the level of cybersecurity is slightly higher. Georgia received maximum NCSI ratings (100%) in five segments of cybersecurity: developing a cybersecurity policy and analysis of cyber threats; protection of basic e-services; protection of personal data and the fight against cybercrime. The following cybersecurity segments require attention: the ability to manage cyber incidents and large-scale cyber crisis, especially education and professional development in the field of cybersecurity; protection of digital services and military cyber operations. Thus, the cyberspace of both NATO aspirant countries remains a weak component of the national security and retains a high degree of vulnerability to cyber threats. Cyber security issues common to Ukraine and Georgia are the low level of development of the segment of the national defense operations (military cyber operations). Another equally important issue is the protection of digital services and the unpreparedness to respond to cyber incidents. The mechanism of public-private partnership in the field of cybersecurity with the owners and operators of private critical infrastructure facilities also requires adjustment.

International cooperation significantly enhances the ability of these countries to counteract all kinds of cyber influences. For example, the CERT-UA team works with other CERT teams in the Member States, as well as with the Cisco Talos Intelligence Team, to address the impact of cyberattacks on critical information infrastructure and identify the causes and circumstances of cyber incidents. Within the framework of Ukraine-NATO cooperation, the Cybersecurity Trust Fund has been set up to strengthen cyber potential, assist Ukraine in developing the defense capabilities for responding to cybersecurity incidents and eliminating their consequences [19]. Such cooperation will help to ensure that countries are prepared to prevent the realization of fundamental cyber threats and manage cyber incidents and large-scale cyber crises.

A necessary condition for the successful digital transformation of the economy and society is counteracting cyber threats and the fight against cybercrime. Among the main obstacles to the promotion of the basic principles of cyber defense, information security experts point out: lack of

| Segment<br>#                          | NCSI components & segments             | Max score   | Ukraine,<br>version as of<br>Jul 14, 2018 | Georgia,<br>version as of<br>Nov 21, 2017 | Estonia,<br>version as of<br>Feb 18, 2019 |  |  |
|---------------------------------------|--|-------------|---|---|---|--|--|
|                                       | GENERAL CYB                            | ER SECURITY | INDICATORS                                |   |   |  |  |
| 1                                     | Cyber security policy development      | 7           | 100                                       | 100                                       | 57  |  |  |
| 2                                     | Cyber threat analysis and information  | 5           | 20  | 100                                       | 80  |  |  |
| 3                                     | Education and professional development | 9           | 89  | 22  | 67  |  |  |
| 4                                     | Contribution to global cyber security  | 6           | 33  | 50  | 50  |  |  |
| BASELINE CYBER SECURITY INDICATORS    |  |             |   |   |   |  |  |
| 5                                     | Protection of digital services         | 5           | 20  | 0   | 20  |  |  |
| 6                                     | Protection of essential services       | 6           | 83  | 100                                       | 17  |  |  |
| 7 E-identification and trust services |  | 9           | 78  | 78  | 67  |  |  |
| 8 Protection of personal data         |  | 4           | 100                                       | 100                                       | 100                                       |  |  |
|                                       | INCIDENT AND CRIS                      | SIS MANAGEM | ENT INDICATO                              | ORS                                       |   |  |  |
| 9                                     | Cyber incidents response               | 6           | 67  | 50  | 67  |  |  |
| 10                                    | Cyber crisis management                | 5           | 0   | 60  | 60  |  |  |
| 11                                    | Fight against cybercrime               | 9           | 100                                       | 100                                       | 100                                       |  |  |
| 12                                    | Military cyber operations              | 6           | 17  | 17  | 83  |  |  |
| Score (                               | points) obtained                       | 77          | 49  | 50  | 70  |  |  |
| NCSI, 9                               | %                                      | х           | 63.6                                      | 64.9                                      | 90.9                                      |  |  |
| DDL                                   |  | х           | 58.1                                      | 59.6                                      | 79.3                                      |  |  |
| Differen                              | nce                                    | х           | 5.5                                       | 5.3                                       | 11.6                                      |  |  |

Source: created by the authors on the basis of [18].

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resources, incompatibility of information security systems, and a shortage of qualified cybersecurity specialists. Nowadays, the staffing challenge for the cybersecurity industry has become global and is showing a tendency to deepen.

International cybersecurity ratings (GCI and NCSI) are useful to make sound decisions about addressing and preventing potential cybersecurity challenges and choose the path to a more secure and sustainable economy in an unstable, cybernetic, and conflict-prone world.

The highest levels of digital transformation and cybersecurity are observed in NATO member countries. Ensuring cybersecurity in the context of global threats, along with the joint efforts of the international community, dictates the importance of monitoring at the national level. Ukraine and Georgia, like all countries in the world, are constantly threatened by cyber-attacks and occasionally face cybersecurity challenges. The main threats to the national cybersecurity of these countries should be considered in the context of Russian information and cyber aggression, in particular, cyber-attacks on vital infrastructure. Therefore, the issue of improving the cyberspace military security systems, which would meet EU and NATO membership criteria and guarantee reliable protection of the states from cybercrime, remains urgent for both NATO aspirant countries.

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#### СТАТИСТИЧНІ ІНДИКАТОРИ РОЗВИТКУ КІБЕРБЕЗПЕКИ В КОНТЕКСТІ ЦИФРОВОЇ ТРАНСФОРМАЦІЇ ЕКОНОМІКИ Й СУСПІЛЬСТВА

**Вступ**. Масштаби й руйнівні наслідки протиправного впливу на кіберпростір є ключовою проблемою сучасної геополітики, а кібернадійність визнається суб'єктами міжнародних відносин як один з найважливіших безпекових пріоритетів.

**Проблематика**. Моніторинг кіберінцидентів та аномалій в інформаційно-комунікаційних системах, оперативне реагування на детерміновані кіберзагрозами ризики потребують формування системи індикаторів і критеріїв оцінювання кібербезпеки.

**Мета.** Узагальнення міжнародного досвіду оцінювання стану кібербезпеки, позиціонування країн за рівнем її розвитку у глобальному просторі, визначення сильних і слабких ланок в управлінні кібербезпекою та забезпечення дієвого захисту кіберпростору на національному рівні.

**Матеріали й методи.** Використано компонентні індекси міжнародних рейтингів, які характеризують потенціал цифрової економіки (ICT IDI, NRI, EGDI) та участь країн у сфері кібербезпеки (GCI i NCSI).

**Результати.** Аргументовано, що рейтинги кібербезпеки виконують роль своєрідного ідентифікатора відносних переваг і вразливих позицій національних кіберстратегій, вказують на необхідність їх перегляду з метою посилення захисту від кібератак і вдосконалення системи управління кіберризиками.

В країнах з високим рівнем економічного розвитку, який значною мірою базується на внеску IT-технологій у національне виробництво, потенціал кібербезпеки значно вищий, незалежно від геолокації. Виявлена кореляція між GCI, індексами розвитку інформаційного суспільства (IDI, NRI, EGDI) та ВВП на душу населення підтверджує, що цифрова трансформація економіки та суспільства відіграє роль ключового драйвера економічного розвитку лише за умови забезпечення інформаційної та кібербезпеки. Висвітлено найкращі практики та зазначено критично слабі сегменти національної кібербезпеки.

**Висновки.** За індикаторами NCSI оцінено готовність Грузії та України запобігати сценаріям реалізації фундаментальних кіберзагроз, керувати кіберінцидентами та масштабними кіберкризами.

*Ключові слова*: кібербезпека, кіберзагроза, кіберзлочинність, глобальний індекс кібербезпеки, національний індекс кібербезпеки, управління безпекою.



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# DIGITAL AND GREEN ECONOMY: COMMON GROUNDS AND CONTRADICTIONS<sup>1</sup>

**Introduction.** The processes of digitalization of an economy, associated with the deployment of technologies of the Fourth Industrial Revolution, are multifaceted and have a significant impact, including on the environment, which affects the interests of future generations.

**Problem Statement.** Acceleration of digitalization is accompanied by contradictory positive and negative effects on the environment. In this regard, the identification of these effects at both the global and national levels is an urgent problem.

**Purpose.** The purpose is to identify the relationship between the digital and green economy and to substantiate ways of environmentally safe development of digital technologies in Ukraine.

Materials and Methods. Clustering of world countries on the basis of economic, industrial, and digital development; econometric analysis of the relationships between the ICT development index and the environmental performance index in the world countries and their groups (clusters) for 2017–2020.

**Results.** It has been established that at the global level, the introduction of state-of-the-art digital technologies has a generally positive relationship with the state of environment: the higher the level of digitalization, the more environment friendly national economies, other things being equal. It has been found that the environmental performance of digitalization depends on the level of manufacturing (tangible) technologies and the overall economic development. In the clusters of less developed coun-tries, including Ukraine that has significant problems in industry and innovation, the spread of digital technologies has less positive impact on the environment than in the clusters of more advanced econ-omies. Therefore, the long-term positive effects of digitalization for Ukraine are not obvious, while the negative ones may have serious negative consequences.

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**Conclusions.** To minimize the environmental risks of digitalization processes in Ukraine, it is necessary to develop a national academic program for comprehensive assessment of effects of various aspects (abiotic, biotic, anthropogenic) of digital technologies on environment, as well as to harmonize economic digitalization programs with the overall strategy for innovation-driven national manufacture.

Keywords: digital technologies, digitalization of economy, industry, sustainable development, ecological footprint, and environmental performance.

In long-term strategies of innovation-oriented industrial advanced economies and emerging markets (USA, European Union, Scandinavian countries, Japan, South Korea, etc.), digitalization and greening of economy are considered complementary and such that promote inclusive, socially responsible and sustainable development. In Communication of the EU Commission to the European Parliament [1], the creation of digital green industrial ecosystems and, consequently, the achievement of climate-neutral digital leadership in industry have been identified as priorities for the upcoming decades to maintain the overall competitive advantage and geopolitical influence of the European Union.

The economy digitalization, like any new understudied phenomenon, is associated not only with ample opportunities but also with challenges, including environmental ones, and with qualitative transformations of the ecological footprint structure. On the one hand, according to European experts, provided that the current trends continue, by 2020 the share of the ICT sector in global CO<sub>2</sub> emissions may increase from today's 2% to 14% [2]. On the other hand, the target use of "green" ICTs to decarbonize the world economy may result in reducing greenhouse gas emissions by 15%, i.e. decreasing the man-made burden on the global ecosystem and achieving carbon neutrality of the ICT industry.

In addition, the ever-growing "digital divide"<sup>2</sup> between the innovative leaders and the less technologically developed economies is contributing to the conservation of outdated environmentally dangerous and resource-intensive technological structures, which casts a role for the latter as raw material colony and hazardous waste endpoint. A clear evidence of such an "institutional-environment trap" is the map of e-waste emigration (Fig. 1).

The logistical flows of e-waste shown in the figure indicate certain patterns in the geopolitical distribution of the links of global value chains. Ecologically "clean" and economically prosperous countries with a strict environment legislation and a high cost of legal disposal of electronic waste, prefer to import them to less developed regions with a relatively loyal attitude to environmentally dangerous economic activities and cheap manual labor. An exception is China, which is both the largest producer of digital products and a place for the accumulation of electronic waste.

The connection between ecology and digitalization manifests itself in the fact that high environment requirements in advanced economies have created barriers to spreading digital technologies. Environment standardization of product life cycle increases the transaction costs of quality control, manufacturing and operating conditions, after-sales environment friendly disposal of electronic products and related infrastructure. Failure (technical and/or financial) to meet the established quality standards is one of the most common market barriers in the international and domestic markets. Influential environment lobbies in central and local government<sup>3</sup>, as well as protest movements by environment organizations, create a negative image of developers of potentially dangerous innovations, hinder economic

<sup>&</sup>lt;sup>2</sup> There are 5 key indicators (per capita), for which the digital inequality between countries is the most obvious: (1) coverage of users by mobile broadband networks; (2) the number of IT professionals; (3) investment in ICT versus GDP; (4) the number of downloaded applications; (5) the number of installed Internet of Things (IoT) databases [3].

<sup>&</sup>lt;sup>3</sup> In France, 68 local authorities, including the mayors of 11 major cities, are demanding that the government ban 5G communications.



Fig. 1. Map of distribution of countries by income and e-waste emigration, according to [4, 14, 23]

development and R&D progress, and increase investment risks and tax burden on business. At the same time, the environmental consequences of digital innovation may be really difficult to predict. For example, increasing intensity of wave radiation as a result of the development of digital communications provokes growing number of congenital genetic mutations in living species (birds, fish, insects, etc.), changes in their basic behavioral responses (especially in the species characterized by social way of life: ants, wasps, bees, termites, bumblebees and etc.), changes in their migration routes and habitats, which disrupts the established food chains in ecosystems and leads to a reduction in biodiversity and, in some cases, to the collapse of ecosystems [29, 12–13, 18–21]. The mass extinction of bees causes a reduction in the pollination of fruit crops and some plant species, which can fatally affect the range and quantity of food [5].

As the European experience has shown [2, 6], combining the imperatives of Industry 4.0 with the imperatives of climate and environment emergencies requires radical reforms in the transport and energy sectors of industry, and, accordingly, huge capital investments. According to preliminary estimates, the European Union needs an investment of about EUR 3 trillion to achieve the ambitious goals of climate-neutral digital industry leadership. For the period from 2021 to 2027, the main financial burden is expected to be shared between the European Investment Bank (about EUR 600 billion), the private sector (about EUR 300 billion), governments of EU member states (about 100 billion euros), and the EU budget (about EUR 7.5 billion). Because of this, this initiative has been criticized in the context of unjustified tax increase and uncontrolled use of budget resources by officials under the pretext of environment goals.

These examples have shown that digital and green economies have obvious points of contact, which, on the one hand, may give a new impetus to the sustainable development of national economies and, on the other hand, may create new problems associated with unpredictable consequences that are different for different countries. In this regard, the purpose of this research is to identify the relationship between digital economy and green economy and to substantiate the ways of environmentally safe development of digital technologies in Ukraine.

# Environment effects of digitalization

The immediate positive environment effect of digitalization is dematerialization. Transition to electronic document control, digital services and products in trade, banking, and administrative spheres, replacement of physical logistics flows by

Table 1. Environment Advantages of Digitalization

remote means of communication based on digital technologies (e-mail and bulletin boards, video conferencing, electronic exchanges, e-government services, etc.) have caused a reduction in time, financial, and material resources extracted from the natural environment. As a result, the amount of waste generated by enterprises, organizations, and end users decreases, which consequently sig-

| Manifestations   | Causal-related environmer   | nt effects   | Consequences for ecosystems       |
|--|---|--|-----------------------------------|
| Transition to electronic document control<br>Expansion of commercial and administra-<br>tive digital services<br>Spread of digital remote means of commu-<br>nication<br>Use of "smart" automatic systems in indust-<br>ry and everyday life | Dematerialization of goods and services<br>Reduction of physical logistics flows<br>Flexible response to changes in envi-<br>ronment conditions in real time to en-<br>sure the most efficient use of resources<br>and to minimize costs<br>Customization of production<br>Improvement of production<br>Improvement of production monitor-<br>ing systems, reduction of risks associa-<br>ted with equipment failures (due to un-<br>detected technical malfunc-tions, hu-<br>man factor, etc.) | Saving of renewable<br>and non-renewable na-<br>tural resources<br>Reduction of pollutant<br>emissions into the en-<br>vironment (emissions,<br>discharges, waste dis-<br>posal)<br>Reduction of risks of<br>manmade disasters | Reduction of<br>mancaused<br>load |

#### Table 2. Environment Disadvantages of Digitalization

| Manifestations   | Causal-related environment effects  | Consequences for ecosystems  |
|--|---|--|
| Expansion of the range of devices<br>Increase in the number of devices as a<br>result of growing demand<br>Increase in the duration of use of de-<br>vices during the day  | Increasing energy consumption (industrial and domestic)<br>Increasing greenhouse gas emissions<br>Increasing industrial consumption of rare earth metals<br>Increasing electronic waste, including that containing to-<br>xic substances<br>Increasing risk of industrial accidents because of the im-<br>perfection of digital technologies and the accumulation of<br>errors and failures in the systems  | Disruption of the cycle<br>of substances in eco-<br>systems<br>Disruption of food chains<br>and reduction of habi- |
| Change / emergence of new technolo-<br>gies of in-formation signal transmis-<br>sion<br>Accelerated change of device genera-<br>tions (early termination of operation)<br>caused by manufacturers' efforts to<br>gain a monopoly quasirent | Increasing intensity of wave radiation per unit area<br>Manifestation of understudied adverse ef-fects in the<br>structure of genomes, the opera-tion of reproductive sys-<br>tems and the behavioral reaction of living organisms<br>Growing consumption of natural resources as a result of<br>aggressive advertising and unfair competition (intentio-<br>nal technological incompatibility of software and hard-<br>ware, industrial espionage, trade wars) | tats of organisms, reduc-<br>tion of biodiversity of<br>ecosystems<br>Distortion of the system<br>of social values |

nificantly reduces the anthropogenic burden on ecosystems in certain areas of resource consumption and pollutant emissions. On the other hand, expanding range of and growing demand for devices, as well as increasing time of their daily use significantly affect (raise) energy consumption and, therefore, entail growth in greenhouse gas emissions.

A more purposeful and environment friendly effect of digitalization is the "smartness" of automated (robotic) industrial systems, which improves real-time monitoring and control systems, increases the efficiency of business processes and reduces costs. Smart power systems, ventilation and climate control systems in smart buildings, 3D printing, automated product quality control systems, industrial robotics, smart logistics, etc., contribute to the customization of production, resource savings, inventory optimization, timely troubleshooting, prevention of failures and emergencies and, as a consequence, reduction in mancaused load on ecosystems.

The most obvious advantages of digitization are given in Table 1.

The environment disadvantages of digitalization (Table 2) are caused by growing demand for smart products and digital services, which provokes an increase in energy consumption and greenhouse gas emissions and accumulation of electronic waste. These negative consequences are exacerbated by unfair competition and attempts to maximize monopoly quasi-rent from pseudo-innovation, when marketing policies that stimulate excessive consumption for prestige reason substitute for real research and development. In addition, the risks to the ecosystem increase as a result of the understudy<sup>4</sup> of the impact of digital technologies on flora and fauna [7].

# Estimate of digitalization effects on environmental performance

The relevance of smart industrial development based on the principles of digitalization and decarbonization of the economy through digital technologies leads to a strong research interest in quantifying the impact of digitalization on the environmental footprint. Depending on the methodology and the approach to forecast, the following estimates have been obtained:

- the share of digital technologies in the total world energy consumption may exceed 3% [9, 10];
- carbon footprint of the ICT industry ranges from 1.1 to 1.4 billion tons of CO<sub>2</sub> equivalent [9, 11, 17, 12, 13, 14, 15];
- ◆ potentially possible reduction of global greenhouse gas emissions due to "green" digital technologies varies within 15%−16.5% of the total projected emissions of all sectors [2, 12].

To confirm the hypothesis of the existence of a direct relationship between digitalization and sustainable development (in terms of its environment component), the authors have assessed the strength of the relationship between the ICT Development Index that characterizes the world achievements in terms of ICT development (Table 3) and the Environmental performance Index (EPI) that reflects the combined effect of preserving the quality of the natural environment and natural resource management (Table 4).

For this purpose, different countries that have different level of economic and R&D development, the specifics of national production, and, accordingly, size and structure of man-made load on world ecosystems have been selected. At the same time, to increase the objectivity of the results of the analysis, the countries with a population of less than 1 million people, the countries that are unable to ensure the regular submission of the necessary statistical information, as well as the countries with atypically high revenues from sale of minerals (primarily, hydrocarbons) are ex-

<sup>&</sup>lt;sup>4</sup> In particular, 5G technology that is critical to the spread of the Internet of Things, including for households [8], because of the peculiarities of signal transmission (millimeter waves and small signal reception / transmission centers), requires a high coverage density ( $\approx 250$  m between cells), which may lead to a critical growth of mutations in some species of birds, as well as to mass death of bees [7], i.e. there is a threat of the destruction of ecosystem food chain and the extinction of species.

| ICT access sub-index   |     | ICT use sub-index   |     | ICT skills sub-index            |     |
|--|-----|---|-----|---------------------------------|-----|
|  |     | Share in the index composition  |     |                                 |     |
| 40%  |     | 40%   |     | 20%                             |     |
| Fixed telephone lines per 100 inhabitants                        |     | Proportion of households with Internet access at home                           |     | Adult literacy rate             |     |
| Mobile cellular telephone sub-<br>scriptions per 100 inhabitants |     | Proportion of house-holds with Inter-<br>net access at home per 100 inhabitants |     | Secondary gross enrolment ratio |     |
| International Internet band-<br>width (bit/s) per Internet user  | 20% | Mobile broadband subscribers per 100 inhabitants                                | 33% | Tertiary gross enrolment ratio  | 33% |
| Proportion of households with a computer                         |     |   |     |                                 |     |
| Proportion of households with<br>Internet access at home         |     |   |     |                                 |     |

Table 3. Quality Structure of ICT Development Index

cluded from the review. As a result, 106 world economies are included in the final sample<sup>5</sup>.

The distribution of the countries by ICT development and environmental performance, as well as the dependence curve are presented in Fig. 2, where Ukraine is ranked 48<sup>th</sup> among the analyzed countries with the ICT Development Index of 5.62 and the Environmental Performance Index of 49.50.

The coefficient of determination ( $R^2 = 0.85$ ) indicates a significant weight of the positive linear relationship between the ICT development (variable x) and the environmental performance (variable y) of the analyzed countries. The Mean Absolute Percentage Error for the environmental performance is 11%, i.e. the equation may be considered satisfactory. The nonparametric Spearman rank correlation coefficient (0.93) also indicates the presence of a statistically significant relationship between the analyzed phenomena.

Thus, the most advanced and innovation-driven economies (Germany, Denmark, Finland, France, Switzerland, Japan, etc.) with a high level of economy digitalization and, accordingly, a high ICT development index, are generally characterized by the best results in terms of ensuring environmental performance (less anthropogenic burden on ecosystems and more effective environmental policy).

| Table 4. Quality Structure of Environmental Performance |  |
|---|--|
| Index   |  |

| Environmental he               | alth | Ecosystem vitality   |     |  |  |  |  |  |
|--------------------------------|------|----------------------|-----|--|--|--|--|--|
| Share in the index composition |      |                      |     |  |  |  |  |  |
| 40%                            |      | 40%                  |     |  |  |  |  |  |
| Air quality                    | 20%  | Climate change       | 24% |  |  |  |  |  |
| Sanitation and drin-           | 16%  | Biodiversity and ha- | 15% |  |  |  |  |  |
| king water                     |      | bitat                |     |  |  |  |  |  |
|                                |      | Ecosystem services   | 6%  |  |  |  |  |  |
| Heavy metals                   |      | Fisheries            | 070 |  |  |  |  |  |
| Waste manage-                  | 2%   | Agriculture          |     |  |  |  |  |  |
| ment                           |      | Pollution emissions  | 3%  |  |  |  |  |  |
|                                |      | Water resources      |     |  |  |  |  |  |

<sup>&</sup>lt;sup>5</sup> Sample composition: Australia, Austria, Albania, Algeria, Argentina, Bangladesh, Belgium, Benin, Belarus, Bulgaria, Bolivia, Bosnia and Herzegovina, Brazil, Burkina Faso, Burundi, Great Britain, Gambia, Guatemala, Guinea, Guinea Georgia, Denmark, Dominican Republic, Ecuador, Estonia, Ethiopia, Egypt, Zambia, Zimbabwe, Israel, India, Indonesia, Ireland, Spain, Italy, Jordan, Kazakhstan, Cambodia, Cameroon, Canada, Kenya, Kyrgyzstan China, Cyprus, Colombia, Costa Rica, Ivory Coast, Laos, Latvia, Lesotho, Lithuania, Lebanon, Myanmar, Mauritius, Madagascar, Macedonia, Malaysia, Morocco, Mexico, Mozambique, Moldova, Mongolia, Namibia, Nepal, Nigeria, Netherlands, Nicaragua, Germany, New Zealand, Norway, Pakistan, Panama, Paraguay, Peru, South Africa, South Korea, Poland, Portugal, Russian Federation, Romania, El Salvador, Senegal, Serbia Slovak Republic, Slovenia, USA, Thailand, Tanzania, Tunisia, Turkey, Uganda, Hungary, Ukraine, Uruguay, Philippines, Finland, France, Croatia, the Czech Republic, Chile, Switzerland, Sweden, Sri Lanka, Jamaica, and Japan.



*Fig. 2.* Relationship between ICT Development Index and EPI (106 world countries, based on data of 2017–2020) *Source*: [17, 25].



Fig. 3. The relationship between ICT development and environmental performance indices by clusters. A - The "leaders" and the "chasers" (with a high level of digitalization); B - The "catchers" (with a medium level of digitalization); C - The "outsiders" (with a low level of digitalization)

At the same time, from the point of view of economic and environmental policy formation, such global dependence has limited value. The fact is that economic institutions (formal and informal rules and norms of conduct) that operate well in some countries cannot be automatically transferred to other countries. Similarly, the transition from one dominant production technology to a new one that determine, in particular, the level of environmental performance, is not a "smooth" process, but is described in terms of technological gaps between countries [18]. Therefore, it is advisable to divide these countries into relatively homogeneous clusters (groups), within which there are certain general patterns of socio-economic and digital processes, on which environmental processes depend.

The clusters have been formed in STATISTI-CA<sup>6</sup>. The following variables are used: (1) income per capita; (2) the share of manufacturing industry in GDP; (3) the Human Development Index (HDI); (4) exports of ICT goods and services; (5) the number of fixed broadband subscriptions and mobile subscriptions; and (6) the number of individual users of the Internet. The first three

<sup>&</sup>lt;sup>6</sup> STATISTICA: Data Mining, data analysis, quality control, forecasting, training, and consulting. *StatSoft Russia*. 2020. URL: http://statsoft.ru/ (last access 01.11.2020).

#### **BRIEF DESCRIPTION OF THE CLUSTERS**

The first cluster includes traditional world leaders in economic development and such a relatively fresh EU member state and former member of the socialist bloc (as part of Yugoslavia) as Slovenia. Accordingly, the countries of the "leaders" cluster are characterized by the highest average values of the 6 studied indices, except for "exports of ICT goods (% of total exports of goods)".

The second cluster (tentatively called "the outsiders") consists of the countries that demonstrate diametrically opposite results: the average values of all indices are the worst among all clusters. The cluster of "outsiders" mainly includes countries that gained independence from the leading countries of Europe (mostly Britain and France), as late as in the 20<sup>th</sup> century, and during the Cold War were considered the Third World countries.

The third cluster is the largest one in terms of the number of countries. It includes the countries that are characterized by a high or an upper middle income and fall behind the "leaders" and the "chasers" in terms of the average indices, but exceed the indices of the "outsiders". They are mainly the former countries of the socialist bloc, as well as the countries belonging to the Third World, which have managed to improve their socio-economic situation since the Cold War. Some of them are currently the EU member states (Cyprus, Greece, and Portugal), which during the period under review (2009–2018) either failed to improve the socio-economic situation up to the leading countries, or because of the influence of various external and internal factors (in particular, the global financial crisis) have lost stability. Conventionally, the countries of the third cluster are called the "catchers".

The fourth cluster includes the countries that in terms of 6 indices, in addition to "exports of ICT goods (% of total exports of goods)" are as close as possible to the leading countries (cluster 1), with this index even exceeding that of the leading countries. This cluster includes the countries that have been actively developing national industry for at least the last 30 years (including through offshoring) and some new EU member states that were part of the USSR or the socialist bloc. Conventionally, the countries of this cluster are called the "chasers".

#### REFERENCE

The "leaders": Switzerland, Ireland, Norway, Denmark, the Netherlands, Sweden, Japan, Germany, Finland, Austria, USA, Great Britain, Belgium, Israel, France, Canada, Australia, Italy, New Zealand, Slovenia, and Spain (21 countries)

The "chasers": South Korea, Czech Republic, Malaysia, Estonia, Slovak Republic, Hungary, China, Philippines, Costa Rica, Thailand, and Mexico (11 countries).

The "catchers": Cyprus, Lithuania, Poland, Latvia, Greece, Portugal, Uruguay, Russia, Croatia, Panama, Argentina, Romania, Chile, Bulgaria, Belarus, Kazakhstan, Mauritius, Brazil, Turkey, Serbia, Tunisia, Georgia, Colombia, Ukraine, Albania, South Africa, Bosnia and Herzegovina, Morocco, Jordan, Peru, Lebanon, Dominican Republic, El Salvador, Ecuador, Jamaica, Moldova, Algeria, Paraguay, Indonesia, Sri Lanka, Egypt Pet, Mongolia, Guatemala, and Kyrgyz Republic (45 countries).

The "outsiders": Namibia, Bolivia, Nicaragua, Honduras, Cambodia, India, Ivory Coast, Laos, Senegal, Lesotho, Gambia, Nepal, Zimbabwe, Bangladesh, Kenya, Nigeria, Zambia, Ben Uganda, Tanzania, Myanmar, Guinea, Burkina Faso, Madagascar, Mozambique, Ethiopia, and Burundi (29 countries).

indices characterize the general level of national economy and industrial sectors development. The rest of them describe the level of development and use of ICT technologies and the Internet. All statistic data on world countries, in terms of digital technologies and digitization indices, are taken from the World Bank website [20].

According to the results of cluster analysis with the use of the method of k-means, there have been formed 4 relatively homogeneous clusters of countries, which are called: "leaders" (typical representatives are the Scandinavian countries, Western EU, and USA), "chasers" (Asian emerging markets such as China, South Korea, etc.), "catchers" (Eastern European and the post-Soviet countries, including Ukraine, etc.), and "outsiders" (underdeveloped African and Asian countries) (Box 1).

As shown by the estimates given in Fig. 3, the global dependencies and trends cannot be directly extrapolated to underdeveloped national economies, as the relationship between ICT development and environmental performance in the catchers and the outsider countries is not strong

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BOX 1



Exports of ICT goods and services, % of the total exports

• GDP in comparative prices per capita, USD million (2010 as reference)



enough. Moreover, as one can see from Fig. 3 (according to the angle of the trend lines), the digitalization of the economy in these clusters has a much smaller positive impact on the environment. That is, digitalization itself, without reference to the general economic development as a whole and particularly the technologies of the real sector, does not provide environmentally sustainable growth. Therefore, to address the problem it is important to take into account the specifics of national R&D development, as well as its general strategic direction.

In particular, with regard to Ukraine, given its strategic geo-economic priorities, individual EU members, similar in size, climate, and population, can be used as references for justifying national policies in the field of environment friendly digitalization. These criteria are met by Germany and France (the "leaders"), as well as by Poland (the "catchers").

As shown by the example presented in Table 5 and in Fig. 4, the largest gap between Ukraine and these countries is observed in terms of GDP per capita: the share of the economies of Germany and France (in comparative prices) exceeds Ukraine almost 15 times. The gap with Poland is slightly lower, 4.7 times. To correctly understand

*Table 5.* Digitalization and Environmental Performance Indices of Ukraine and the Reference Countries (averaged for 2009–2018)

| Cluster<br>type   | Rank<br>in the<br>internal<br>clus-ter<br>rating<br>in terms<br>of digita- | Country | GDP<br>(in compara-<br>tive prices)<br>per capita,<br>USD million<br>(2010 as<br>reference | Share<br>of pro-<br>cessing<br>industry<br>in GDP,<br>% | HDI *,<br>points | Export<br>of ICT goods<br>and servi-<br>ces, %<br>of total<br>exports of<br>goods | Fixed<br>telephone<br>line<br>subscribers<br>(per 100<br>inhabitants) | Mobile<br>subscribers<br>(per 100<br>inhabitants) | Individual<br>users<br>of Internet<br>(% of popu-<br>lation) | EPI **,<br>points |
|---|--|---------|--|---|------------------|---|---|---|--|-------------------|
| lizatio   |  |         | Indices  |   |                  |   |   |   |  |                   |
| Leaders   | 8  | Germany | 44.4   | 20.0  | 0.93             | 4.7   | 36.1  | 121.7   | 84.1   | 77.2              |
|   | 15   | France  | 41.7   | 10.3  | 0.88             | 4.1   | 39.2  | 100.1   | 79.4   | 80.0              |
| Catchers  | 3  | Poland  | 14.1   | 16.7  | 0.85             | 7.6   | 17.8  | 136.1   | 67.0   | 60.9              |
|   | 25   | Ukraine | 3.0  | 12.2  | 0.74             | 1.0   | 9.3   | 130.7   | 41.6   | 49.5              |
| Ukraine, difference in the indices as compared with the reference countries |  |         |  |   |                  |   |   |   |  |                   |
| Leaders   | 8  | Germany | -41.4  | -7.8  | -0.19            | -3,7  | -26,8   | +9.0  | -42,5  | -27,7             |
|   | 15   | France  | -38.7  | +2.1  | -0.14            | -3,1  | -29,9   | +30.6   | -37,8  | -30,5             |
| Catchers  | 3  | Poland  | -11.1  | -4.5  | +0.11            | -6,6  | -8,5  | -5.4  | -25,4  | -11,5             |
| Average difference  |  | -30.4   | -3.4   | -0.07   | -4.5             | -21.7   | +11.4   | -35.2   | -23.2  |                   |
| Ukraine, % of averaged indices  |  |         | 9.0%   | 77.9%   | 83.5%            | 18.3%   | 30.0%   | 109.6%  | 54.1%  | 68.1%             |

\* HDI is Human Development Index; \*\* EPI is Environmental Performance Index. *Source*: [19].



*Fig. 5.* Comparative estimate of the digitalization indices of Ukraine and the reference countries *Source*: [19].

the situation, it is also important to take into account a large gap, especially from the "leaders" cluster, in terms of the share of ICT exports, which well characterizes national technological level (Fig. 5). At the same time, in terms of the number of mobile subscriptions per 100 inhabitants, Ukraine is ahead of Germany and France, which is typical for low-income countries, where population actively uses mobile communications, equipment, and technologies of more advanced economies. As a consequence, there is a significant gap between Ukraine and the countries under review in terms of EPI.

If we analyze environmental indices more thoroughly (Table 6), it can be noted that Ukraine has the worst air and water quality, including because of poor development of wastewater treatment infrastructure, and the best ecological purity of agriculture, due to a relatively low use of mineral fertilizers [20].

## **Consequences for Ukraine**

In general, as the analysis has shown, the economy digitalization cannot yet be considered as a

| T. 1 / .1 . 1.  | "Leaders" |        | "Catchers" |         | Ukraine, difference in the indices as compared with the reference countries |        |        |                        | Ukraine, % |  |
|---|-----------|--------|------------|---------|---|--------|--------|------------------------|------------|--|
| Indices/ sub-indices  | Germany   | France | Poland     | Ukraine | Germany   | France | Poland | Averaged<br>difference | indices    |  |
| EPI. points   | 77.2      | 80.0   | 60.9       | 49.5    | -27.7   | -30.5  | -11.4  | -23.2                  | 68.1       |  |
| Environmental health  | 89.6      | 91.5   | 58.9       | 49      | -40.6   | -42.5  | -9.9   | -31.0                  | 61.3       |  |
| Air quality   | 81.1      | 88.1   | 44.7       | 39.8    | -41.3   | -48.3  | -4.9   | -31.5                  | 55.8       |  |
| Sanitation and drinking water   | 99        | 96.2   | 71.7       | 55.1    | -43.9   | -41.1  | -16.6  | -33.9                  | 61.9       |  |
| Heavy metals  | 90.7      | 84.0   | 65.3       | 69.3    | -21.4   | -14.7  | +4.0   | -10.7                  | 86.6       |  |
| Управління відходами  | 97.9      | 94.8   | 91.1       | 73.1    | -24.8   | -21.7  | -18.0  | -21.5                  | 77.3       |  |
| Ecosystem vitality  | 68.9      | 72.3   | 62.3       | 49.9    | -19.0   | -22.4  | -12.4  | -17.9                  | 73.6       |  |
| Biodiversity and habitat  | 88.8      | 88.3   | 89         | 37.7    | -51.1   | -50.6  | -51.3  | -51.0                  | 42.5       |  |
| Ecosystem services  | 39.7      | 36.1   | 27.1       | 30.2    | -9.5  | -5.9   | +3.1   | -4.1                   | 88.0       |  |
| Fisheries (condition of reserves,<br>trophic index, environmental friend-<br>liness of fishing methods) | 14        | 12.1   | 8          | 12.4    | -1.6  | +0.3   | +4.4   | +1.0                   | 109.1      |  |
| Climate change (preventive measures)  | 71.5      | 81.9   | 65.4       | 69.2    | -2.3  | -12.7  | +3.8   | -3.7                   | 94.9       |  |
| Pollution emissions (preventive mea-<br>sures)  | 96        | 100.0  | 89.6       | 76.6    | -19.4   | -23.4  | -13.0  | -18.6                  | 80.5       |  |
| Agriculture (ecological purity)   | 61.9      | 65.2   | 57.4       | 79.5    | +17.6   | +14.3  | +22.1  | +18.0                  | 129.3      |  |
| Water resources (waste water treat-<br>ment)  | 97        | 88.0   | 60.9       | 14.1    | -82.9   | -73.9  | -46.8  | -67.9                  | 17.2       |  |

Table 6. EPIs of Ukraine and the Reference Countries, in 2020

Source: [17].

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reliable means of solving environmental problems in Ukraine. First, digitalization itself has limited transformational potential, unless in the country there is innovation-driven development of national production, with modern production processes and products designed and implemented [21].

Second, the possible environmental consequences of economy digitalization need further indepth analysis, as the long-term positive effects of national economy digitalization are not obvious (as for many countries in the "catchers" cluster), while the adverse ones can have a significant impact. Ukraine, as part of Eastern Europe, has been already part of the region that receives e-waste [30, 14]. In addition, the introduction of new digital technologies, including 5G (a critical technology for the development of the Internet of Things), may have negative consequences not only for the advanced economies that have strict environmental standards, but also for Ukraine, given its present-day institutional realities (high corruption risks, significant gaps in the field of legal regulation of intellectual property, environmental protection) and relevant infrastructure [22, 69-72]).

While solving this problem, one cannot rely solely on private business, as it is subjectively motivated to maximize profits. In view of this, there is a need for a special national academic program to assess various aspects of the impact (abiotic, biotic, man-made, anthropogenic) of the advanced digital technologies on the environment.

Its important element can be the formation of a representative database on the status and parameters of digitalization of Ukraine's economy, including: the intensity of R&D in the digital sector, the density of digital technologies in industry, their productivity, environmental impact (energy balance and energy saving), carbonization or decarbonization, dynamics of accumulation, movement, and utilization of electronic waste, etc. It is also appropriate to take into account the existing approaches to assessing the economy digitalization, in particular, the EU's Digital Economy and Society Index (DESI)7<sup>7</sup> that integrates several different indicators of digital Europe and monitors the evolution of EU member states in terms of their digital competitiveness.

Third, it is important to form a digitalization program as part of the overall strategy of innovation-driven sustainable development of national production, which involves the formation of strong development institutions, similar to those already used successfully in other emerging markets [24].

In addition, it is necessary to adapt the European public-private partnership practices that have proven viability and to finance projects that are important to the national economy on a longterm basis. According to [26], more than EUR 20 billion are expected to be invested in the EU's single digital market by 2020. The current EU public-private partnership projects cover such important areas as: cybersecurity of energy and power engineering, transport, financial, and health sectors; high-performance computing; robotics; fifth generation mobile communication (5G); development of electronic components and firmware. It should be emphasized that their strategic goal is to help European industry meet the growing global consumer demand for greener, more individualized and better products by ensuring the necessary transition to demand-oriented industries with less waste and better use of resources [26]. Obviously, Ukraine's industry also needs similar support.

# Conclusions

1. The introduction of state-of-the-art digital technologies in various spheres of public life has a profound and diverse impact (both positive and negative) on the surrounding environment. The

<sup>&</sup>lt;sup>7</sup> DESI was first calculated in 2014; in 2018, in addition to the 28 EU member states, DESI was temporarily extended to 17 non-European countries (within the Interstate Index of Digital Economy and Society, I-DESI), including the United States, Canada, China, Japan, and Brazil., South Korea, Turkey, and Russia.

positive environmental effects of economy digitalization are associated with dematerialization of goods and services, improvement of production technologies, decrease in physical logistics flows, reduction of pollutant emissions, etc. The adverse effects are growing industrial and household energy consumption (and, consequently, increasing greenhouse gas emissions), accumulating electronic waste, understudied negative effects on the reproductive systems, genome structure, behavioral responses of living organisms, and so on.

2. The studies made by influential international organizations (OECD, European Commission, Asian Development Bank, etc.) have confirmed the growing changes in the size and structure of the ecological footprint caused by the introduction of digital technologies. In their assessments, digitalization is a generally positive phenomenon, as it may reduce global greenhouse gas emissions, among others. At the same time, it should be borne in mind that most of the estimates are predictive. Despite the world's prevailing desire to ensure climate neutrality and environmental loyalty of digital innovations, as a result of the lack of representative observations and because of delayed effects of technological interference in the functioning of ecosystems, the real environmental consequences of digitalization may be underestimated.

3. The empirical estimates presented in the research based on the economic analysis of ICT development and environmental performance indices in 106 countries have also showed a generally positive relationship between the introduction of digital technologies and the state of the environment: the higher the level of digitalization, the cleaner the economy. At the same time, from the point of view of substantiation of national policy, this general relationship is rather limited. This is because of the fact that the environmental performance of digitalization processes is determined by local economic development and production technologies, which in different countries (groups of countries) are characterized by their own characteristics rather than by global patterns.

4. To identify the local relationship between environmental performance and digitization, the analyzed countries have been divided into the four relatively homogeneous clusters (groups). Their analysis has showed that in clusters of less developed countries (including Ukraine), the relationship between ICT implementation and environmental performance is not strong, and the development of digital technologies has a much smaller positive impact on the environment than in the groups with advanced economies.

5. Based on this, the possible environmental consequences of digitalization of Ukraine's economy require further analysis, as its long-term positive effects in the specific conditions of the national economy are not obvious, while the negative ones can have a significant impact. Ukraine, as part of Eastern Europe, has been already part of the region that hosts e-waste. In addition, the introduction of new digital technologies may have undesirable consequences in the context of biology, the risks of man-made disasters, and so on. Therefore, there is a need to develop and to implement a national academic program to assess various aspects (abiotic, biotic, man-made, anthropogenic) of the impact of new digital technologies on the environment. In addition, it is critical to incorporate the digitalization of the economy into the overall strategy of innovation-driven sustainable development of national production, because being separated from the real sector, digitalization loses its effectiveness. Consequently, this requires the formation of national development institutions similar to those already used successfully in other emerging markets and the adaptation of best European practices in public-private partnerships for the selection and funding of the most important digital projects on a long-term basis.

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#### ЦИФРОВА І ЗЕЛЕНА ЕКОНОМІКИ: ТОЧКИ ДОТИКУ Й СУПЕРЕЧНОСТІ

**Вступ**. Процеси цифровізації економіки, пов'язані з розгортанням технологій Четвертої промислової революції, є багатоаспектними й чинять суттєвий вплив, зокрема й на навколишнє середовище, що зачіпає інтереси майбутніх поколінь.

**Проблематика**. Прискорення цифровізації супроводжується суперечливими позитивними і негативними ефектами для довкілля. Зважаючи на це, актуальною проблемою є визначення цих ефектів як на глобальному, так і на національному рівнях.

**Мета.** Виявити взаємозв'язки цифрової та зеленої економіки й обґрунтувати шляхи екологічно безпечного розвитку цифрових технологій в Україні.

**Матеріали й методи.** Кластеризація країн світу за ознаками економічного, промислового й цифрового розвитку; економетричний аналіз залежностей між показниками розвитку інформаційно-комунікаційних технологій і екологічної ефективності в країнах світу та їх групах (кластерах) за 2017—2020 рр.

**Результати.** Встановлено, що на глобальному рівні впровадження сучасних цифрових технологій має загалом позитивний зв'язок зі станом довкілля: чим вищим є рівень цифровізації, тим більш екологічно чистими, за інших рівних умов, є національні економіки. З'ясовано, що екологічна ефективність цифровізації залежить від рівня виробничих (фізичних) технологій та загального економічного розвитку держави. У кластерах менш розвинених країн, зокрема й в Україні, яка має суттєві проблеми у сферах промисловості й інновацій, поширення цифрових технологій має менший позитивний вплив на екологію, ніж у кластерах більш розвинених країн. Тому довгострокові позитивні ефекти цифровізації для України не є очевидними, а негативні можуть бути серйозними.

**Висновки.** Для мінімізації екологічних ризиків цифровізації в Україні потрібно розробити національну академічну програму комплексної оцінки різних аспектів (абіотичних, біотичних, техногенних, антропогенних) впливу новітніх цифрових технологій на довкілля, а також узгодити програми цифровізації економіки із загальною стратегією розвитку національного виробництва на інноваційній основі.

*Ключові слова*: цифрові технології, цифровізація економіки, промисловість, сталий розвиток, екологічний слід, екологічна ефективність.



# **RESEARCH AND ENGINEERING INNOVATION PROJECTS OF THE NATIONAL ACADEMY OF SCIENCES OF UKRAINE**

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# APPROACH TO STUDYING THE STRENGTH AND DETERMINING THE YIELD STRESS OF ROCKET AND SPACE ENGINEERING STRUCTURES

Introduction. Designing rocket structures requires computer modeling of their mechanical behavior in operating conditions. Based on the optimal design drawings obtained from computational experiments, a physical prototype has been made and tested. Depending on how successful the prototype passes the tests, the serial production of such structures is launched. The share of computer modeling in this process is constantly growing, since experimental studies are quite limited and extremely expensives.

**Problem Statement.** Estimates of structural strength significantly depend on the accuracy and reliability of data on their stress-strain state under operating conditions. Therefore, the development of software for assessing the stress-strain state of structures based on adequate mathematical models is extremely relevant.

**Purpose.** The purpose is to develop a method for studying the strength of complex structures of rocketry under intense loads and to determine ultimate breaking loads according to the results of computer modeling.

Materials and Methods. The problem is formulated within the framework of the geometrically nonlinear theory of thermoelastic plasticity, assuming that displacements and strains are large and stresses exceed the ultimate breaking load of materials. To solve the formulated problem, the finite element method has been used.

**Results.** A method for studying the stress-strain state of rocket complex structures under intense loads has been developed to estimate the ultimate breaking loads of such structures according to the results of computer modeling based on high-precision mathematical models. It has been successfully tested at the Yangel Pivdenne Design Office while designing fuel tanks of a launch vehicle.

**Conclusions.** The developed method makes it possible to significantly reduce or to completely abandon experiments during which the structure is carried to failure.

Keywords: mathematical and computer simulation, space rocket technology, strength, and failure.

Designing modern structures is associated with a complex multi-stage process of mathematical and computer simulation of their mechanical behavior under operating condi-

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tions. In cyberspace, engineers and researchers practically look for a rational or optimal design of structure, study its mechanical behavior under different load conditions, materials, and parameters of its geometric shape by computer modeling. Based on the drawings of the optimal design obtained as a result of computational experiments, a physical prototype is made and subjected to comprehensive trials. As a result of successful tests, serial production is launched. The share of mathematical and computer simulation in this process is constantly growing, as experimental studies of the mechanical behavior of complex structures are quite limited and costly.

Estimates of the service life of structures significantly depend on the accuracy and reliability of data on their stress-strain state under operating conditions. Therefore, their mechanical behavior under operating conditions is studied with the use of refined mathematical models that, in addition to the conventional properties of elasticity of materials, take into account their plastic properties. This problem is especially relevant for the design of structural elements of rocket and space technology, in which contradictions between the requirements for strength and minimum material consumption are most striking. Designing structural elements, when the task is to determine the ultimate breaking load, at which the material of a significant part of the mentioned objects is in an elastic-plastic state, with strains and displacements reaching significant values, may be an example. This state of the material, which does not cause any failure of the functional purpose of the structure and the operation of its equipment, is allowed in some structural elements of disposable rocket and space technology and in the case of long-term operational load.

The study of structures given plastic strains and large displacements and strains allows the use of additional material resources, which makes it possible to increase the operational load in the design estimates.

Obtaining reliable results for the strength of real structures of rocket and rocket-and-space tech-

nology is associated with difficulties caused primarily by their subtlety and the presence of different types of geometric concentrators in the form of frames, stringers, and so on. In particular, the reinforcing elements essentially complicate the application of shell theories, because the stressstrain state in their vicinity during loading is significantly three-dimensional. The use in these areas of the assumptions of the theory of shells may lead to the difference of the obtained solutions from the actual stresses and strains. On the other hand, under intense loads, thin shells are strongly displaced as a rigid whole. Most finite elements of the general type react to such a displacement by the appearance of false shear and membrane strains, which often leads to a slowdown in convergence and "locking" of solutions [1]. The situation worsens as ratio of the finite element length to its thickness increases [2].

Many aspects of the behavior of complex mechanical structures are associated with the interaction of their various components. Often, they cannot be predicted or traced experimentally (either in computational or in field experiments) with individual separated elements [3]. As a rule, actual stresses in real structures significantly differ from those predicted by partial experiments with individual structural elements (because of structural continuity and availability of alternative load paths for individual elements).

The researchers of Pidstryhach Institute for Applied Problems of Mechanics and Mathematics (IAPMM) of the NAS of Ukraine have developed a method for studying the stress-strain state of rocket and space technology structures under the action of intense force load and for determining the ultimate breaking loads and zones from which they may start breaking up, based on the results of computer simulation within the general model of a geometrically nonlinear elastic-plastic body [3–8], with the use of the finite element method. The obtained results have been tested in operating conditions, in the course of tests of large fuel tanks and introduced into production at Yangel's *Pivdenne* Design Office.



*Fig. 1.* Strain curves of materials of the cylindrical part of the tank (solid line) and bottoms (dash line)

The method for studying the strength of the structure is as follows. The study begins with simple 2D models. With the use of the documentation, a finite element model of the structure is built for chosen dimensions of its components and a model is designed from the bottom upwards, i.e. from points, lines to areas.

In numerical modeling of deformation processes, we use, as a rule, finite elements with a quadratic approximation of displacements [6]. While building a discrete model, we check to be certain that there are no strongly distorted or elongated finite elements (with a height-to-width aspect ratio that does not exceed 1: 2).

Experimental strain curves of the structure materials are used as input data as well. The strain curves are set pointwise, as interpolation splines [7, 8].

The conditions of fixing the structure are simulated and the load steps for the computational experiment are set.

After the successful computational experiment, we have analyzed the obtained values of displacements, strains, and stresses in the nodes, determined the critical areas of the structure with the highest stresses, strains, and strength criteria as well as the places from which failure is likely to start (where the corresponding strength criteria reach maximum). Having analyzed the results, we build a 3D fragment of the structure in the area with maximum values of parameters (stresses, strains, and criteria), for which we repeat the operations done for the 2D models (build a 3D finite element model, starting from points, lines, surfaces to volumes, set the conditions for fixing the fragment and the load). Having completed the computational experiment, we proceed to the analysis of the stress-strain state of a 3D fragment of the structure (determined the critical local areas of the structure with the largest deformations, stresses, strength criteria).

After a series of computational experiments, having determined the ultimate breaking load and the most stressful areas of the structure by computer simulation, we may perform a field experiment on a physical prototype for loads that are significantly less than the ultimate breaking ones. While performing these experiments, to measure deformations while applying loads, strain gages shall be placed in the most stressful places of the structure, as determined by computer simulation. After this, the experimental values of strains and stresses in these places shall be compared with similar values of the computational experiment. If the results of computational and field experiments coincide for loads less than the ultimate breaking ones, there is no need to increase the load to the ultimate breaking one in the physical prototype of the structure. This allows significantly reducing the costs of studying the strength problems of the elements of rocket and space technology.

To illustrate the proposed method, let us consider a large rocket structure, an eighteen-meter fuel tank of a space launch vehicle under the action of internal pressure.

The fuel tank is designed as a 3.9 m diameter cylindrical body closed by the upper and the lower spherical bottoms, each having a radius of 2.5 m. The body consists of eleven cylindrical shells of different types, with intermediate thickened zones between them for welding. As a result of the presence of circular frames and longitudinal strin-



*Fig. 2.* Distribution of equivalent stresses in the tank as a whole body at a pressure of 0.84 MPa

Fig. 3. Equivalent stresses in the vicinity of the most stressed area

gers, the inner surface of the shells has a wafer structure. The strain curves for the materials of which the wafer cylindrical shells and bottoms are made are shown in Fig. 1.

In order to quickly determine the strength and ultimate breaking load in the lower part, the whole tank deformation processes have been simulated based on the axisymmetric model, with the stringers neglected. For this purpose, we have used eight-node biquadratic finite elements [2].

Several computational experiments have been performed for different values of internal pressure. Fig. 2 shows the intensity of equivalent von Mises stresses in the tank at an internal pressure of 0.84 MPa. These stresses reach their absolute maximum (379.7 MPa) at the front of the rounded coupling of the first (immediately after the transition zone from the adjacent shell) frame with the inner surface (see Fig. 3) of the fifth shell (with a base thickness of 3 mm).

The stress distribution on the inner surface of the fifth shell is generally shown in Fig. 4. As one can see, there are local surges in the vicinity of



*Fig. 4.* Distribution of equivalent (solid line), axial (dash line) and circular (dash-and-dot line) on the inner surface of the fifth shell

each frame. The maximum stresses in the shell are mainly the circular ones that are highest in the middle of the shell. The axial stresses are generally lower, but in the vicinity of the extreme frames bordering the transitional thickened parts for welding individual shells, one can see their significant concentration. In the vicinity of these areas, they exceed the maximum circular stresses. In these places, equivalent von Mises stresses reach their maximum (at the level of the ultimate strength at a pressure of 0.84 MPa).

It should be noted that the absolute maximum stress in the fifth shell is greater than other local maxima in similar places of other shells of the same type by values of the order of computational error (maximum stresses in other shells range from 378.2 to 379.7 MPa). Practically, almost all these maxima can be considered equivalent, with the general trend being as follows: the local stress maxima are located in the vicinity of the extreme frames adjacent to the transition areas for welding individual shells. The stresses in the three lower shells (4.4 mm thick) and in the bottoms are significantly lower. The equivalent von Mises strain at the places of maximum stresses is 5.987%.

It should be noted that with a thickness of the upper bottom of 2.8 mm, the total displacement of the top part of this bottom reaches a value that is 73 times greater than the thickness of the bottom. The stresses at this point also exceed the ultimate strength for the bottom material (320 MPa, see Fig. 1). Increasing the thickness of the lower bottom by 0.2 mm eliminates this problem (at a thickness of 3 mm, the equivalent stresses in the upper bottom are less than the ultimate strength). The maximum deflections of the cylindrical shells in the central part of the tank reach twenty minimum thicknesses of these shells.

Therefore, having analyzed the results, we conclude that within the model of geometrically nonlinear, elastically and plastically deformable axisymmetric body (excluding longitudinal stringers) at a pressure of 0.84 MPa the equivalent von Mises stresses exceed the ultimate strength in the vicinity of the extreme frames of 3 mm thick shells. The axial stresses being highest at these local maxima, the tank breaks up in the circular direction (unlike in the case of conventional axial propagation of cracks in cylindrical shell-type bodies, when fracture is caused by circular stresses).

The results of the computational experiment based on the axisymmetric model have also shown that the action of the spherical bottom on the cylindrical part of the tank may be replaced by appropriately setting axial stresses at the end of the cylindrical component, distributing the whole load on the bottom at the ends of the transition area of the cylindrical part, i.e. by setting the axial stresses  $\sigma_z = p (R - h)^2/(R^2 - (R - h)^2)$  at the end, where R is the outer radius of the cylindrical part of the tank and h is the thickness of the transition area.

It should be pointed out that the axisymmetric finite-element model has been analyzed for convergence. The calculations for different sizes of finite elements have been done. For 0.5 mm and 1 mm elements, the differences in the maximum equivalent von Mises stresses are less than 0.25%. This difference is also within 1% for 1 mm and 2 mm elements.

To study the effect of longitudinal stringers on the stress state of the tank, a similar study has been performed, with the effect of frames neglected. For this purpose, the tank's cross section in the middle of the area between the frames has been analyzed. From the symmetry conditions, half of the longitudinal stringer and half of the waffle cell in the circular direction have been considered (within the framework of plane strain problem). Local stress concentrations in the vicinity of the stringer have been found significantly lower than in approaches to the frames.

Given the current capabilities of computers, on the one hand, and the complexity of geometrically and physically nonlinear problems in 3D formulation, on the other hand, the tank strength in the vicinity of structural components in which maximum stresses occur has been studied on partial models in the axisymmetric formulation, and the comparative analysis of the obtained solutions with similar ones for the whole structure has been made. In particular, the stress-strain state of a shell fragment of five wafer cells has been studied. The action of the bottoms is replaced by the axial force at one end; the conditions of equality of displacements in the axial direction to zero are set on the opposite edge of the fragment.

Fig. 5 shows the general distribution of equivalent von Mises stresses in such a fragment of the shell at a pressure of 0.84 MPa. As you can see, in this formulation, we reach the same level of maximum internal pressure as while considering the whole tank of eleven shells. The maximum stress equivalents are reported in the vicinity of the rounded coupling of the first (after the thickened part) and the last (before the thickened part) frames of the considered fragment, as a result of surging axial stresses in these areas.

Therefore, based on the obtained results, we conclude that for the considered fragment of the five cells we reach the ultimate strength at a pressure of 0.84 MPa. Moreover, the obtained results are consistent with those obtained for the whole tank of 11 shells with an accuracy of 0.7%. Similar results have been obtained for structures consisting of one and two complete shells (10 waffle cells in each).

To summarize the obtained results, the stress state of the same fragments of the shell of five cells has been calculated based on the model of a 3D



Fig. 5. Equivalent stresses in the five-cell shell fragment

geometrically nonlinear elastic-plastic body. From the circular symmetry conditions, the sector corresponding to half of the wafer cell (dimensions 0.137 m x 0.136 m) has been considered (see Fig. 6). The *Y* axis is directed along the axis of the cylindrical part of the tank; the *X* axis is oriented along the thickness; the Z axis coincides with the cylindrical angular coordinate at z = 0. Axial stresses that take into account the influence of the spherical bottom and zero axial displacements are set at the lower edge of the cylindrical part and at the opposite edge, respectively.

The nature of the stresses on the inner surface in the middle between the longitudinal stringers (in the plane of circular symmetry) is similar to that of those previously obtained within the axisymmetric model. The maximum stresses are the circular ones. In the vicinity of the extreme frames, in front of the transition area, there recorded a surge of the axial stresses. However, while studying the 3D stress state of the tank fragment under pressure, it has been established that the equivalent Mises stresses reach their absolute maximum in



Fig. 6. Equivalent stresses in 3D shell fragment at a pressure of 0.88 MPa



*Fig. 7.* Equivalent stresses in the median wafer cell of the shell at a pressure of 0.88 MPa



*Fig. 8.* Equivalent stresses in the cylindrical body at a pressure of 0.87 MPa in the framework of the shell model

other places, namely, in the middle of the studied fragment, on the inner surface of the central cell, 5 mm from the stringer (see Fig. 7). The same qualitative result has been obtained for a cylindrical fragment of the tank which consists of two whole shells, under similar load conditions.

Having made calculations for different values of internal pressure within the 3D model representation, the pressure (0.88 MPa) at which the maximum equivalent von Mises stresses reach the ultimate strength is determined. The highest value of the maximum stress criterion for the critical load is 0.985, which also indicates approaching failure according to this strength criterion.

It should be noted that as we approach the ultimate breaking load, the stresses over the tank thickness in the areas of maximum stresses even up, and the stress gradient through thickness practically disappears, as the difference between equivalent stresses on the inner and the outer surfaces is about 1-2 MPa, while in the area of elastic strain, it exceeds 20 MPa.

The influence of variation of geometrical parameters of shells, frames, and stringers on the stress state of the tank in the framework of the 3D model has been also studied. For example, the thickness of the thinnest shell should range within 3-3.35 mm; the thickness of frames and stringers should not exceed 6.4-6.9 mm. The computational experiment has been performed for the case where the thickness of shells, frames, stringers, and transition areas is taken at the upper limit of their allowable variation. Pressure at which the equivalent stresses approach the ultimate strength under such conditions is equal to 0.92 MPa.

Similarly, the tank strength has been studied within the framework of the six-modal theory of shells [9]. Based on the cyclic symmetry conditions, one cell of the shell is considered in terms of the angular coordinate. The surface of the shell, parts of the frames and stringers are represented by shell elements (in each node of the finite element division of the considered area, we have three displacements, two angles of rotation of the normal and its compression). The impact of the bottom on the cylindrical body is replaced by the axial stresses set at the upper edge of the body; at the other edge zero axial displacements are set. The conditions of cyclic symmetry are given at the edges as  $\alpha = 0$  and  $\alpha = Room2 / R$ , where Room2is the linear size of the cell in the circular direction, R is the tank radius. The pressure is set on the inner surface of the cylindrical body.

The computational experiments have shown that the equivalent stresses are almost close to the ultimate strength at a pressure of 0.87 MPa (see Fig. 8). As one can see, the maximum stresses are recorded in the middle of the fifth shell and they are the circular ones.

It should be pointed out that finite-element solutions in the case of the shell model are quite stable in terms of the size of finite elements. The same value of ultimate breaking load has been obtained for maximum finite element size of 2 mm and 5 mm.

The developed method and the corresponding software have been tested and implemented in the Yangel *Pivdenne* Design Office. With their help, the stress-strain state of fuel tanks has been studied. The comparative analysis of the results of computer simulation and field experiments has shown a good agreement in terms of the location and the nature of failure, as well as the value of ultimate breaking pressure. The last measured value of pressure before the failure of physical prototype is 0.89 MPa (in the computational experiment based on the 3D model a critical load of 0.88–0.92 MPa, depending on the tolerance for the shell thickness, has been obtained). On practice, the tank prototype starts failure with the fifth shell, as predicted by the computer simulations.

Hence, a method for studying the strength of structures and for determining ultimate breaking load by computer simulation and non-destructive experiments has been developed. Assuming that displacements and strains may be large and stresses significantly exceed the the yield stress of materials, the problem has been formulated within the geometrically nonlinear theory of thermoelastic plasticity. The finite element method has been used to solve the problem stated. Appropriate software has been developed on this basis. Within the framework of the developed method, the stress-strain state of a fuel tank of launch vehicle under the action of internal pressure has been studied for different model assumptions: the tank has been considered an axisymmetric structure, a composed shell, and a 3D elastic-plastic body. Quantitative estimates of its strength have been obtained; the ultimate breaking load and the most loaded local areas have been determined.

The analysis of the results of computer simulation of the fuel tank deformation processes allows us to state that the maximum stresses at ultimate breaking loads are located in the cylindrical part of the tank at the level of the fifth shell; in the vicinity of the spherical bottoms and spacer frames to which the cylindrical part of the tank is attached, the stresses are less than in its cylindrical part. It is the fifth shell from which the tank starts breaking up as the load increases, which has been confirmed by experimental tests. The stresses in the lower wafer shells are significantly lower.

With the transition to the area of plastic strains, as the load increases, the difference between the stresses on the inner and the outer surfaces decreases, which may also indicate an approach to failure (in the early stages, the stress on the inner surface is significantly higher).

The proposed method makes it possible to sharply reduce, or even to abandon, the full-scale experiments, during which the structure is carried to failure. After computational experiments and determination of the ultimate breaking load and the most stressful places of the structure by computer simulation, one may perform a field experiment on a physical prototype for loads that are significantly less than the ultimate breaking one. In these experiments, the sensors shall be placed in the most stressful places of the structure, as determined by computer simulation. The experimental values of strains and stresses in these places shall be compared with similar values of the computational experiment. In the case of coincidence of the results of computational and field experiments for the loads less than the ultimate breaking one, there is no need to increase the load to the ultimate breaking one in experiments with a physical prototype of the structure. This enables saving valuable materials and money.

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#### МЕТОДОЛОГІЯ ДОСЛІДЖЕННЯ МІЦНОСТІ ТА ВИЗНАЧЕННЯ РУЙНІВНОГО НАВАНТАЖЕННЯ КОНСТРУКЦІЙ РАКЕТНО-КОСМІЧНОЇ ТЕХНІКИ

Вступ. Проєктування ракетних конструкцій передбачає процес комп'ютерного моделювання їхньої механічної поведінки за умов експлуатації. За кресленнями оптимального проєкту, отриманого в результаті обчислювальних експериментів, виготовляють фізичний прототип, який піддають випробуванням, за результатами успішності яких переходять до виготовлення серійної продукції. Питома вага комп'ютерного моделювання в цьому процесі постійно зростає, позаяк експериментальні дослідження є доволі обмеженими і високовартісними.

**Проблематика**. Оцінки міцності конструкцій істотно залежать від точності й достовірності даних про їхній напружено-деформований стан за умов експлуатації. Тому розроблення програмного забезпечення для оцінювання напружено-деформованого стану конструкцій на основі високоточних математичних моделей є надзвичайно актуальним.

**Meta.** Розроблення методології адекватного дослідження міцності складних конструкцій ракетної техніки за інтенсивних силових навантажень та визначення руйнівних навантажень за результатами комп'ютерного моделювання.

**Матеріали й методи.** За припущення, що переміщення й деформації є великими, а напруження перевищують межу пластичності матеріалів, задачу сформульовано в межах геометрично нелінійної теорії термопружно-пластичності. Для її розв'язування використано метод скінченних елементів.

**Результати.** Розроблено методологію дослідження напруженого стану складних конструкцій ракетної техніки за інтенсивних силових навантажень з метою оцінювання руйнівних навантажень таких конструкцій за результатами комп'ютерного моделювання на основі уточнених математичних моделей, яку успішно апробована на Державному підприємстві «Конструкторське бюро «Південне» ім. М.К. Янгеля» при проєктуванні паливних баків ракети-носія.

**Висновки.** Розроблена методологія дає можливість суттєво скоротити або й взагалі відмовитись від натурних експериментів, під час яких конструкцію доводять до руйнування.

Ключові слова: математичне й комп'ютерне моделювання, ракетно-космічна техніка, міцність, руйнування.


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# ESTIMATES OF METHANE EMISSIONS IN THE OIL-AND-GAS INDUSTRY OF UKRAINE: PROBLEMS AND WORLD EXPERIENCE IN THEIR SOLUTION

**Introduction.** Given the possible impact of economy decarbonisation policy decisions on the future of the oiland-gas industry, it is necessary to develop a strategy for its further development, taking into account both carbon dioxide and methane emissions.

**Problem Statement.** In recent years, many countries have been making efforts for reducing methane emissions in the oil-and-gas industry, several national and international initiatives have been formed. In Ukraine, not enough attention is paid to this matter.

**Purpose.** The purpose is to analyze the state of monitoring of methane emissions from the oil-and-gas industry of Ukraine and to generalize experience of other countries in this field.

**Materials and Methods.** Analysis of official estimates of methane emissions from the oil-and-gas industry of Ukraine. Review of authoritative literature sources and documents of international organizations on the estimate of methane emissions from the industry, technological and institutional measures for monitoring and verification of these emissions.

**Results.** Comparative analysis of estimates of greenhouse gas emissions in the oil-and-gas industry based on the National GHG Inventory annual reports of the Naftogaz of Ukraine Group has been made. The peculiarities of methane emission sources in the industry and the problems of quantification of its emissions have been considered. Technological means and measures implemented in different countries to solve the problems of methane emissions monitoring have been analyzed.

**Conclusions.** It has been concluded that there is a wide range of available technologies for detection and quantification of methane emissions in the industry. The need to use national coefficients for estimating fugitive emissions from oil-and-gas industry for the National GHG Inventory has been shown. An important factor in reducing methane emissions from the industry shall be government policy that aims at developing and implementing regulatory standards and special economic tools.

Keywords: greenhouse gases, oil-and-gas industry, identification of methane emission sources, methane emission estimation, and technology.

Much of the world's attention has been paid to climate change that is associated with greenhouse gas (GHG) emissions. Ukraine has been an official party to Annex I of the United Nations Framework Convention on Climate Change (UNFCCC), since 1997; a party to

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Annex B to the Kyoto Protocol, since 2004; and a party to the Paris Agreement that amends the Kyoto Protocol and defines its commitment to reduce GHG emissions, since 2016. As part of the climate process, the Cabinet of Ministers of Ukraine by its order of 16.09.2015 no. 980 approved the expected national contribution to the draft of the new global climate agreement, which is not to exceed 60% greenhouse gas emissions of 1990 in 2030 [1]. In 2018, GHG emissions (excluding the sector Land use, rezoning, and forestry) accounted for only 31.6% of 1990 [2]. At the same time, according to the Paris Agreement, every five years, the member countries shall report on their contributions to the UNFCCC Secretariat and set new, more ambitious goals. The first such report is to be submitted in 2023.

Another important argument in favor of strengthening GHG emission reduction in the oil-andgas industry is a significant transformation of approaches to energy development in the world, the so-called green energy transition that is accompanied by a reduction in the share of extractive industries in economy. According to [3], political decisions regarding decarbonization, which are made in the next 5-10 years, will irreversibly affect the future of not only oil but also natural gas. To ensure that natural gas is included in Europe's energy balance after 2030 and remains competitive with other low- or zero-carbon energy sources, gas companies need to develop appropriate strategies for further development over the next five years. If the situation in the gas sector remains unchanged, it will be the beginning of its decline in the future after 2030, as options for the formation of non-methane energy may be adopted.

Today, the only widely available document that contains official information on GHG emissions in our country is the National Inventory of Anthropogenic Emissions from Sources and Absorption of Greenhouse Gases in Ukraine (hereinafter referred to as the National Inventory). According to the National Inventory for 1990–2018 [2], in 2018, methane ( $CH_4$ ) emissions in Ukraine amounted to 67.54 million tons of  $CO_2$ -eq, which was

about 20% of total GHG emissions. The largest sources of methane emissions are power engineering (65.1% of total emissions), agriculture (13.9%), and waste management (16.4%). In the Energy sector, according to the Intergovernmental Panel on Climate Change (IPCC), the largest fugitive emissions are from coal, oil and natural gas. Thus, in the oil-and-gas industry of Ukraine, it is necessary to pay attention to reducing emissions of both carbon dioxide (CO<sub>2</sub>) and methane.

In recent years, much attention has been paid to reducing methane leaks and emissions in the oil-and-gas industry, and several national and international initiatives have been launched to this end. First and foremost, the United States Environmental Protection Agency's Natural Gas STAR Program that encourages oil-and-gas corporations to use proven, cost-effective technologies and practices that improve performance and reduce methane emissions [4]. Reducing methane emissions from the oil-and-gas sector has attracted focused attention of the UN [5–7], the International Energy Agency [8], the European Commission [9], and many non-governmental organizations. At the same time, there have been almost no publications on this important subject in Ukraine, and when it comes to reducing GHG emissions, first of all, we mean carbon dioxide. Even in such an important document as the Strategy for Low Carbon Development of Ukraine until 2050, measures for reducing greenhouse gas emissions other than carbon dioxide are presented very formally [10].

Table 1 shows the amount of carbon dioxide and methane emissions in 2017–2018 from the oil-and-gas industry (excluding oil refining) along the entire technological chain from exploration to consumption.

From Table 1 shows that the main GHGs generated in the industry are carbon dioxide and methane, as their shares made up 2.6% and 43.8% of the total emissions of these GHGs across the country, in 2017, and 2.4% and 45%, in 2018, respectively, The main part of carbon dioxide emissions is generated from hydrocarbon extraction and fuel combustion operations by gas-compressor units of main gas pipelines. The main sources of methane emissions are natural gas production, distribution, and consumption in the residential and commercial sectors. This structure of methane emissions suggests, in particular, that in contrast to the country's gas transportation system, the conditions of gas distribution networks require much attention.

In Ukraine, information on GHG emissions from oil-and-gas facilities in addition to the National Inventory is provided in the annual reports of *Naftogaz of Ukraine* Group (Table 2).

The data given in Table 2 differ significantly from the data of the National Inventory, especially with regard to methane emissions. Thus, in 2017, according to the inventory, methane emissions from hydrocarbon production amounted to 356.5 thousand tons, and according to *Naftogaz*, the total methane emissions of JSC *Ukrnafta* and JSC *Ukrgazvydobuvannya* came to only 14.4 thousand

tons. According to the National Inventory, methane emissions from these operations amounted to 371.98 thousand tons, while according to Naftogaz, they totaled 24.9 thousand tons. In 2017, JSC Ukrnafta and JSC Ukrgazvydobuvannya extracted 16.4 billion m<sup>3</sup>, and in 2018, 16.6 billion m<sup>3</sup>, which accounted for about 80% of gas production in Ukraine. Since in accordance with the Law of Ukraine on Environmental Impact Assessment [12], at each stage and project of the technological chain of the development of hydrocarbon resources, both public and private corporations shall develop Environmental Impact Assessment given the norms defined in the laws of Ukraine, industry regulations, and standards of enterprises, the emissions from extraction by private corporations may be taken similar to methane emissions by Naftogaz of Ukraine Group corporations. Hence, according to Naftogaz estimates, the total annual methane emissions from hydrocarbon pro-

| Table 1. | GHG Emission | s in the Oil-aı | nd-Gas Industry | y of Ukraine in | 2017-2018 |
|----------|--------------|-----------------|-----------------|-----------------|-----------|
|          |              |                 | •               | /               |           |

|  |         | GHG, thousand tons |                 |        |  |  |
|--|---------|--------------------|-----------------|--------|--|--|
| Operation  | 20      | )17                | 2018            |        |  |  |
|  | $CO_2$  | $CH_4$             | CO <sub>2</sub> | $CH_4$ |  |  |
| Exploration and production of oil and condensate   | 150.72  | 56.13              | 162.50          | 60.53  |  |  |
| Flaring in oil operations  | 88.55   | 0.05               | 95.47           | 0.06   |  |  |
| Venting in oil operations  | 0.21    | 1.56               | 0.22            | 1.68   |  |  |
| Exploration and production of natural gas  | 1751.69 | 281.53             | 1815.89         | 291.84 |  |  |
| Flaring in natural gas operations  | 77.25   | 0.05               | 80.08           | 0.05   |  |  |
| Processing of natural gas  | 5.44    | 17.19              | 5.64            | 17.82  |  |  |
| Total extraction of hydrocarbons   | 2073.86 | 356.51             | 2159.80         | 371.98 |  |  |
| Pipeline transportation of oil   | 0.01    | 0.10               | 0.01            | 0.10   |  |  |
| Pipeline transportation and storage of natural gas, including:                               | 3730.46 | 26.61              | 3473.99         | 26.05  |  |  |
| fugitive emissions   | 0.31    | 26.54              | 0.30            | 25.99  |  |  |
| combustion of fuel by gas-compressor units   | 3730.15 | 0.07               | 3473.69         | 0.06   |  |  |
| Natural gas distribution   | 5.72    | 496.74             | 6.50            | 568.11 |  |  |
| Natural gas consumption by the residential and commercial sectors                            | 0.91    | 236.58             | 0.94            | 249.94 |  |  |
| Total transportation, distribution, and consumption of hydrocarbons                          | 3737.10 | 760.03             | 3481.44         | 844.20 |  |  |
| Total oil-and-gas industry   | 5811    | 1117               | 5641            | 1216   |  |  |
| Total GHG emissions (without capture)  | 223200  | 2548               | 231700          | 2700   |  |  |
| The share of emissions from the oil-and-gas industry from total GHG emissions in the country | 2.6     | 43.8               | 2.4             | 45.0   |  |  |

Source: based on the data of Ukraine's Greenhouse Gas Inventory 1990-2018 [2].

duction may be estimated at 20 thousand tons, in 2017, and 32 thousand tons, in 2018, which is an order of magnitude higher than the data given in the National Inventory. At the same time, methane emissions from the transportation of natural gas through main gas pipelines differ much less.

The significant difference in estimates of methane emissions in the industry is explained by several factors. First, to date, both in Ukraine and in other countries, the problem of determining the sources and amount of methane emissions in the oil-and-gas industry has not been addressed. This is due to the following features that are clearly defined in [5, 6]:

- a large number of emission sources. For example, studies in Canada have shown that compressor stations have an average of 6 leakage points, while gas extraction plants comprise several ten thousand components, a few percent of which typically has leakages, assuming an average of 19 leakage points;
- geographical dispersion of emission sources. Equipment at fields, compressor stations, pipelines are located on a large area and in remote places, which increases the cost of measurements, often physical availability of emission sources for measurements is limited;
- variability of emissions. Emission indicators from equipment and processes vary significantly depending on the type and age of the equipment, its technical condition, operating condi-

*Table 2.* GHG Emissions by Corporations of Naftogaz of Ukraine Group in 2017–2018, thousand

| Corporations of Naftogaz | 2017    | 7      | 2018    |        |  |
|--------------------------|---------|--------|---------|--------|--|
| of Ukraine Group         | $CO_2$  | $CH_4$ | $CO_2$  | $CH_4$ |  |
| Ukrgazvydobuvannia       | 862.7   | 10.0   | 1 715.2 | 20.3   |  |
| Ukrnafta                 | 1 022.8 | 4.4    | 631.1   | 4.6    |  |
| Ukrtransgaz              | 3 818.5 | 30.4   | 3 707.9 | 30.2   |  |
| Ukrtransnafta            | 1.7     | 0.1    | 2.9     | 0.1    |  |
| Other corporations       | 1.5     | 0.6    | 1.9     | 0.6    |  |
| Total emissions          | 5 707   | 45.5   | 6059    | 55.7   |  |

*Source*: annual reports of *Naftogaz of Ukraine* Group for 2017 and 2018 [11].

tions and maintenance practices, climatic conditions. In addition, many emission points are intermittent sources. Therefore, the widespread use of emission factors from a limited number of sites or equipment may lead to significant uncertainties;

• Methane emissions are invisible and in most cases odorless, which makes it difficult to determine and to estimate emissions without the use of specialized equipment. This leads to additional costs of monitoring, reporting, and verification.

Second, according to the authors of the National Inventory, the Tier 1 simplest methodological approach and the average default emission factors according to the IPCC recommendations of 1996 and 2006 are used to estimate emissions in category 1.B.2 Fugitive emissions [13]. The Tier 2 approach recommended by the IPCC is similar to Tier 1, but instead of default emission factors. it uses national factors determined on the basis of research and analysis of the results of special measurements. The National Inventory of 2019 states that a "national method" based on the use of state statistical reporting, namely, the 4-MTP form, was developed to assess GHG leakage during the transportation of natural gas through main gas pipelines [2]. The 2-step approach was also used to estimate leakage during natural gas distribution with the use of gas distribution networks (GDN). It seems, the authors of the document mean the application of the Tier 2 approach, but readers do not understand this. In particular, in [5, 6] it is noted that for the National Inventory, in 2019, in Ukraine, only the Tier 1 approach was used to estimate emissions from hydrocarbons.

In addition, the application of the 2-step approach proposed by the authors of the National Inventory leads to the fact that the natural gas leak rates during transportation and distribution differ significantly for neighboring years, which has not been justified by the authors of the document and raises doubts about their correctness (Table 3).

It should be noted that both Tier 2 and Tier 3 approaches as well as Tier 1 approaches are used in the inventory of methane emissions from oil and natural gas operations in different countries. According to the National Inventory 2019 Reports [14], the USA and Canada applied the Tier 2 and Tier 3 approaches, and so did Australia for most categories of emission sources. While preparing National Inventories 2019, twelve EU member states used Tier 1 approaches, whereas the others applied coefficients from different tiers for different operations with hydrocarbons. Kazakhstan used Tier 1 for the preparation of the National Inventory for 2019; in 2019, the Russian Federation applied Tier 2 for natural gas production and transportation operations and Tier 1 for other operations with hydrocarbons. It should be noted that in 2016, in this country, upon the request of the Ministry of Power Engineering of the Russian Federation, a survey was conducted and national factors for carbon dioxide and methane emissions from certain categories of sources of the oil-and-gas industry were developed [15]. These coefficients were used to estimate methane and carbon dioxide emissions during the production and processing of natural gas, as well as during its transportation through main gas pipelines. Because of the use of national Tier 2 emission factors instead of the Tier 1 default factors, the estimate of methane emissions from the oil-and-gas sector, for example, in 2016 decreased from 24.9 million tons to 6.3 million tons.

So, Ukraine shall move to Tier 2, while preparing National Inventories.

Third, it cannot be said that the methane emission estimates given by *Naftogaz* in its annual reports are more accurate than the estimates of the National Inventory. Today, in Ukraine, even at the level of industry corporations, the quantitative estimates of methane leaks are rarely based on direct measurements, more often they are derived from the estimates or requirements of industry standards (so-called "certified" or "nominal" value of leaks).

Thus, until the system of monitoring, reporting, and verification of GHG emissions start operating

in Ukraine, it is impossible to talk about the development of national methane emission factors.

It should be noted that, in 2019, the process of improving the 2006 IPCC Guidelines was completed [7]. In the Energy sector, all methodological updates concern the categories of fugitive emissions, including those from the oil-and-gas industry. In particular, methods and coefficients for determining emissions from liquidated wells were added. The introduction of this source in the inventories may significantly increase estimates of methane emissions from the oil-and-gas industry, as in Ukraine, especially in the Carpathian Region, there are many liquidated and abandoned wells in many old oil fields. Another important amendment in the Guidelines is that there is no longer a difference between Tier 1 emission factors for advanced economies and developing countries.

With regard to the system of monitoring, reporting, and verification of GHG emissions, Verkhovna Rada of Ukraine adopted the Law of Ukraine on the *Principles for Monitoring, Reporting, and Verification of Greenhouse Gas Emissions* in compliance with international obligations under the Association Agreement with the European Union [16]. The law is expected to be introduced since 01.01.2021. However, this law is a framework, the methods and procedures for preparing a monitoring plan, as well as emission calculation methodologies will be determined by bylaws to be app-

*Table 3.* Natural Gas Leak Rates During Transportation and Distribution in Ukraine

| Year | Natural gas leak rate<br>during transportation,<br>billion m³/million tons | Natural gas leak rate<br>during distribution,<br>billion m³/ billion m³ |
|------|--|---|
| 2012 | 0.00071  | 0.01151   |
| 2013 | 0.00101  | 0.00893   |
| 2014 | 0.00150  | 0.01042   |
| 2015 | 0.00057  | 0.01386   |
| 2016 | 0.00140  | 0.01623   |
| 2017 | 0.00039  | 0.01984   |
| 2018 | 0.00040  | 0.02386   |
|      |  |   |

Source: Ukraine's Greenhouse Gas Inventory 1990–2018 [2].

roved by the relevant resolutions of the Cabinet of Ministers of Ukraine. According to the draft resolution of the Cabinet of Ministers of Ukraine on Approval of the List of Operations Covered by

Monitoring, Reporting, and Verification of Greenhouse Gas Emissions, and Specific Features of Its Application [17], at the first stage of implementation, this system will apply only to operations

| r. | i i i i i i i i i i i i i i i i i i i                          |   |   |  |
|----|--|---|---|--|
|    | Method   | Principle of the method   | Capital expenses, USD   | Analysis of price factors  |
| ĺ  |  | Leak detection methods  | 3   |  |
|    | Optical video<br>recording sys-<br>tem (infrared<br>cameras)   | Hydrocarbon emissions absorb infrared light with a cer-<br>tain wavelength, the camera uses this feature to detect<br>the presence of hydrocarbon emissions in real time  | 85 000 — 115 000<br>for portable device   | High cost and labor expenses   |
|    | Laser Leak<br>Detector   | Uses an adjustable infrared LED tuned to a frequency that is absorbed by methane  | 15 000  | Relatively cheap equip-<br>ment, but high labor ex-<br>penses                |
|    | Soap bubble<br>screening                                       | Soap solution is applied to the place where there is a sus-<br>picion of leakage. In the case of leakage, bubbles are<br>formed, which are observed visually  | Less than 100   | Relatively low costs, but<br>high labor inputs                               |
|    | Organic va-<br>por analyzers<br>and toxic va-<br>por analyzers | Portable hydrocarbon detectors are generally capable of measuring organic vapor concentrations in the range from 9 to 10,000 ppm  | Less than 10 000  | Limited use, complexity.<br>May require expensive<br>software                |
|    | A c o u s t i c<br>Leak Detec-<br>tors                         | Record the acoustic signal that is generated when a gas<br>leaks under pressure. Most detectors have the ability to<br>adjust the frequency, which allows adjusting the sensor to<br>the leaks of specific objects  | 1 000–20 000, depen-<br>ding on sensitivity, si-<br>ze, and availability of<br>additional equipment | Limited use and high<br>complexity when using<br>a hand-held device          |
|    |  | Leak quantification metho   | ods   |  |
|    | Calibrated<br>vent bag   | Measures the time to complete the bag of the calibrated<br>volume. The gas temperature is measured to adjust the<br>volume to standard conditions. The gas composition shall<br>be analyzed to determine the methane content  | 50  | Low cost method, major<br>costs are labor expenses<br>(requires 2 operators) |
|    | High-volume<br>sampler   | Absorbs atmospheric air and hydrocarbon gas leaks. The<br>thermal anemometer monitors the mass flow rate of the<br>air-hydrocarbon mix. Two-element hydrocarbon detec-<br>tor measures the concentration of combustible hydrocar-<br>bons in the captured stream.                                 | 17 500, additional 1.200<br>(calibration kit)   | Relatively expensive me-<br>thod given labor costs                           |
|    | Gas flowme-<br>ters  | There are different technical versions of flowmeters: vo-<br>lumetric, thermal, rotary, ultrasonic, vortex, etc.  | 4 000-8 500, depen-<br>ding on the type and<br>size of the meter                                    | Cost-effective, especial-<br>ly for measuring large<br>and long-term leaks   |
|    | Vane anemo-<br>meters  | Consist of a paddle speed sensor and a hand-held unit<br>that displays the measured speed of the gas passing<br>through the device  | 1 400-5 500   | Low cost and cheap main-<br>tenance  |
|    | Hotwire ane-<br>mometer  | A heated wire inserted into the gas stream is used to mea-<br>sure its speed. The hotwire anemometer measures the<br>electric current passing through the wire, as the heat is<br>dissipated due to the gas flow, and the heat lost as a result<br>of convection is proportional to the gas flow. | 1 400-5 500   | Low cost and cheap main-<br>tenance  |

| Table 4 Methods for Detection and         | Quantification of M  | lethane Leaks in the | <b>Oil-and-Gas Industry</b> |
|---|----------------------|----------------------|-----------------------------|
| <i>Table 4.</i> Methods for Detection and | Qualitilication of M | lethane Leaks in the | Oll-allu-Gas Illuusti y     |

*Source:* based on [4–6, 20].

that lead to emissions of carbon dioxide: fuel combustion in plants with a total rated thermal capacity of more than 20 MW, oil refining, metallurgy, production of coke, building materials, nitric acid, and ammonia. Monitoring and verification of methane emissions has not been implemented yet.

At the same time, given the structure of GHG emissions from the oil-and-gas industry, the main priority is to reduce methane emissions from natural gas, which is typical for the gas industries of other countries as well. Preventing and reducing methane emissions is first and foremost a safety requirement. In addition, the global warming potential of methane is 28 times higher than that of carbon dioxide, but it has a shorter life, averaging up to 12 years, as compared with CO<sub>2</sub> that is stored in the atmosphere for centuries. Thus, methane emissions have a much greater impact on the climate in the short term [18]. It is also possible, in many cases, to sell the captured methane in the natural gas market, thereby avoiding emissions and making a profit.

Today, in the world, there is a wide range of methods and measures for timely detection and quantification of methane leaks in the gas industry [4-6, 8, 9, 19, 20] (Table 4).

The analysis of the characteristics of methane emission sources and methods for their detection has shown that continuous monitoring of a large number of emission sources in the oil-and-gas industry is currently impossible. However, many new methods that will allow it in the near future, primarily, through remote sensing have been being developed.

Quantitative estimation of methane emissions requires a combination of operational measurements and calculation methods. Currently, there are two groups of the calculation methods: the bottom — up and the top — down ones [4-6, 8]. The former provides a quantitative estimate of emissions from individual sources directly at the emission site. These methods give the most accurate information on specific emission sources at the equipment level, but are costly and time consuming as compared with the computational or top - down approaches. The top - down estimation methods measure methane concentrations in the atmosphere with the use of, for example, satellites, aircraft, or drones. These methods use the values of the measured environment parameters and weather conditions and mathematical models to determine emissions from a specific facility or from a specific region. Scaling such data to a corporation or a regional level is cheaper and may be more accurate than the use of bottom - up approaches. Such estimation methods can provide more frequent quantification of methane emissions and identify the largest sources of emissions. Although according to research [6], one of the key problems related to the top - down methods is that they do not allow the identification of specific equipment that is a source of emissions, but today analytical methods for building emission distributions are developing very rapidly.

Also in research [6] it is noted that today no country may completely deviate from the general methods for estimating individual emission sources. Therefore, it is important to involve research institutions for independent verification of emissions through actual measurement programs.

The studies conducted in different countries [5, 6, 8, 19] allow us to identify several key measures that can contribute to the formation of reliable national estimates of methane emissions:

- organization of qualitative direct measurement of emissions, which is critical for the localization of emission sources and estimates of their reduction levels;
- clear formulation of the emission reduction target, which shall be expressed both in broad, qualitative and in specific, quantitative and time terms;
- attraction of innovative technologies, first of all, low-cost technological solutions, and use of advanced digital technologies;
- ensuring of maximum transparency through the exchange of measurement protocols and their analysis by industry corporations and national regulator;

- encouragement of cooperation with international and national oil companies, which facilitates the introduction of best practices;
- ensuring of effective control over the implementation of established legal norms governing the organization of supervision and regulation, determination of institution entrusted with regulation or control, provision of powers and resources for this institution, determination of penalties for non-compliance with legal norms.

The world experience summarized in [6, 8] also has shown that the main government policies and regulations important for the reduction of methane emissions in the oil-and-gas industry are as follows:

1. Standards that require the use of specific technologies and / or operational practices and quantify emission limits. The most common are technical standards. For example, this category includes the requirement to implement regular programs to detect and to eliminate methane leaks.

2. Economic tools covering emissions charges, taxes, and penalties for exceeding the permitted level of emissions, emissions trading systems, tax rebates and financial subsidies for specific investments in emission reductions. However, the introduction of a methane emission charge requires confidence in the accuracy of a certain amount of emissions, as there may be situations in the industry where the reliability of the estimated emissions are not verifiable.

3. Public-private partnership and agreements between industry and political authorities or the regulator, which may take various forms: from a weakly defined partnership with voluntary objectives to formalized agreements with the subsequent introduction of mandatory rules if specific quantitative targets are not met.

At the same time, there is no single best practice for regulating methane emissions. Each country shall develop its own rules, given world experience and its own institutional conditions and economic opportunities.

In recent years, several countries have developed policies to reduce methane emissions, in particular, the report of the International Energy Agency for 2020 [8] refers to the following examples:

- ♦ Canada has introduced standards to reduce methane emissions by 40—45%, by 2025, as compared with the reference year 2012. In the provinces of Alberta, British Columbia, and Saskatchewan, additional regulatory measures have been being taken to address ventilation and flare leaks in oil and natural gas production;
- In the United States, several states (California, Colorado, Ohio, Pennsylvania, Utah, and Wyoming) have their own regulations and standards for methane emissions that accompany or reinforce federal obligations. They vary in terms of scale, but all require mandatory control of objects at different intervals;
- Several European countries have provisions on reporting and limiting methane emissions. For example, in Norway, each oil-and-gas complex shall annually give report on methane emissions with the use of a common estimation methodology based on standard emission factors; methane emissions from ventilation are taxed.

An example of public-private partnership is the commitment to reduce methane emissions, which is assumed by oil-and-gas corporations. Some companies have set a target of reducing methane emissions from oil-and-gas production by 2025, depending on the amount of natural gas supplied to the market. For example, British Petroleum aims to achieve methane emissions of 0.2% of natural gas sales during this period; Shell and Total have similar targets; *Pemex* and *OGCI* aim to achieve 0.2-0.25% methane emissions from the total amount of natural gas released to the market [19]. Other companies have set as a target reducing in methane emissions by a percentage of a given reference year. For example, Eni aims to reduce methane emissions from extraction by 80% by 2025 as compared with 2014; *ExxonMobil* aims to reduce methane emissions from operating activities in 2020 by 15% as compared with 2016; the Netherlands Oil and Gas Exploration and Production Association undertakes to reduce methane emissions from offshore production by 50%, as compared with 2017 [19], in 2020—2024. These commitments can be a guide for other companies that have not yet set their methane reduction targets.

It should be noted that NJSC *Naftogaz of Ukraine* declares its participation in reducing greenhouse gas emissions. However, so far, the official documents of *Naftogaz* and its subsidiaries, which are available to the general public [21–25], have not contained any specific commitments to reduce GHG emissions in general or methane in particular.

At the same time, according to the information contained in the annual reports of Naftogaz of Ukraine [11], the company has applied some measures and technologies to reduce methane emissions, in particular, detection of natural gas leaks is carried out by electronic indication and acoustic leak detection. In 2019, within the framework of the tripartite Memorandum between NJSC Naftogaz of Ukraine, the European Bank for Reconstruction and Development, and the Ministry of Environment and Natural Resources of Ukraine [26], the first detection and measurement of methane leaks into the atmosphere with the use of drones were implemented at the facilities of JSC Ukrgazvydobuvannia and JSC Ukrtransgaz. The contractor was Carbon Limits (Kingdom of Norway). It was this company that, in 2017, conducted a study for reducing methane emissions at the industrial facilities of ISC Ukrgazvudobuvannia, but no information about the results of this study has been published in open sources.

With regard to gas distribution networks and gas consumers in the residential and commercial sectors, which are the main sources of methane emissions from the oil-and-gas industry, the efforts for reducing emissions are not sufficient. To estimate methane emissions, gas distribution companies use the Methodology approved by the Ministry of Energy and Coal Industry of Ukraine in 2003 [27]. This Methodology defines productionrelated (normalized) gas losses as "the maximum gas leakage which does not prevent ensuring reliable operation and conditional standard tightness of gas pipelines, connecting parts, fittings, compensators, gas equipment, appliances, etc." However, the current technical condition of the GDN equipment is significantly different from the state of "conditional standard tightness". Also, it should be noted that the Methodology covers only the regular operation leaks of the equipment, while the unforeseen leaks of methane from the GDN equipment are not estimated at all. Given the fact that as of 2017, in Ukraine 1% of the total length of GDN and 8% of gas control points were in a critical condition [28], and the entire gas distribution system is suboptimal because of reduced natural gas consumption, the most relevant is the use of advanced technologies for detecting natural gas leaks in these networks. However, today, most often, both GDN and consumers use the soaping method and the calibrated ventilation bag technique for detecting gas leaks and for measuring the amount of leakage, respectively.

Thus, the analysis of greenhouse gas emissions in the oil-and-gas industry has shown that it is a major source of methane emissions that, in 2018, according to the National Inventory, accounted for 45% of emissions of this greenhouse gas in the country as a whole. Hence, the main priority for the industry is to reduce methane emissions, which is typical for oil-and-gas industries in other countries.

It has been shown that the oil-and-gas industry is very difficult in terms of identification and quantification of methane leaks and emissions because of a large number of emission points, their geographical dispersion, physical inaccessibility, variability of emission levels. Quantifying methane emissions is a global problem that has not yet been addressed so far. Today, it is advisable to use a combination of measurements, computational methods, and simulation. It has been established that technologies that facilitate the detection and quantification of methane leaks are available and shall be used by corporations and authorities for monitoring, reporting, and verification of emissions.

It has been established that until the system of monitoring, reporting, and verification of methane emissions starts operating in Ukraine, it is impossible to say which of the estimates, the National Inventory or the reports of the *Naftogaz of*  *Ukraine* group, are more accurate and reliable. Meanwhile, it is necessary to move to Tier 2 (use of national coefficients) while forming the National Inventory in terms of estimating fugitive emissions from oil and natural gas operations.

An important measure to reduce methane emissions from the oil-and-gas industry shall be government policy that aims at developing and implementing regulatory standards, economic tools, agreements between industry and government, and promoting the exchange of best practices.

Extensive implementation of measures to reduce methane emissions from the oil-and-gas industry may allow Ukraine to achieve more ambitious GHG emission reduction targets under the Paris Agreement and to prepare the industry for operation in the context of energy decarbonization.

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#### ОЦІНКИ ВИКИДІВ МЕТАНУ В НАФТОГАЗОВІЙ ГАЛУЗІ УКРАЇНИ: ПРОБЛЕМИ ТА СВІТОВИЙ ДОСВІД ЇХ ВИРІШЕННЯ

**Вступ**. Враховуючи можливий вплив на майбутнє нафтогазової галузі політичних рішень стосовно декарбонізації економіки, потрібно розробити стратегію її подальшого розвитку з урахуванням необхідності зменшення викидів не тільки двоокису вуглецю, а й метану.

**Проблематика**. Останніми роками у багатьох країнах ведеться активна діяльність зі скорочення викидів метану у нафтогазовій галузі. Для вирішення цієї проблеми сформовано низку національних та міжнародних ініціатив. В Україні зазначеному питанню не приділяється достатньо уваги.

**Мета**. Проаналізувати стан моніторингу викидів метану від нафтогазової галузі України та узагальнити досвід інших країн з цього питання.

**Матеріали й методи.** Аналіз офіційних даних щодо викидів метану від нафтогазової галузі України; огляд авторитетних літературних джерел та документів міжнародних організацій щодо оцінки викидів метану від підприємств галузі, технологічних та інституціональних заходів, спрямованих на вирішення проблем моніторингу та верифікації цих викидів.

**Результати.** Виконано порівняльний аналіз оцінок викидів парникових газів у нафтогазовій галузі відповідно до Національного кадастру парникових газів та річних звітів групи «Нафтогаз України». Розглянуто особливості джерел викидів метану в галузі та проблеми кількісного визначення обсягів його викидів. Проаналізовано технологічні засоби та заходи, які запроваджуються в різних країнах для вирішення проблем моніторингу викидів метану.

**Висновки.** Встановлено, що існує широкий спектр доступних технологій для виявлення та кількісного оцінювання викидів метану в галузі. Визначено необхідність переходу до використання національних коефіцієнтів при формуванні Національного кадастру парникових газів в частині оцінки летучих викидів від діяльності з вуглеводнями. Важливим чинником зменшення викидів метану від галузі має стати політика держави, акцентована на розробленні та запровадженні регуляторних стандартів і спеціальних економічних інструментів.

*Ключові слова*: парникові гази, нафтогазова галузь, ідентифікація джерел викидів метану, оцінка викидів метану, технологія.



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# SPECTROMETER-IDENTIFIER BASED ON A SOLID DETECTOR FOR NFC FACILITIES

**Introduction.** The Chornobyl accident resulted in radiation contamination of a large area. In order to prevent the release of radioactive elements into the environment and food, it is necessary to use specialized devices that allow monitoring of the radiation situation.

**Problem Statement.** One of the most effective ways to quickly detect and identify sources of ionizing radiation in the environment is to control the spread of radionuclides that are present in food and construction materials.

**Purpose.** The purpose is to develop modern domestic equipment for automated operational detection, identification, and monitoring of ionizing radiation sources in the environment in real time.

**Materials and Methods.** Methods of mathematical and computer modeling, full-scale modeling, machine design have been used. To study the specifications of the system and its features, field tests of its individual channels in the exclusion zone of the Chornobyl NPP have been carried out.

**Results.** An experimental system for automated operational detection, identification, and monitoring of ionizing radiation sources in the environment in real time, as well as for identification of detected radioactive isotopes and reliable estimate of their activity has been created and tested.

**Conclusions.** The created spectrometer-identifier is a new generation rapid response system based on advanced technologies, synthesis of principles of radiometry, spectrometry, and mathematical simulation. It is used for effective control of specific activity of liquid, viscous, bulk food and non-food samples and for identification of their radionuclide composition.

The introduction of the spectrometer-identifier significantly reduces the time for operational mass study of food and non-food samples and identification of their radionuclide composition, which raises the environmental safety in the era of widespread operation of nuclear fuel cycle facilities.

Key words: nuclear radiation accident, gamma radiation, spectrometer, radiation monitoring, and radiation safety.

Any facility of the nuclear fuel cycle (NFC) infrastructure, while operating, is a source of radionuclides that pollute the environment. The long-term operation of NFC facilities brings additional radioactivity to the adjacent territories, with its elemental composition being identical to the natural radioactivity accumulated in the environment. Most emis-

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sions because of a short half-life of radionuclides and their limited mobility in the environment have local or regional importance. Some radionuclides (<sup>3</sup>H, <sup>14</sup>C, <sup>129</sup>J, etc.) are characterized by a long half-life and a high mobility [1].

Thus, as a result of human activity, the content of natural and artificial radionuclides in the environment has increased. The concentration of radionuclides in food also has grown. The level of food contamination depends on the intensity of radioactive fallout, their bioavailability, and on the soil and climatic conditions that determine the migration of radionuclides [2].

The separation of technogenic radioactivity from the background natural one that accumulated in the environment, for example, in the soil, is a rather complicated analytical task, and ways to solve it have not been sufficiently developed. Also, there have been no methods to correctly determine relative contributions into the pollution of each individual enterprise or a cluster of enterprises located within a limited area, which can be sources of additional radioactivity discharged into the environment.

Reliable information on the levels of radioactive contamination of the environment is a necessary condition for assessing the dose load on the population and for making decisions on measures to ensure radiation safety.

The estimation of radiation doses is an extremely complicated biological problem because of the difficulty of obtaining statistically significant values of dose loads, especially when they are less than 0.1 Gy (doses that do not lead to the development of clinically defined non-random effects on human or animal health). Irradiation in such doses may be dangerous because of delayed somatic and genetic effects characterized by probabilistic nature of their manifestation. There have been almost no reliable experimental data on small doses.

In order to prevent the ingress of radioactive elements into the environment and food, it is necessary to use specialized instruments and measuring systems for monitoring the radiation situation and, having analyzed it, for predicting and preventing emergencies.

This is especially relevant now, when the design resource of many NPPs has already been exhausted, and decisions are being made to extend it. That is, there is a need for specialized devices and measuring systems that allow monitoring the radiation situation.

The existing approaches, methods, and devices cannot be effectively used to detect and to identify sources of ionizing radiation. This is primarily because of a low functionality of existing technical systems, the ability to register only limited characteristics of radiation fields, unsatisfactory level of automation of control procedures, underdeveloped information exchange, and "closed" architecture. The limiting factors for the modernization of these systems and their integration into other monitoring systems are unsatisfactory level of identification of ionizing radiation sources, the inability to integrate them into a common system because of the lack of a common principle and method for their design.

Given the importance and urgency of controlling the radiation situation, researchers of the Nuclear Physics Department of IEG of the NAS of Ukraine have created a new generation measuring system that allows quick detection and identification of radionuclides in the measured sample.

The purpose of this research is to design, create, and to evaluate the parameters of a compact, inexpensive, wireless spectrometer-radiometer for realtime detection, identification, and monitoring of ionizing radiation sources in the environment.

# 1. Engineering solutions

The spectrometer-identifier may be considered as a rather sophisticated autonomous system that operates in real time. Like all such systems, it consists of disparate components: analog and digital electronic circuits, measurement algorithms, and structural elements, i.e. a set of hardware and software designed for automatic solution of the tasks assigned to them for effective identification of gamma radiation sources. The spectrometer-identifier has a modular structure and consists of the following elements:

- detection unit;
- microcontroller for data control, collection, and pre-processing;
- unit for transmission and exchange of information with an external user;
- data selection and record unit; and
- power control unit.

A scintillation crystal of cesium iodide activated by thallium CsI (Tl) is used as a detector in the spectrometer-identifier. This crystal has the property of radioluminescence: charged particles and high-energy photons (X-ray and gamma range) excite the glow in it, with photons emitted as a short, about a microsecond, flash of light — scintillation. The scintillation crystals are chosen in as much as they can be compact, inexpensive, provide efficient record of gamma rays, and operate in spectrometric mode.

Typically, photoelectric multipliers (PEMs) the main advantage of which is a high sensitivity are used to capture such weak light pulses. The maximum sensitivity of PEM coincides with the maximum wavelength of the scintillator. However, PEM has several significant disadvantages:

- the need for high voltage power supply;
- large dimensions;
- ♦ high cost;
- the need for magnetic shielding.

Today, semiconductor photodetectors that are able to compete in sensitivity with PEMs, but do not have the above disadvantages have appeared on the market.

A multipixel silicon photodiode with p-i-n junctions, which has a maximum spectral sensitivity in the infrared region is used as a photodetector. Each pixel is a p-n junction to which a reverse bias voltage exceeding the breakdown voltage (<60 V) is applied. The charge gain of an individual pixel is ~ 10<sup>6</sup> and is determined by the amount of accumulated charge at the p-n junction of the pixel. The magnitude of the charge at the output of such a photomultiplier is determined by the sum of the charges of all its pixels trig-



Fig. 1. Configuration of the detector

gered by the light flash of the scintillator. This photodetector has several advantages, in particular, a high internal gain, a low reverse bias voltage and a weak dependence of the internal gain on bias voltage and temperature variations. These advantages allow it to be used as a photodetector for scintillation detectors designed for solving spectrometric problems.

A solid photomultiplier with a total area of  $1 \times 1 \text{ mm}^2$  consists of 576 independent pixels, each having a size of ~  $40 \times 40 \mu m$ .

The CsI (Tl) scintillator is coupled with a solid PEM with optical glue to remove the air gap between the crystal and the photodetector window, and to ensure maximum light collection by the photodetector. The crystal and solid PEM are surrounded from all sides by a reflector made of fluoroplastic powder. This coating has a very high diffuse reflection coefficient. To be protected against external influences, the detector is placed in a cylindrical aluminum housing that provides protection and water-proofing, since the cesium iodide crystal is sensitive to moisture that may destroy it (Fig. 1).

#### The detector has the following electric parameters:

| Voltage, V                         | + 5.0   |
|------------------------------------|---------|
| Detector's maximum bias voltage, V | + 5.0   |
| Supply current, mA                 | 100     |
| Supply current, mA                 | 24 - 27 |



Fig. 2. Stand for gamma-spectrometric measurements

| Amplifier conversion factor, mV / MeV      | 80       |
|--|----------|
| Front of the amplifier output signal, ns   | ~ 5      |
| Gain ratio (adjustable)                    | 20 - 20  |
| Polarity of the output pulse at a positive |          |
| bias on the detector                       | Positive |
| Output pulse FWHM, µs                      | 5.0      |
| Maximum magnitude of output pulse, V       | + 3.2    |

# The detection unit is built on the basis of a solid detector and has the following specifications:

| Relative resolution on 661 keV line ( <sup>137</sup> Cs),                    |    |
|--|----|
| % At most 7  |    |
| $\label{eq:linearity} Integral nonlinearity, \%. \dots \qquad At most \pm 1$ |    |
| Instability for 8 hours of continuous ope-                                   |    |
| ration, % $\pm 2$  |    |
| Maximum input static load, s <sup>-1</sup> 50 000                            |    |
| Operating mode setting time, min At most 30                                  |    |
| Number of channels 1024  |    |
| Operating temperature range, $^{\circ}C$ from $-10$ to $+$                   | 40 |

The signals of required amplitude and duration from the detector are digitized, encoded, and stored in the form of a digital code in the memory of the microprocessor unit.

The microprocessor unit (MPU) provides collection and processing of information in real time, storage of information on a memory card (microSD), transfer of information to the host (personal computer or other device), execution of commands from it, support of the Ethernet network interface, various expansion modules (UEXT interface, Olimex-compatible), device power, and user interface. The MPU is based on a microcontroller of the Cortex M4 family with a core clock speed of 168 MHz, has 1 MB internal Flash memory and 196 KB RAM [3]. The MPU performs all control functions of other modules; it is a hardware platform for executing algorithms for processing and organizing the user interface.

## 2. Algorithm solutions

According to the measurement model used in the registration of particles with energy spectrum  $\Phi(E)$ , we obtain some signal distribution U(V) that is called the hardware spectrum. The relationship between  $\Phi(E)$  and U(V) is described by the following integral relation

$$U(V) = \int_{0}^{\infty} G(V, E) \Phi(E) dE.$$
(1)

When working with a spectrometer, the main task is to find the true energy spectrum  $\Phi(E)$  based on the hardware spectrum U(V). In the general case, for this purpose it is necessary to know the response function of the detector G(V, E) and to solve the above integral equation.

The problem of identifying the radioisotope composition of the spectrum  $\Phi(E)$  is reduced to finding the peaks of full absorption in the spectrum U(V) in the hardware spectrum.

From formula (1) it follows that the identification is based on a comparison of the energy distribution of the measured hardware spectrum U(E)with the energy distribution of individual radionuclides  $g_i(E)$ .

The energy distribution of the sample to be analyzed may be represented as the sum of the distributions of radionuclides in the sample:

$$f_N^* = \sum_{i=1}^N \alpha_i g_i, \tag{2}$$

where  $g_i \subset \Phi$ ,  $i = \overline{1, N}$  are basic expansion functions;  $\alpha_i \in R$ ,  $i = \overline{1, N}$  are coefficients of the series expansion;  $f_N^*$  is approximation of certain function y with the use of N various basic expansion



Fig. 3. Spectra of tested sources of 137Cs and 60Co

functions from set  $\Phi$ ;  $y = \{y_1, ..., y_L\}$  is known function obtained from measurements;  $M \le N$  is the number of functions in set  $\Phi$ .

It is necessary to choose basis  $\{g_1, ..., g_N\} \subset \Phi$ and respective coefficients  $\{a_1, ..., a_N\} \in \mathbb{R}^N$  in such a way as to minimize the quadratic residual:

$$RSS = ||R_N||^2 = ||y - f_N^*||^2 = \sum_{i=1}^{L} (y_i - f_N^*(x_i)). \quad (3)$$

To ensure the (mathematically) optimal solution to this problem, it is necessary to search through *T* bases  $\{g_1, ..., g_N\} \subset \Phi$  and to find *T* times the respective coefficients  $\{a_1, ..., a_N\} \in \mathbb{R}^N$ , where *T* is defined from the formula

$$T = 2^N. \tag{4}$$

For an arbitrary basis, the respective coefficients that minimize the quadratic residual (3) have been found with the use of the least squares method, provided that the free term of the corresponding linear regression equation (2) is equal to zero [4].

#### 3. Testing of solutions

A stand for gamma spectrometric measurements has been designed to verify and to test the solutions, algorithms, and software of the spectrometer-identifier.

The design of the stand consists of a spectrometer-identifier, a personal computer with a program for processing and visualization of spectra,



Fig. 4. Spectra of tested sources of 152Eu and 133Ba

and a positioning system for sources of ionizing radiation (Fig. 2).

Using radioisotope sources 241Am, 137Cs, 60Co, 152Eu, 133Ba, and 40K, the detection unit of the spectrometer-identifier has been tested.

According to the measurement results, the optimal forming time constant, in terms of signal / noise ratio, has been determined. Its value is  $\tau = 1 \ \mu s$ , despite the fact that the total illumination time of the scintillator CsI (Tl) is ~  $3-4 \mu$ s. Reducing the forming time constant allows increasing the record capacity of the detector based on the "slow" scintillator CsI (Tl). The discrete sensitivity (number of counted pulses per unit dose) of the detection unit may be adjusted both by selecting the detector volume together with varying the operating bias voltage and by varying the discrimination (or amplification) of the signal in the measuring path. Figs. 3–4 show the results of background radiation and test radionuclide record, which characterize the most typical energy regions of the detector hardware spectra. The range of their gamma radiation, from 81 keV (133Ba) to 1460 (40K), practically covers the range of gamma radiation of Chornobyl genesis radionuclides.

The energy resolution of the gamma spectrometer at an energy of 661.6 keV is 6.5%. The energy calibration of the gamma spectrometer has been validated by reference spectrometric gamma sources (RSGS) 137Cs and 60Co (Fig. 5).



Fig. 5. Calibration curve of energy channel

The measurement is performed upon the operator's command; the measurement results are processed automatically. The implemented isotope identification algorithm has showed good results. For test samples, it unmistakably determines the available isotopes in the total spectrum (Table 1). The response functions of the detector have been obtained on the stand of gamma spectrometric measurements.

The high energy capacity of the detector (6.5%) increases the accuracy of radionuclide identification. The wide spectral range of measurements from 0.5 KeV to 3 MeV increases the ability to detect different types of radionuclides.

#### Conclusions

1. As a result of the research, an experimental sample of spectrometer-identifier based on a solid detector has been designed for real-time control and prevention of the spread of radionuclides that are present in food and construction materials, as well as for identification of detected radioactive isotopes and reliable determination of their activity.

2. Due to the use of a scintillation crystal with a high radiation detection as a detection unit and a PEM based on a semiconductor diode with a high quantum efficiency and readout speed, the gamma-ray spectrometer has excellent spectrometric and operational characteristics.

3. Modern element base and perfect circuitry, which are used in the creation of recording equipment (pre-amplifier, analog-to-digital converter, microprocessor unit), allow real-time obtainment of the spectra of any gamma radiation source with subsequent processing and analysis.

4. The microprocessor unit with a modern signal processor *Cortex*, on the basis of which the device is built, provides statistical processing of measurement results at the same rate as they come

| Sample | Isotope | Energy, keV | Confidence | Identification error | Activity, Bq/sample |
|--------|---------|-------------|------------|----------------------|---------------------|
| P-1    | CS-137  | 661.66      | 1.0        | 1.1134806E-03        | 1.7200047E+02       |
|        | EU-154  | 123.07      | 0.998      | 5.7892155E-02        | 8.8093251E+01       |
|        |         | 1274.43     |            |                      |                     |
|        | EU-155  | 105.31      | 1.0        | 7.8731112E-01        | 1.2195589E+01       |
|        | AM-241  | 59.54       | 1.0        | 5.2484277E-03        | 8.2756083E+02       |
| P-2    | CS-137  | 661.66      | 0.992      | 8.281543E-003        | 3.951950E+002       |
|        | EU-154  | 123.07      | 0.988      | 1.070405E-002        | 4.626154E+000       |
|        |         | 1274.43     |            |                      |                     |
|        | AM-241  | 59.54       | 1.0        | 7.357731E-002        | 4.277017E+001       |
|        | CO-60   | 1173,24     | 0.996      | 1.817543E-003        | 2.619645E+002       |
|        |         | 1332,5      |            |                      |                     |
| P-3    | CS-137  | 661.66      | 0.992      | 8.281543E-003        | 3.951950E+002       |
|        | EU-154  | 123.07      | 0.988      | 1.070405E-002        | 4.626154E+000       |
|        |         | 1274.43     |            |                      |                     |
|        | AM-241  | 59.54       | 1.0        | 7.357731E-002        | 4.277017E+001       |

Table 1. Results of Gamma Spectra Processing

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from the detector, prompt display of results, comparison of measurement results with the tolerances, alarming in the case where these results go beyond the established limits, and archiving of measurement results.

5. The resulting spectrometer-identifier based on a solid detector, which is designed for real-time

control and prevention of the spread of radionuclides present in food and construction materials, as well as for identification of detected radioactive isotopes and reliable estimation of their activity, may be used as a basic element of the automated system for continuous safety control of radiation in the areas affected by the Chornobyl disaster.

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#### СПЕКТРОМЕТР-ІДЕНТИФІКАТОР НА ОСНОВІ ТВЕРДОТІЛЬНОГО ДЕТЕКТОРА ДЛЯ ОБ'ЄКТІВ ЯДЕРНО-ПАЛИВНОГО ЦИКЛУ

**Вступ**. Наслідком аварії на Чорнобильській АЕС стало радіаційне забруднення значної території. З метою запобігання потрапляння радіоактивних елементів в довкілля та продукти харчування необхідним є використання спеціалізованих приладів, що дозволяють здійснювати контроль радіаційної обстановки.

**Проблематика**. Одним з найбільш ефективних способів оперативного виявлення та ідентифікації джерел іонізуючого випромінювання в довкіллі є контроль за розповсюдженням радіонуклідів, присутніх у продуктах харчування та будівельних матеріалах.

**Мета.** Розробка сучасного вітчизняного обладнання для автоматизованого оперативного виявлення, ідентифікації та моніторингу джерел іонізуючого випромінювання в середовищі в режимі реального часу.

**Матеріали й методи.** Використано методи математичного та комп'ютерного моделювання, натурного макетування, машинного проєктування. Для дослідження технічних характеристик системи, її особливостей проведено натурні випробування окремих її каналів в зоні відчуження Чорнобильської АЕС.

**Результати.** Створено та апробовано експериментальну систему автоматизованого оперативного виявлення, ідентифікації та моніторингу джерел іонізуючого випромінювання в навколишньому середовищі в режимі реального часу, а також ідентифікації виявлених радіоактивних ізотопів та достовірної оцінки їхньої активності.

**Висновки.** Створений спектрометр-ідентифікатор є системою швидкого реагування нового покоління на базі сучасних технологій, синтезу принципів радіометрії, спектрометрії та математичного моделювання для ефективного контролю питомої активності рідких, в'язких, сипучих харчових і нехарчових проб, ідентифікації їхнього радіонуклідного складу.

Впровадження ідентифікатора-спектрометра сприятиме суттєвому скороченню часу на проведення оперативної масової перевірки харчових і нехарчових проб та ідентифікації їхнього радіонуклідного складу, що, в свою чергу, підвищить рівень екологічної безпеки населення в епоху широкої експлуатації об'єктів ядерно-паливного циклу.

*Ключові слова*: ядерно-радіаційна аварія, гамма-випромінювання, спектрометр, радіаційний моніторинг, радіаційна безпека.



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# INNOVATIVE APPROACH TO THE CREATION OF TEXTILE MATERIALS WITH ANTIMICROBIAL PROPERTIES

**Introduction.** In recent years, there has been a constant search for more advanced and environmentally friendly means for antimicrobial treatment of cellulose-containing tissues of various intended uses in the textile industry.

**Problem Statement.** The problem of protection of textile materials and products from microbiological destruction is complex and multifaceted and needs to be solved. Today, one of the methods of protection is to provide textile materials with biocidal properties, which not only prevents the growth of bacteria, but can also ensure a high level of tissue safety. Therefore, we are faced with the task of finding new safe biocidal products.

**Purpose.** The research has been made to determine the level of safety of textile materials treated by biocidal substances with the thiosulfonate structure including Ethylthiosulfanilate, Methylthiosulfanilate and Allylthiosulfanilate.

**Materials and Methods.** The fabrics of different chemical composition were used in the study, designed for the manufacture of overalls. New preparations of thiosulfonate structure were chosen for impregnation: ethylthiosulfanilate (ETS), methylthiosulfanilate (MTS) and allylthiosulfanilate (ATS). The presence of heavy metals and pesticides was determined by atomic absorption spectrometry with the use of a ZEENIT 650P spectrometer (Germany).

**Results.** It has been established that the detected level of heavy metals and pesticides in the studied textile materials is insignificant and is within the regulatory requirements. It has been confirmed that the studied biocidal substances are low-toxic and environmentally friendly, because before and after treatment they did not change

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the hygienic parameters of tissues. A method for imparting biocidal properties to textile materials for the manufacture of overalls, in particular by impregnating textile materials with an alcoholic solution of biocidal products, has been developed. Also due to this treatment, the water absorption of materials decreases by an average of 40%. **Conclusions.** The treatment of textile materials with biocidal preparations of the thiosulfonate structure allows obtaining simultaneously two desired effects for these fabrics: the appropriate bioresistance and water resistance. K e y w or ds: environmental responsible, heavy metals, biocides, hygienic properties, and thiosulfonates.

In recent years, textile industry specialists have been paying attention to the problem of determining the level of environmental responsible and hygiene of clothing and other types of textile materials. Until recently, the demands of consumers and producers of textiles have been related to fashion, shape stability, ease of care and low cost. The negative influence of the textile material was not discussed or discussed last of all.

However, publications on the negative effects of textiles on the human body are appearing increasingly in the world scholarly research literature, also great attention is paid to textile materials with antimicrobial properties because textiles can contribute to the transmission of pathogens [1-6].

In particular, the issue about the development of antimicrobial fibers has been consider by the textile industry since 1941 (Hirschmann and Robinson 1941).

In [1], it is shown the possibility of survival of 60 bacteria strains including four species (*Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Staphylococcus aureus*, and *Enterococcus faecium*) on untreated cotton textiles in clinically significant incubation periods. The antibacterial efficacy of the textiles treated with *Sanitized T99-19* and *Sanitized T27-22*, which contain quaternary ammonium salts (QAC) has been established. The mentioned samples have shown a high influence on the action of bacterial test cultures of the most of grampositive pathogens and ineffectiveness against multiresistant gram-negative bacteria (*Escherichia coli*) [2].

As is known, organic antimicrobial reagents of both natural (chitosan, cyclodextrins and natural dyes) and synthetic origin (various Quaternary ammonium salts, triclosan, halogenated phenols and organometallic compounds) are used for the processing of cellulose textiles. The interaction between cellulose and antimicrobial reagents, mechanisms of their biological action and the influence of various factors on the biocidal activity of textile carriers are illustrated by researchers in the work [3]. In order to improve durability and mechanical properties of textiles it is need to conduct a preliminary activation of its cellulose component or to use linker agents. As antimicrobial agents it is advisable to use environmentally friendly compounds of prolonged action, in particular resistant to hygienic care [3].

The effect of biocides 3-methylol-2,2,5,5-tetramethylimidazolidinone (MTMIO) and 1,3-dimethylol-5,5-dimethylhydantoin (DMDMH) and their compositions in various ratios for chemical modifications of cellulose was studied by Californian researchers. The use of such compositions for cellulose treatment improves the strength and stability of biocidal functions of tissues treated with these preparations, in addition, these tissues can withstand repeated washing and long shelf life [4].

Another achievement in this direction is cyclodextrins, which are widely used for tissue processing, because due to their unique chemical structure they exhibit the good absorption capacity, namely, they form inclusion complexes with different antimicrobial and other biologically active substances. Therefore, this is undoubtedly important to provide textiles with antimicrobial properties in further studies [5, 6].

Many compounds with a wide spectrum of antimicrobial attributes, high bactericidal and fungicidal activity [7] have been found among thiosulfonates of the general formula  $RSO_2SR'$ , which are close to structural analogues of natural phytoncides including garlic *Allium sativum*, *Allium*  *cepa onion*, various types of cabbage, especially cauliflower [8, 9].

The synthetic thiosulfonic acid esters are known to exhibit a wide range of biological activity, which often exceeds the efficiency of natural analogues. Some of them are offered as effective antifungal substances, promising perspective substances of another direction, preservatives of fruits and vegetables, effective remedies for plants, growth regulators, biocidal additives and insecticides. Esters of thiosulfonic acids are effective sulfenylating reagents in organic synthesis, having valuable properties for solving the complex problems of molecular biology and biochemistry [7, 10–11].

But today, the searching of the new environmental ways for providing antimicrobial properties to textile materials does not lose its relevance, despite the existence of numerous studies in this field.

The textile materials can be a source of negative effects of chemicals complex during production. For example, dyes, compounds, and preparations containing heavy metals are used to decorate and provide textiles with specific properties. Their application not only reduces the level of environmental friendliness of the product, but also adverselv affects the environment. These substances can be complex multi-component systems, which are not always completely removed from products and materials at different stages of the technological process. During the operation of clothing under the influence of various factors products of destruction can be also released into the clothing space, which in turn adversely affects the human body, causing various biological effects [12, 13].

All over the world, much attention is paid to the development of various methods for obtaining and studying the antimicrobial properties of textile materials and their safety. Therefore, the issue of creating environmentally friendly textile materials with antimicrobial properties resistant to wet treatments, washing, and solar insolation when the textiles are used in real conditions [14– 16], remains quite relevant. Given these facts, it is obvious that textile products require a great attention to quality and safety.

In Ukraine, ecological safety of textile products is defined in the framework of the draft CMU Resolution on *Approval of the Technical Regulation on Environmental Criteria for the Eco-labeling of Textile Products* as strategic directions and tasks for the implementation of state policy in the field of environmental protection, preservation of the health of the state population.

Also, in 2013, the State Sanitary norms and rules "Textile, leather and fur materials and products" came into force. The basic hygiene requirements were developed for harmonization of domestic standards with the standards of the International Association for Research and Testing in the field of Textile Ecology (OECO-TEX).

The basic hygiene requirements are divided into groups:

- rationing of chemicals in products;
- rationing of indicators such as hygroscopicity, air permeability, specific surface electric resistance and pH level;
- normalization of harmful substances and their migration from the products into the human body and the environment (the content of free formaldehyde and formaldehyde which is able to partially excrete, residues of heavy metals able to extract, pesticide content, the content of pentachlorophenol, azo dyes and organochlorine carriers, the presence of odor, etc.) [16].

The natural fiber fabrics provide excellent conditions for the development and growth of microorganisms through the ability to retain moisture and microbial enzymes that can easily hydrolyze polymer bonds. Cellulose is known throughout the world as the most common, renewable and almost inexhaustible polymeric material with an exciting chemical structure and properties. Consequently, cellulose polymer is characterized by its chirality, high functionality, biodegradation, the ability to broadly chemical modification and the formation of universal semi-crystalline fibers. Therefore, the functionalization of cellulose textiles is the aim of researchers [15–18].



Fig. 1. The synthesis of used thiosulfonates

Consequently, the study of environmental safety of cellulosic textile materials with antimicrobial properties, obtaining new data on the protective properties of such materials, expanding their scope of application used to be urgent scientific tasks with a great practical importance.

The need of development of new biocidal materials with antimicrobial properties is caused by the changing general biological resistance of the human body. Studies show that there are new types of microorganisms which are resistant to most antimicrobial agents. Also pathways, modes of transmission and the duration of their lives are changing [11, 12, 19–21].

The purpose of the research is to develop the antimicrobial textile materials with the use of biocide compounds of the thiosulfonate structure such as Ethylthiosulfanilate (ETS), Allythiosulfanilate (ATS), Methylthiosulfanilate (MTS) preparations, study their properties and environmental safety in order to use it in seaports and docks. These biocidal preparations are tested and effectively used as biocides to protect paintwork materials, component of anticorrosive composition for pipelines of circulating water supply systems, petroleum products, building materials and constructions, algaecides for surface protection, packaging materials, for sterilization of culture fluid in biotechnological manufactures [22–23]. To our knowledge ETS, MTS, ATS preparations were used firstly to produce environmentally friendly fabrics according to international indices of safety.

*Collection of textiles.* The object of our research was cotton and cotton polyester fabrics produced by *Toctals Fabrics* and *Ten Cate Protect*, respectively (Table 1). All samples of fabrics are treated by the new species of biocidal preparations possessing thiosulfonate structure, which plays an important role in ensuring safe working conditions in various industries, as well as in seaports and docks. The main functions of such clothes are the preservation of human health, the creation of favorable conditions, protection against the negative influence of the environment, fungal and bacterial microflora.

The biocide preparations. To protect cellulosecontaining textile materials and clothing products from the negative effects of fiber-destroying and pathogenic microorganisms, we selected new biocidal preparations having the thiosulfonate structure: Ethylthiosulfanilate (ETS), Allylthiosulfanilate (ATS), Methylthiosulfanilate (MTS), which exhibit a wide spectrum of antimicrobial activity,

| Table 1. | <b>Properties</b> | of the | Studied | Textile | <b>Materials</b> |
|----------|-------------------|--------|---------|---------|------------------|
|----------|-------------------|--------|---------|---------|------------------|

| Sample | ple<br>Fibrous composition, % Surface<br>density, |                  | Density, P, tl<br>threads p | ne number of<br>per 10 cm | Linear densi<br><i>T</i> , | ty of threads,<br><i>tex</i> | Type of coloring |
|--------|---|------------------|-----------------------------|---------------------------|----------------------------|------------------------------|------------------|
| number |   | g/m <sup>2</sup> | Warp                        | Weft                      | Warp                       | Weft                         |                  |
| 1      | Cotton, 100                                       | 245              | 307                         | 292                       | 49                         | 38                           | smooth-dyed      |
| 2      | Cotton-polyester, 50/50                           | 245              | 292                         | 220                       | 42                         | 25                           | smooth-dyed      |

are non-toxic, and can be used for antimicrobial protection in various industries.

These thiosulfonates are synthesized at the Department of Technology of Biologically Active Compounds, Pharmacy and Biotechnology in the Lviv Polytechnic National University in accordance with Fig. 1 [22, 23].

Indicators of the minimum concentration of thiosulfonate biocidal preparations for fungicidal (A) and fungistatic (B) treatment of cotton-polyester cloths for their protection against biodestruction by fibrous and pathogenic microorganisms are presented in Table 2.

**Methods.** In order to determine the environmental quality of textile materials treated with biocidal preparations content of toxic substances, heavy metals, pesticides, measurements have been made at the Kovalevsky Institute of Biology of the Southern Seas of the NAS of Ukraine (Odesa) and at the laboratory of chemical analytical research of the Ukrainian R&D Center of Ecology (Odesa) under the Ministry of Ecology and Natural Resources of Ukraine.

Antimicrobial treatment of cotton-polyester cloths was carried out at the Analytical and Research Testing Laboratory *Textile-TEST*, Kyiv (Kyiv National University of Technology and Design). Samples of tissues were treated by water alcoholic solution (60/40) of ETS, MTS and ATS preparations in padding dyer at room temperature (18–20 °C) and relative humidity of the air 63– 65%. Subsequently, these test specimens were pressed with the use of padding dyer to a residual moisture content of 6–8% and dried at 75, 60 and 50 °C. The minimum concentration of ETS, MTS and ATS in water alcoholic solutions was 0.5%. Before all determinations of textile quality, fabric samples were being dried for 5–7 min.

The concentrations of heavy metals were detected by atomic absorption spectrometry (AAS) with the help of spectrometer *ZEENIT 650P* (*Analytik Jena AG*, Germany) including separation/ preconcentration procedures, solid phase extraction and coprecipitation. The principle of the spectrometer functionality was based on atomization of the test sample, measuring the optical density of the atomic vapor and further determining the mass concentration of the elements to be determined with the use of calibration curves. All chemicals were purchased in Merck (Darmstadt, Germany).

Another way of detection of heavy metals in textiles was Wet Digestion Procedure (WDP) described by Sungur Ş. and Gülmez F. [24] with the help of MP-AES Analysis. The method was provided by *Agilent 4200 MP-AES (Agilent Technologies*, USA).

The pesticide content and the toxic substances are determined with the help of *Agilent 4200 MP-AES* (*Agilent Technologies*, USA). Also a detector was used to capture electrons (a temperature rise of 1.2 °C per min). The content of organic solvents (benzene, toluene, and xylene) was determined based on the equilibrium concentration of the vapor phase.

The odor intensity of fabrics was determined by 6 experts at the laboratory of sensory analysis in the Odesa National Academy of Food Techno-

Table 2. Minimum Concentration of Thiosulfonate Preparations for Fungicidal (A)and Fungistatic (B) Treatment of Cotton-Polyester Fabrics

|  | Minimum concentration, % |                |                   |                |               |               |  |
|--|--------------------------|----------------|-------------------|----------------|---------------|---------------|--|
| Country                                      | ET                       | S              | MTS               |                | A             | ATS           |  |
|  | А                        | В              | А                 | В              | А             | В             |  |
| Trichoderma viride                           | 0.055                    | 0.006          | 0.055             | 0.012          | 0.025         | 0.012         |  |
| Penicillium funiculosum                      | 0.055                    | 0.0185         | 0.0185            | 0.008          | 0.05          | 0.008         |  |
| Paecilomyces variotii<br>Chaetomium globosum | 0.0185<br>0.055          | 0.006<br>0.006 | $0.0625 \\ 0.055$ | 0.003<br>0.006 | 0.625<br>0.12 | 0.003<br>0.03 |  |

logies. The intensity of smell is determined based on the five-point scale (Table 3).

The chemical research takes into account that the main pollutants are bismuth, cadmium, cobalt, manganese, copper, zinc, nickel, mercury, lead, antimony, chromium, among which lead, mercury and cadmium are global the first class of danger pollutants for the environment. They can remain on the surface or in the structure of textile material, which also affects the human body, causing various biological effects (allergens, skin irritants) with different duration of action and the time of detection [25]. The heavy metals can accumulate in bones and various organs, causing their dysfunction. They can also help to eliminate the beneficial elements from the organism such as magnesium, calcium and others. High concentration of heavy metals in the organism can lead to the following diseases: cancer, acute and chronic renal insufficiency, autism, fetal death, cardiovascular and nervous system diseases, metabolic disorders [30].

In addition, raw materials and products of natural origin are treated with fungicides and insecticides against the destructive action of microorganisms, moths, rodents during storage of textile materials and clothing in warehouses and transportation. Moreover, the heavy metals have particular hygienic significance which can also contaminate textile materials and clothing as a result of the use of dyes, the specifics of technological

#### Table 3. Odor Scale

| Score  | Patents in n   |  |  |  |
|--|--|--|--|--|
| 0  | absent odor that is not detected by any expert   |  |  |  |
| 1  | barely noticeable odor that is detected by experts ha-<br>ving the most sensitive organs of senses |  |  |  |
| 2  | faint odor that is detected by experts if they aimed at its definition                             |  |  |  |
| 3  | pronounced odor that is detected by experts if they do not pay attention to it                     |  |  |  |
| 4  | powerful odor that is detected by experts easily   |  |  |  |
| 5  | heavy odor that is detected by experts without smelling  |  |  |  |
| processes, due to contamination of the ecosystem |  |  |  |  |

[27]. The content of heavy metals in fabrics determined with the help of WDP is presented in Table 4.

Copper (26.3–26.4 mg kg<sup>-1</sup>) was detected in the highest concentrations in cotton-polyester fabrics (Samples No. 2). Also higher content of Chromium (1.29–1.30 mg kg<sup>-1</sup>) was determined in all cotton-polyester textiles in comparison to samples of cotton fabrics. The levels of Arsenic and Mercury were found to be considerably less than the values demanded by *Oeko-Tex*. However, all concentrations of heavy metals in extract of 0.07M HCL were determined to be within the normal limits.

The content of heavy metals in the studied fabrics measured with the use of AAS is shown in Table 5.

Table 4. Effect of Biocide Treatment on the Presence of Heavy Metals in Fabrics

|               | Poquiromonts  |                      |        | I      | Metal conte | ent, µg kg <sup>-1</sup> |        |        |        |
|---------------|---|----------------------|--------|--------|-------------|--------------------------|--------|--------|--------|
| Metals        | of Oeko-Tex   |                      | Sample | Nº1    |             |                          | Sample | Nº2    |        |
|               | <i>Standard</i> [28],<br>at most, μg kg <sup>-1</sup> | Without<br>treatment | ETS    | MTS    | ATS         | Without<br>treatment     | ETS    | MTS    | ATS    |
| Co (Cobalt)   | 4.0   | < 0.05               | < 0.05 | < 0.05 | < 0.05      | < 0.05                   | < 0.05 | < 0.05 | < 0.05 |
| Cr (Chromium) | 2.0   | 0.54                 | 0.535  | 0.58   | 0.537       | 1.30                     | 1.296  | 1.30   | 1.29   |
| Cu (Copper)   | 50.0  | 8.84                 | 8.84   | 8.83   | 8.84        | 26.3                     | 26.3   | 26.4   | 26.4   |
| Ni (Nickel)   | 4.0   | 0.38                 | 0.348  | 0.35   | 0.348       | 0.195                    | 0.196  | 0.195  | 0.194  |
| Pb (Lead)     | 1.0   | 0.41                 | 0.406  | 0.045  | 0.406       | 0.384                    | 0.379  | 0.384  | 0.384  |
| Cd (Cadmium)  | 0.1   | 0.045                | 0.045  | 0.045  | 0.045       | 0.070                    | 0.070  | 0.070  | 0.070  |
| As (Arsenic)  | 1.0   | < 0.05               | < 0.05 | < 0.05 | < 0.05      | < 0.05                   | < 0.05 | < 0.05 | < 0.05 |
| Hg (Mercury)  | 0.02  | < 0.01               | < 0.01 | < 0.01 | < 0.01      | < 0.01                   | < 0.01 | < 0.01 | < 0.01 |

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| Matala        | Sample No.1, µg kg <sup>-1</sup> |       |       |       | Sample No.2, µg kg <sup>-1</sup> |       |       |       |
|---------------|----------------------------------|-------|-------|-------|----------------------------------|-------|-------|-------|
| Metals        | Without treatment                | ETS   | MTS   | ATS   | Without treatment                | ETS   | MTS   | ATS   |
| Cr (Chromium) | 1.01                             | 1.00  | 1.00  | 1.00  | 1.37                             | 1.37  | 1.37  | 1.37  |
| Cu (Copper)   | 10.9                             | 10.9  | 10.89 | 10.87 | 40.2                             | 40.2  | 40.2  | 40.3  |
| Ni (Nickel)   | 0.372                            | 0.371 | 0.370 | 0.372 | 0.5                              | 0.034 | 0.036 | 0.036 |
| Pb (Lead )    | 0.454                            | 0.454 | 0.453 | 0.453 | 0.416                            | 0.42  | 0.413 | 0.416 |
| Cd (Cadmium)  | 0.083                            | 0.083 | 0.082 | 0.083 | 0.084                            | 0.086 | 0.081 | 0.082 |
| Hg (Mercury)  | 0.018                            | 0.017 | 0.018 | 0.018 | 0.012                            | 0.012 | 0.012 | 0.012 |

| Table 5 | . Total | Content | of Heavy | Metals in | the S  | Studied | Fabrics |
|---------|---------|---------|----------|-----------|--------|---------|---------|
| 10000 2 | · ioui  | content | ormoury  | meetens m | UIIC N | Juanca  | Labitos |

The total content of Copper  $(40.2-40.3 \,\mu g \, kg^{-1})$ in cotton-polyester fabrics (Sample  $\mathbb{N}_{2}$ ) was the highest among another metals as well as concentration of it found in extract of 0.07M HCL. Also in accordance with literature values of heavy metals in different cotton fabrics the less content of Copper was detected, especially: 0.28–0.84 µg kg<sup>-1</sup>, 0.26-0.78 µg kg<sup>-1</sup> [29], 0.05-0.21 µg kg<sup>-1</sup> [30]. However, in study [31] concentration of Copper was three times higher in comparison with the results of our research (until 340 µg kg<sup>-1</sup>). Lead was detected in the less concentration (0.413–  $0.454 \ \mu g \ kg^{-1}$ ) in all fabrics of the present research in comparison with the results of another research  $(1.23-1.83 \ \mu g \ kg^{-1})$ . In the studied fabrics, all concentrations of other heavy metals (Sample No.1 and No.2) were determined identically, by cont-

Table 6. Influence of Biocide Treatmentson the Content of Organochlorine Pesticides

| Influence<br>of Biocide<br>Treatments             | Requirements<br>of standard [28], | The content of<br>organochlorine pesticides<br>in tissue samples, µg kg <sup>-1</sup> |                |  |
|---|-----------------------------------|---|----------------|--|
| on the Content<br>of Organochlorine<br>Pesticides | μg kg <sup>-1</sup> ,<br>not more | Sample<br>No.1  | Sample<br>No.2 |  |
| DDT   | 1.0                               | < 0.1   | 23.0           |  |
| DDD   | 1.0                               | 0.05  | 5.6            |  |
| DDE   | 1.0                               | 2.8   | < 0.1          |  |
| Heptachlor  | 0.5                               | 7.40  | < 0.1          |  |
| Lindan (γ-HCH)                                    | 1.0                               | 0.28  | < 0.1          |  |
| (α-HCH)   | 1.0                               | < 0.1   | < 0.1          |  |
| (β-НСН)   | 1.0                               | < 0.1   | < 0.1          |  |
| Dieldrin  | 0.2                               | < 0.1   | < 0.1          |  |
| Aldrin  | 0.2                               | <0.1  | < 0.1          |  |

rast to ones without treatment. Arsenic and Cobalt contents were not detected according to method of AAS.

According to data shown in Table 4 and 5 the concentrations of heavy metals in the studied textile materials treated by ETS, MTS, and ATS preparations were virtually the same in comparison with samples of fabrics without treatment and met the requirements of international standard. Obtained results proved that biocide preparations are non-toxic and its use in textile industry does not lead to danger to human health or life.

Organochlorine pesticides in textiles. In order to increase yields, in the traditional method of cultivating raw materials for textiles, not only fertilizers, but also large amounts of insecticides are utilized. Approximately 10% of all pesticides used in the world are in cotton-growing areas. Due to active irrigation, these substances penetrate into groundwater, which leads to the risk of contamination for local sources of drinking water and soils. Approximately 10% of them remain in the can-

| Ten a af teachtra ant | Evaluation of samples, scores                                   |   |  |  |
|-----------------------|---|---|--|--|
| Type of treatment     | Sample No.1   | Sample No.2                                 |  |  |
| Without treatment     | 1 - without odor  | 1 - without odor                            |  |  |
| ETS                   | 2 - faint odor of garlic 2 - faint odor of $2 - faint odor of $ | 2 - faint odor of garlic  2 - faint odor of |  |  |
| MTS                   | cabbage   | cabbage                                     |  |  |
| ATS                   | 2 - faint odor of garlic and onion                              | 2 - faint odor of garlic and onion          |  |  |

vas and can lead to the development of skin diseases and allergic reactions.

Influence of biocide treatments on the content of organochlorine pesticides with mean values is presented in Table 6.

Heptachlor was found in the highest concentration (7.40  $\mu$ g kg<sup>-1</sup>) in cotton fabric samples from comparative to ones from cotton-polyester. It is associated with presence of Heptachlor in soil that contributes to its content in cotton plant during growing [30]. Heptachlor is highly effective in controlling insects thereby it is used for plants but now in the lowest concentrations according to statements of Stockholm Convention on Persistent Organic Pollutants. The content of DDE (2,8  $\mu$ g kg<sup>-1</sup>) also was detected higher than standard norm that is associated with agricultural use.

*Study of textile odors*. After treatment by ETS, MTS and ATS preparations fabrics had special odors. The results of odor studies are presented in Table 7.

All fabric samples differed by the biocide preparation used. The faint odor of garlic is found in textiles treated by ETS preparation, while faint odor of cabbage is reported for textiles treated by MTS

| Table 8. Results of Chemical Analysis of Textile Materials |
|--|
| on the Presence of Toxic Substances                        |

|                      | Requirements   | Measured value, µg kg <sup>-1</sup> |              |  |
|----------------------|--|-------------------------------------|--------------|--|
| substances           | of standard [28],<br>µg kg <sup>-1</sup> , not<br>more | Sample No.1                         | Sample No.2  |  |
| Formaldehyde         | 0.05   | < 0,02                              | < 0,01       |  |
| Hexamethyle-         |  |                                     |              |  |
| nediamine            | 0.01   | not detected                        | not detected |  |
| Caprolactam          | 1.0  | not detected                        | not detected |  |
| Propyl alcohol       | 0.25   | not detected                        | not detected |  |
| Isopropyl<br>alcohol | 0.25   | not detected                        | not detected |  |
| Butyl alcohol        | 0.1  | not detected                        | not detected |  |
| Isobutyl<br>alcohol  | 0.15   | not detected                        | not detected |  |
| Benzene              | 0.5  | not detected                        | not detected |  |
| Toluene              | 0.5  | not detected                        | not detected |  |
| Xylene               | 0.05   | not detected                        | not detected |  |
| Acetone              | 2.2  | not detected                        | not detected |  |
|                      |  |                                     |              |  |

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preparation and faint odor of garlic and onion was a characteristic for textiles treated by ATS.

*Toxic substances in textiles.* An important characteristic of textile materials is their ecological cleanliness, namely the absence of toxic substances, and, accordingly, the threats to consumers' health. The results of the presence of toxic substances in textile materials for the production of overalls are shown in Table 8.

The content of formaldehyde in the studied textile materials was within the normal limits, and other toxic substances were not detected at all. The concentrations of formaldehyde in Chinese cotton textiles are higher by several times (89.6  $\mu$ g kg<sup>-1</sup>, 72.3  $\mu$ g kg<sup>-1</sup>) in comparison with our values, even for different methods of its determination. Such fact means that using of biocide preparations for textiles is safe to human life.

*Study of the hygienic properties of textiles.* Hygroscopicity of textile materials is characterized by their ability to adsorb and desorb hygroscopic and capillary moisture during changing of environmental conditions. It is known that hygroscopicity depends on the fiber composition of the product, the structure of the material and the operating conditions of the product. Influence of biocide treatment of studied materials on change of their hygienic properties is presented in Table 9.

The analysis of the obtained results showed that the biocidal treatment of the studied cellu-

*Table 9.* Effect of Biocide Treatment of Studied Materials on Change in Their Hygienic Properties

| No. | Samples           | Hygro-<br>scopicity,<br>% | Water<br>Resistance,<br>Pa | Water<br>absorption,<br>% |
|-----|-------------------|---------------------------|----------------------------|---------------------------|
| 1   | Without treatment | 8.5                       | 0                          | 33.7                      |
|     | ETS               | 8.5                       | 760                        | 15.6                      |
|     | MTS               | 8.4                       | 750                        | 20.9                      |
|     | ATS               | 8.4                       | 750                        | 20.5                      |
| 2   | Without treatment | 7.0                       | 0                          | 29.7                      |
|     | ETS               | 7.2                       | 600                        | 12.3                      |
|     | MTS               | 7.0                       | 590                        | 13.5                      |
|     | ATS               | 7.0                       | 590                        | 14.2                      |
|     | Aldrin            | 0.2                       | < 0.1                      | < 0.1                     |

losic textile materials leads to increasing of their hygienic parameters associated with keratolytic action and insoluble properties of used preparations. The protective layers are lipophilic, that also prevents the penetration of water. Particularly high effect was achieved in samples of textile materials treating by ETS as made from cotton as well from cotton-polyester.

In general, the results of studies on the provision of antimicrobial properties with new low toxic biocidal substances of the ETS, MTS and ATS suggest that the treatment with these preparations allows obtaining at the same time two desired effects on these tissues (appropriate bio resistance and water resistance) and improving their environmental safety, in general.

Consequently, according to the results of the research, samples of cotton and cotton-polyester textile materials treated with new types of biocidal preparations met the criteria for human health safety. Also the present study has confirmed that

the biocidal substances of the ETS, MTS and ATS are low-toxic and environmentally safe, because during treatment with them, the hygiene indices of tissues have not changed. In addition, thiosulfonate biocides do not increase the content of heavy metals, pesticides and other toxic substances used in the cultivation of cotton plant and the production of textiles and can be recommended for the provision of antimicrobial properties to textiles.

*Further research.* In order to improve the method for applying thiosulfonate biocide compounds to textile materials, it is advisable to develop highly stable nanosize water oligomer systems with thiosulfonates [32, 33] as well as to improve the method for providing textile materials with antimicrobial properties and to ensure their stability and durability. The obtained results may be the source data for the development of scientifically substantiated requirements in the production of clothing for special and technical purposes.

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#### ІННОВАЦІЙНИЙ ПІДХІД ДО СТВОРЕННЯ ТЕКСТИЛЬНИХ МАТЕРІАЛІВ З АНТИМІКРОБНИМИ ВЛАСТИВОСТЯМИ

**Вступ**. У текстильній промисловості постійно ведеться пошук більш досконалих та екологічних засобів для антимікробної обробки целюлозовмісних тканин різного цільового призначення.

**Проблематика**. Проблема захисту текстильних матеріалів та виробів від мікробіологічної деструкції складна та багатогранна і потребує рішення. На сьогодні одним із способів захисту є надання текстильним матеріалам біоцидних властивостей, що не тільки запобігає розвитку бактерій, а й може створити високий рівень безпечності тканин. Зважаючи на заначене, постає задача пошуку нових безпечних біоцидних препаратів.

**Мета.** Визначити рівень безпечності текстильних матеріалів, оброблених біоцидними речовинами тіосульфонатної структури.

Матеріали й методи. Використано тканини різного хімічного складу, що призначені для виготовлення спецодягу. Для просочування було обрано нові препарати тіосульфонатної структури: етилтіосульфанілат (ETC), метилтіосульфанілат (MTC) та алілтіосульфанілат (ATC). Наявність важких металів та пестицидів визначали методом атомноабсорбційної спектрометрії із застосуванням спектрометру ZEENIT 650P (Німеччина).

**Результати.** Встановлено, що виявлений рівень важких металів та пестицидів у досліджуваних текстильних матеріалах незначний та знаходиться у межах нормативних вимог. Підтверджено, що досліджувані біоцидні речовини є малотоксичними й екологічно безпечними, оскільки до та після обробки ними гігієнічні показники тканин не змінилися. Розроблено спосіб надання біоцидних властивостей текстильним матеріалам для виготовлення спецодягу, зокрема шляхом просочування текстильних матеріалів спиртовим розчином біоцидних препаратів. Також завдяки такій обробці водопоглинання матеріалів знижується в середньому на 40 %.

**Висновки.** Обробка текстильних матеріалів біоцидними препаратами тіосульфонатної структури дозволяє отримати одночасно два бажані ефекти для цих тканин: біо- та водостійкість.

Ключові слова: екологічна безпека, важкі метали, біоциди, гігієнічні властивості, тіосульфонати.



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## UPGRADE OF CONVEYOR LINE FOR COAL CHARGE PREPARATION WITH THE USE OF MODERN GRADING-AND-MIXING EQUIPMENT

**Introduction.** In the current market conditions, when the demand for metallurgical products remains constant or declines, the metallurgical industry may develop due to optimizing operating costs. A significant component of the cost of final products is the cost of electricity. Its average growth rate over the past five years amounted to 125%. Therefore, there is a need for analysis of electricity consumption with its subsequent optimization.

**Problem Statement.** In the existing coke production process line, the most energy-intensive technological operation is crushing coal charge, which does not provide for prior screening of the finished grade. The analysis of the particle size distribution of coal concentrates has showed that only 12.5% of the input charge fractions needs to be crushed The gross flow of coal concentrate entering the crushers, the efficiency of the crushers does not exceed 16... 18%. In addition, there is re-crushing of coal concentrates, which increases the content of the 0-0.5 mm fraction and, consequently, adversely affects the quality of resulting coke.

**Purpose.** The purpose of this research is to develop practical recommendations for improving the process of coal charge preparation for coking and equipment in it in order to reduce electricity consumption and to increase the quality of resulting coke.

*Materials and Methods.* Empirical research methods with the use of the mathematical apparatus of statistical data processing.

**Results.** As a result of the research, an improved process flowchart for coal charge preparation has been proposed. It allows improving the quality of blast furnace coke and reducing electricity costs per unit of product, at least, 48 times.

**Conclusions.** Improving the quality of coal charge preparation for sintering and reducing the electricity consumption of equipment may be implemented through upgrading the existing conveyor lines by organizing screening sections of the finished grade before crushing.

Keywords: coke, crushing, screening, mixing, and electricity consumption.

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## Introduction

Currently, world industry is in the era of the socalled "New Normality" when no major events that can provoke a steady increase in consumption of metallurgical products are expected. In these conditions, the development of industry is possible through the introduction of new technologies to optimize operating costs [1].

Given that over the past five years, the average growth rate of electricity prices for non-household consumers in Ukraine reached 123.9% [2], there is a need to analyze electricity consumption for its further optimization, especially at the stages of preparation of the coal charge for coking, which requires energy-intensive technological operations, such as coal charge crushing.

Technological schemes of coke production at corporations of the European Union and India [3— 5] provide preliminary enrichment of coking coal, as a result of which technological operations on coal charge crushing are necessarily preceded by material size grading on vibrating screens and there is no need for mixing operation since a singlecomponent charge is used.

While preparing a coal charge for coking, Ukrainian corporations mainly use the processes of charge crushing (CC) and group crushing of components (GCC). The main difference between the processes used is that the charge crushing requires fewer crushers, because in the GCC case, the performance rate of crushing department is chosen on the condition that it shall be not lower than the coal intake capacity that is much higher than

| Table 1. Specific Parameters | of Crushing | Processes |
|------------------------------|-------------|-----------|
|------------------------------|-------------|-----------|

|   | Crushing process |      |        |      |  |
|---|------------------|------|--------|------|--|
| Parameter   | СС               | 2    | CGG    |      |  |
|   | Design           | Fact | Design | Fact |  |
| Specific productivity, $t/(g \cdot m^2)$                              | 18.4             | 2.3  | 23.2   | 3    |  |
| Electricity consumption,<br>(kW · g)/t<br>Metal consumption of equip- | 1.8              | 14.3 | 1.7    | 13   |  |
| ment, $t/(g \cdot t)$   | 15.6             | 2    | 19.4   | 2.4  |  |



Fig. 1. Variability of averaged particle size composition of coal concentrates

the capacity of the conveyor line that supplies coal to the coke-oven battery where the department for charge crushing process is located. In addition, in the case of GCC process, the installation of mixing equipment is required, while in the case CC process, the mix is stirred during its crushing in hammer crushers. Table 1 shows the main design parameters of the used processes of charge crushing [6].

Given the variability and deterioration of the raw material, the particle size distribution of coal concentrates that are processed for the last seventeen years (Fig.1) has been analyzed. The obtained graphs show that the content of fractions +6and 6-3 mm decreases by 33 and 4%, respectively. So the input charge contains only 12.5% of fractions that need to be crushed (+6; 6-3 mm). Since the process trains do not provide for screening, the gross flow of coal concentrate goes to the crushers that actually play a role of mixers, which is not effective both in terms of quality of the mix (the degree of mixing in terms of quality averages 75%, which does not correspond to the optimal value [7] and in terms of the parameters (see Table 1), as a result of which the crusher efficiency does not exceed 16... 18%. In order to reduce electricity consumption, several processes use of hammer crushers without grate [8, 9], which allows raising the efficiency up to 25... 27%.

In addition, the crushing of the charge with specified particle size distribution leads to its recrushing and increasing the share of 0-0.5 mm

Fig. 2. Dependence of electricity consumption and efficiency of the hammer crusher on the reduction of the content of the 0–3 mm fraction in the coal charge with moisture content W = 11.2 %: 1 - idle power of the crusher; 2 - experimental electricity consumption of the crusher with grate; 3 - experimental electricity consumption of the crusher without grate; 4 - efficiency of a hammer crusher with a grate; 5 - hammer crusher efficiency without grate



Given the above, the purpose of this research is to develop reasonable recommendations for improving conveyor line for the preparation of coal charge for coking and the necessary equipment in order to reduce electricity consumption and to improve the quality of blast furnace coke.

## Main Part of the Research

At the first stage of research, we study the influence of 0-3 mm fraction content on electricity consumption and hammer crusher efficiency and the influence of 0-0.5 mm fraction on the coke quality. The research is carried out in the coal preparation shop at the coke production facilities of



PJSC *ArcelorMittal Kryoyi Rih.* The grade and particle size distribution of coal charge and its mechanical properties are given in Table 2.

The given dependences (Fig. 2) show that the crusher efficiency for the grade and size distribution content of coal charge does not exceed 17%. The reduction in the content of 0-3 mm fraction in the charge that is fed for crushing leads to a decrease in electricity consumption by the hammer crusher and increases its efficiency.

As a result of reducing the content of the 0-3 mm fraction before crushing by 51%, electricity consumption of the hammer crusher with a grate decreases by 37% (from 412 to 260 kW) and by 19% (from 267 to 216 kW) for the crusher without a grate. The efficiency of the crusher increases by 10%, with the use of grate, and by 6% without it.

Thus, the screening of 0-3 mm fraction from the coal charge before crushing significantly reduces the electricity consumption of the hammer

Table 2. Grade and Size Distribution Content of Coal Charge in the Coal Preparation Shop at the Coke Production Facilities of PJSC ArcelorMittal Kryvyi Rih

| Charge, %                             | Particle size composition (%) by grades, mm |     |       | Coal elasticity | Coal         | Average imaginary       |                                       |
|---------------------------------------|---|-----|-------|-----------------|--------------|-------------------------|---------------------------------------|
|                                       | +6  | 6-3 | 3-0.5 | -0.5            | modulus, MPa | breaking<br>stress, MPa | density of coal,<br>kg/m <sup>3</sup> |
| Ж/27; К/35; К+КО+ОС/12;<br>К+КО+КЖ/26 | 106   | 22  | 132   | 47              | 47           | 47                      | 47                                    |

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*Fig. 3.* Nomogram for determining the coke quality indicators of M25 and M10 depending on the content of the 0–0.5 mm dust fraction and the bulk density of coal charge at different moisture content: 1 - strength in terms of crushability (indicator M25); 2 - strength in terms of abrasion (M10); 3 - the content of the 0–0.5 mm grade at an average moisture content in the charge W = 11.2 %; 4 - the content of 0–0.5 mm at an average moisture content in the charge W = 5.6 %

crusher, both with a grate and without it. However, when using standard screens, the screening efficiency of which is 50% for 0-3 mm fraction, it is impossible to increase the efficiency of the crusher by more than 32%, which is quite low for the equipment used.

Based on the results of studying the effect of 0-0.5 mm fraction on the bulk density of the coal charge, as well as experimental coking, a nomogram has been obtained (Fig. 3). The nomogram allows assessing the quality of coke for "cold" strength in terms of crushability (M<sub>25</sub>) and abrasion (M<sub>10</sub>), given the preliminary screening

of 0-3 mm fraction at different humidity of the coal charge.

The obtained nomogram shows that as the content of dust fraction 0-0.5 mm in the coal charge increases, its bulk density and quality of coke decreases. For example, as a result of reducing the content of 0-3 mm fraction in the coal charge with a moisture content of W = 11.2% and W = 5.6% (curves 3, 4), the strength of coke increases in terms of crushability by 1.1% and 1.2% (from 85.4 to 86.5% and from 86.3 to 87.5%), respectively, and in terms of abrasion by 0.8% (from 9.2 to 8.4% and from 8.6 to 7.8%), respectively.



Fig. 4. Power of the reversible hammer crusher and average specific consumption of electricity depending on its productivity

The hot strength also improves: reactivity (CRI) decreases by 2.6% (from 40.1% to 37.5%), and post-reaction strength (CSR) increases by 3.3% (from 43.1% to 46.4%).

The studies show that reducing the content of the defined grade in coal charge before crushing in the hammer crusher may improve the quality of the resulting coke, but the efficiency of this process remains low, indicating the need to use a reversible hammer crusher of other size or other type of crusher.

Having studied the market offer of hammer reversible crushers used for crushing coal of different grades before coking (Fig. 4) [11-13], we conclude that economically justified reduction in electricity consumption may not be achieved unless the productivity in terms of oversized product is, at most, 250 t/g, which, given the productivity of the process line of 700 t/h and the existing particle size distribution of the coal charge, requires the use of screens with an efficiency of, at least, 80%.

Ensuring the above efficiency of screening on existing structures of domestic and foreign screening facilities in a limited production area, as well as preventing the clogging of the sieving surface with initial coal concentrate that has average moisture content of 10... 12%, as a result of its sticking, are complicated tasks.

In connection with the above, a group of engineers of the Kryvyi Rih Metallurgical Institute of the National Metallurgical Academy of Ukraine has proposed a configuration of steep vibration-impact screen (Fig. 5), the main elements of which are box 1 with sieving surface 2 supported by rubber shock absorbers 3. The box vibrations are transmitted by two kinematically unbound inertial vibration generators 4 operating in selfsynchronization mode. Given research [14], the sieving surface is formed by a freely supported plate with round holes, which performs periodic shock-pulse oscillations in the vertical plane limited by support 5. To prevent the longitudinal movement of the sieving surface it is fixed by stoppers 6 [15].

To assess the efficiency of the separation of the defined grade before crushing, in the existing pro-



*Fig. 5.* General view of steeply inclined vibrating-impact screen with freely supported screening surface



Fig. 6. Histogram of changes in the particle size composition



Fig. 7. Power of two-roll-gear crusher drive and average specific electricity consumption depending on its productivity

duction conditions, the changes in the particle size distribution of the coal charge with a moisture content of W = 11.2%, during the motion along the conveyor line, have been analyzed (Fig. 6).

The obtained histogram shows that the screening of 0-3 mm fraction from the coal charge with its subsequent crushing on hammer crushers both with a grate and without it, leads to a decrease in the content of -0.5 mm grade by 8 and by 9% respectively, however, the effect of coal crushing with the formation of this grade, is not removed. In addition, the use of hammer crushers with a capacity of less than 320 t/h, because of a 1.5 times increase in the electricity consumption per a ton of finished product (see Fig. 4) is not effective.

An alternative type of crushers used for crushing coal charge, with a productivity of up to 400 t/h is two-roller-toothed crushers. The study of the market range of sizes (Fig. 7) [16] has showed that this type of equipment is more efficient, because it has a lower electricity consumption (specific electricity consumption does not exceed 0.75 (kWh)/t) and prevents re-crushing of the material.

In some processes, hammer crushers act as mixers for incoming coal concentrates in addition to crushing. However, if screening of more than 75% of the defined grade is ensured, practically there is no mixing, so it is necessary to use equipment for forced mixing.

Table 3 presents the main types of mixers that may be or are used in coal processing facilities [6, 17, 18].

Table shows that the revolving-arm and disc stack mixers are less energy-intensive, but they require significant additional space, which in the


conditions of existing coal preparation facilities not always may be realized. Alternative options are beater-type and rotary mixers. The beatertype mixer, like the revolving-arm or disc stack mixer, requires additional space for mounting and operation, while the rotary mixer is mounted directly above the conveyor and does not require re-design of the existing lines in coal preparation facilities.

Disadvantages of the existing rotary mixer configuration is poor quality of the mix and the

| Table 3. Equipment for | Coal Charge N | Mixing |
|------------------------|---------------|--------|
|------------------------|---------------|--------|

possibility of significant damage to the conveyor belt in the case where metal objects or non-shredding materials fall between the belt and the finger rotor formed by metal pins welded to its shaft.

To remove these disadvantages, an engineer team of the Kryvyi Rih Metallurgical Institute of the National Metallurgical Academy of Ukraine has proposed a rotary mixer configuration (Fig. 8). The mixer is mounted directly above the belt conveyor and consists of welded frame 1 and sections 2. Two rotor are installed on bearing sup-

|  | Type of mixer          |                     |                      |                               |                                  |                 |  |  |
|--|------------------------|---------------------|----------------------|-------------------------------|----------------------------------|-----------------|--|--|
| Parameters   | Revolving-arm<br>mixer | Disc stack<br>mixer | Beater-type<br>mixer | Disintegration-<br>type mixer | Organized charge<br>mixing plant | Rotary<br>mixer |  |  |
| Power, kW  | 6                      | 6                   | 15                   | 75                            | 110                              | 23              |  |  |
| Productivity, t/g                                  | 700                    | 500                 | 400                  | 750                           | 1100                             | 600             |  |  |
| Mixer weight, t                                    | 1.4                    | 0.3                 | 0.4                  | 11.4                          | 4.09                             | 5.65            |  |  |
| Area with electromotor included, m <sup>2</sup>    | 2.4                    | 3.24                | 1.96                 | 12.5                          | 6.6                              | 17.1*           |  |  |
| Specific electricity consumption, $(kW \cdot g)/t$ | 0.009                  | 0.012               | 0.038                | 0.1                           | 0.1                              | 0.038           |  |  |
| Specific quantity of metal, $t/(g \cdot t)$        | 500                    | 1667                | 1250                 | 66                            | 269                              | 106             |  |  |
| Specific productivity, $t/(g \cdot m^2)$           | 175                    | 154                 | 255                  | 60                            | 167                              | 0               |  |  |

Note: \* does not require additional space, mounted above conveyor

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*Fig. 9.* The offered CC process chart for coal charge preparation: 1 - bunker; 2 - belt dispenser; 3 - charge conveyor; 4, 5 - screens; 6 - roller crusher; 7 - rotary mixer; 8 - main conveyor

ports 3 of each section. The rotors with flexible cable elements 4 are moved by electric motors 5 connected via V-belt transmission 6. On the opposite side, blade rotors 8 are moved by means of V-belt transmission 7. For ensuring tight coupling of the sections, laminated rubber elements 9 and 10 are used. At the mixer input and outlet, on the end walls, there are installed sealing rubber curtains 11. Adjusting screws 12 are used to maintain and to adjust the gap between the belt and the rotors. The side walls of the sections are protected with shields 13 and 14 to prevent injuries from rotating actuators. Depending on the needs and process requirements, additional sections may be added or detached [19].

Thus, the research allows us to conclude that the process flowcharts used to prepare the coal charge for coking are energy-consuming, and, moreover, do not enable improving the quality of the resulting coke. In our opinion, it is possible to reduce electricity consumption and to make better the quality of coal charge preparation before sintering by improving the existing conveyor line through preliminary screening of the finished grade 0-3 mm with its subsequent blending with coal concentrate that has been crushed on roller crushers.

For example, proceeding from the primary particle size distribution of the coal charge (Fig. 1) and its flows along the conveyor line at the coal preparation facilities of *ArcelorMittal* Kryvyi Rih, the following generalized improved process chart for CC may be offered (Fig. 9).

In the proposed flowchart, screening is realized by two steeply inclined inertial screens with a freely supported screening surface having a capacity of 350 t/g with a cell of 5 mm, which allows achieving efficiency of 80-90% for 3 mm grade (due to a high absorption capacity for class 0-3 mm). A standard range of such screens has been developed by *KVMSH PLUS* together with the Industrial Machine-Building Engineering Depart-

|  | Equipment of the proposed CC process flowchart                                     |              |  |              |  |
|--|--|--------------|--|--------------|--|
| Parameters                               | Steeply inclined vibrating-impact screen with a freely supported screening surface | Roll crusher | Rotary mixer of improved configuration | process line |  |
| Power, kW                                | $25 \times 2 = 50$   | 150          | 23                                     | 223          |  |
| Actual performance, t/h                  | $350 \times 2 = 700$   | 250          | 700                                    | 700          |  |
| Specific electricity consumption (kWh)/t | $0.08 \times 2 = 0.16$   | 0.6          | 0.038                                  | 0.3          |  |

Table 4. Parameters of the Proposed CC Flowchart

ment of the Kryvyi Rih Metallurgical Institute of the National Metallurgical Academy of Ukraine specifically for materials with a high moisture content, tending towards clogging and sticking to screen surfaces. In addition, the scheme provides for the use of a roll crusher with a capacity of 250 t/h that is sufficient for processing the oversized product after screening. After the crushing stage, a multi-section rotary mixer is mounted above the main conveyor. The capacity of the proposed grading & crushing & mixing equipment, as estimated based on the specifications, is 223 kW (Table 4).

Having compared the obtained capacity of all equipment in the proposed process flowchart for the option with the crushing equipment currently used for the CC scheme (see Table 1), i.e. the two crushers each having a capacity of 630 kW, with their actual productivity of 88 t/h caused by a low content of the fractions to be crushed in charge, it may be concluded that the specific electricity consumption of coal concentrate processing at the crushing and mixing site may be reduced at least 48 times, from 14.3 kWh/t to 0.3 kWh g/t.

The use of additional screening sites in the proposed process flowchart leads not only to reducing electricity consumption, but also to improving the quality of coke due to the prevention of re-crushing of the finished product and, as a consequence, reduction in the content of 0–0.5 mm fraction, which increases coal load density. This causes decreasing CRI (coke reactivity index) and growing CSR (coke strength after reaction) of the resulting coke by 3%, on average. The forced mixing of all charge components, as foreseen in the proposed process flowchart, increases the homogeneity of the chemical composition and the physical and mechanical properties of the resulting coke.

# Conclusions

The research has shown that with the existing raw material base and those coal concentrates that are supplied for processing to the coal preparation facilities of coke plants, the existing conveyor lines are low-efficient and energy-intensive. Improving the quality of coal charge preparation for sintering and reducing electricity consumption of the equipment may be realized through improving the existing conveyor lines by organizing sites for prescreening of the finished grade 0-3 mm before crushing followed by crushing of screened sorted material to 0-3 mm and subsequent mixing of the entire product on the main conveyor.

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### УДОСКОНАЛЕННЯ ТРАКТІВ ПІДГОТОВКИ ВУГІЛЬНОЇ ШИХТИ ДО КОКСУВАННЯ ШЛЯХОМ ВИКОРИСТАННЯ СУЧАСНОГО СОРТУВАЛЬНО-ЗМІШУВАЛЬНОГО ОБЛАДНАННЯ

Вступ. В умовах існуючої кон'юнктури ринку, коли попит на металургійну продукцію залишається сталим або знижується, розвиток металургійної галузі можливий за рахунок оптимізації операційних витрат. Оскільки значною складовою собівартості готової продукції є витрати на електроенергію, середній темп зростання цін на яку за останні п'ять років склав 125 %, виникає необхідність у виконанні аналізу енергоспоживання з подальшою його оптимізацією.

**Проблематика**. В діючій технологічній лінії виробництва коксу найбільш енергоємною технологічною операцією є подрібнення вугільної шихти, в якій не передбачено попереднє відсівання готового класу. Аналіз гранулометрично-

го складу вугільних концентратів показав, що вхідна шихта містить лише 12,5 % фракцій, які потребують дроблення. Зважаючи що, валовий потік вугільного концентрату надходить до дробарок, це призводить до того, що коефіцієнт корисної дії використовуваних дробарок не перевищує 16—18 % та відбувається переподрібнення вугільних концентратів, що збільшує вміст фракції 0—0,5 мм, яка негативно впливає на якість коксу.

**Мета.** Розробка науково-обґрунтованих рекомендацій щодо вдосконалення тракту підготовки вугільної шихти до коксування та використовуваного в них необхідного обладнання задля зниження споживання електроенергії та підвищення якості доменного коксу.

**Матеріали й методи.** Використано емпіричні методи досліджень із застосуванням математичного апарату обробки статистичних даних.

**Результати.** Розроблено технологічну схему підготовки вугільної шихти, яка дозволяє підвищити якість доменного коксу та зменшити питомі витрати електроенергії орієнтовно в 48 раз.

**Висновки.** Підвищення якості підготовки вугільної шихти до спікання з одночасним зниженням енерговитрат обладнання, що виконує її переробку, може бути реалізовано удосконаленням існуючих технологічних трактів шляхом організації ділянок попереднього відсіву готового класу перед дробленням.

Ключові слова: кокс, дроблення, грохочення, змішування, енергоємність.



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# INFORMATION TECHNOLOGY FOR TRAJECTORY DATA MINING

**Introduction.** Advanced technologies allow almost continuous tracking and recording the movement of objects in space and time. Detecting interesting patterns in these data, popular routes, habits, and anomalies in object motion and understanding mobility behaviors are actual tasks in different application areas such as marketing, urban planning, transportation, biology, ecology, etc.

**Problem Statement.** In order to obtain useful information from trajectories of moving objects, it is important to develop and to improve mathematical methods of spatiotemporal analysis and to implement them in high-quality modern software.

Purpose. The purpose of this research is the development of information technology for trajectory data mining.

**Materials and Methods.** Information technology contains the three main algorithms: revealing key points and sequences of interest with the use of density-based trajectories clustering of studied objects; detecting patterns of an object movement based on association rules and hierarchical cluster analysis of its motion trajectories in the time interval of observations, similarity measure of the motion trajectories has been proposed to be calculated on the basis of the DTW method with the use of the modified Haversine formula; new algorithm for revealing permanent routes and detecting groups of similar objects has been developed on the basis of clustering ensembles of all studied trajectories in time. The clustering parameters are selected with multi-criteria quality evaluation.

**Results.** The modern software that implements the proposed algorithms and provides a convenient interaction with users and a variety of visualization tools has been created. The developed algorithms and software have been tested in detail on the artificial trajectories of moving objects and applied to analysis of real open databases.

**Conclusions.** The experiments have confirmed the efficiency of the proposed information technology that may have a practicable application to trajectory data mining in various fields.

Keywords: information technology, pattern mining, trajectory of motion, points and sequences of interest, cluster analysis, and similarity measure.

In today's world, where everything is in constant motion, mobility is a key concept. Prevalence of GPS-enabled devices and wireless communication technology leads to the accumulation of huge amounts of information about the movement of objects in space and

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time. Having analyzed these data, we may better understand the features of the motion and behavior of objects, as well as other interesting patterns.

One example of practical application is the analytics or marketing industry, where it is important to correctly analyze the audience and categorize it fairly precisely by interest category in order to be able to more accurately engage a new target audience or draw conclusions based on the interests of an existing audience. Consider, for example, the trajectory of human movement. We can determine which areas may be important for him: work, gyms, shopping malls, etc. On the basis of several trajectories, it is even possible to track some habits and patterns of human behavior: go to the cafe every morning, an evening jog around the park every Friday, and so on.

Most mobile apps installed on mobile devices occasionally request access to a user's location. The location and movement of the users is used in operating systems and mobile applications to provide various quality promotional recommendations for nearby places of interest or, for instance, timely notification of traffic jams.

Analyzing the trajectories obtained by tracking the movement of animals, it is interesting to determine which geographic areas are important for an animal, in which it spends a certain part of its time or movement patterns such as spatio-temporal expression of behaviours, e.g. in flocking sheep or birds assembling for the seasonal migration, migration patterns of traveling for better access to food, water, and shelter.

In transportation field — tracking vehicle movement, traffic planning, detecting hotspots, for taxi pick-up point recommendation; in ecology tracking down pollution incidents etc.

There are also some successful examples in various AR applications: such as Ingress or PokemonGO, where user location analysis is the main mechanism for managing the gameplay.

Raw trajectory data in the form of geographical coordinates and timestamps are meaningless to humans. All these data are of great value only if it is properly processed. Therefore, the task of trajectory data mining is of interest among researchers and very popular in practical applications.

Trajectory data mining is the process of interesting, useful knowledge and patterns discovery in large data sets of objects` motion history. The mathematical apparatus of spatial-temporal analysis methods is used to study the trajectories of motion [1-3]. In [4] the authors divided the methods into two categories: primary (clustering, classification) and secondary (pattern mining, outlier detection, prediction) and showed relationships between them.

A systematic review of different methods and examples of practical application of trajectory analysis was performed in [4-6]. In [6] links to different datasets can also be found.

An important task is finding points of interest or points of stops [7-8]. Generalizing the various methods, the fact can be noticed, that in most cases density algorithms (DBSCAN and its modifications) are used for solving this problem. In cases where there is no access to the entire amount of data, for example, in real-time analysis, the algorithms based on analysis of the spatial and temporal differences between individual segments of trajectories are used in order to highlight the centroids as points of interest. Due to their low computational complexity, they are widely used in mobile devices. Sometimes a probabilistic approach is used based on models such as a mixture of Gaussian distributions, Bayesian and Markov models.

In many pattern mining tasks, it is necessary to determine the similarity of trajectories. Most approaches to determining it are distance measures that can be divided into two categories: spatial ones that focus only on spatial changes and ignore the temporal attribute, and spatio-temporal ones that use data of both spatial and temporal changes. Spatio-temporal distance measures, for the most part, have the same camputation principles as when dealing with time series. Widely used approaches to distance measure are, for example, DTW, LCSS, TWED and so on. Among the spatial measures of distance, three types are most com-



Fig. 1. Determination of points clusters on the trajectory

mon: proximity to the direction of motion, proximity of geometric shapes and spatial proximity.

Visualization and visual analytics is an important and effective tool for the study of trajectories that has been addressed, for example, in [9-10].

Although there are a lot of theoretical works in this area, there are few software solutions and most of them are for highly specialized tasks.

The object of study is trajectories of objects' motion in space and time.

The subject of study is methods of revealing useful information and pattern mining in trajectory databases.

The purpose of the work is to study existing approaches for solving the problem, to develop the information technology for trajectory data mining and to apply the created software to the analysis of real datasets from different subject areas.

# **Materials and Methods**

Let a set of objects of observation be given as  $O = \{O_k; k = \overline{1, N_{obj}}\}$ , each object is characterized by a set of trajectories  $O_k = \{T_i^k; i = \overline{1, N^k}\}, T_i^k = \{p_{ij}^k; j = \overline{1, N^k}\} - i$ -th trajectory of the *k*-th object of observation,  $p_{ij}^k = \langle t_{ij}^k, x_{ij}^k, y_{ij}^k \rangle$ , where  $x_{ij}^k, y_{ij}^k -$ latitude and longitude of the *j*-th point in the *i*-th trajectory of the *k*-th object of observation,  $t_{ij}^k -$ the moment of time corresponding to the *j*-th point in the *i*-th trajectory of the *k*-th object.

To analyze this data, it is necessary to develop algorithms and software for:

- searching for key points and sequences of interest;
- detecting objects movement patterns in the period of observation;
- revealing permanent routes, identifying groups of similar objects based on an analysis of all studied trajectories over time.



*Fig. 2.* Transition from the initial trajectory to sequence of key points (interests)

The first step in analyzing trajectories is to identify key points or so-called points of interest. It can be interesting to researchers as an independent task (identifying visited by an object places that are, places of particular interest to him) and may be used as an ancillary task to reduce data dimensions and to eliminate noise.

To determine the points of interest, we first apply the DBSCAN dense clustering algorithm, which will allow us to find clusters of points on the trajectory (Fig. 1):

1. Set the parameters of the algorithm  $\varepsilon$  (allowable neighborhood of a point during cluster formation) and *minP* (the minimum number of points for cluster formation). All points of the studied trajectory are considered as a set of nonclustered points *S*.

2. Of the set *S* choose an arbitrary point *r* and calculate distances  $d_n$ ,  $i \in S$ . As geo-position coordinates are analyzed, we propose using a modified Haversine formula as a measure of distance:

 $d_{ij} = \arctan \left\{ \frac{...\sqrt{[\cos x_j \sin \Delta y]^2 + }}{+ [\cos x_i \sin x_j - \sin x_i \cos x_j \cos \Delta y]^2} \frac{...\sqrt{[\cos x_j \sin x_j - \sin x_i \cos x_j \cos \Delta y]^2}}{\sin x_i \sin x_i + \cos x_i \cos x_j \cos \Delta y} \right\}$ 

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3. Identify *countP* — the number of points contained in  $\varepsilon$ -neighborhood of point *r*, that is, such that  $d_n \leq \varepsilon$ ,

- if *countP* < *minP*, then denote the point *r* by noise and proceed to item 2,
- otherwise, from the point *r* and its ε-neighborhood form a cluster and proceed to item 4.

4. For each point belonging to the cluster find points belonging to its  $\varepsilon$ -neighborhood and add them to the cluster.

5. All points of the formed cluster exclude from the set *S*.

6. If there are non-noise objects in the set *S*, proceed to item 2, otherwise finish the clustering.

For each cluster  $c_l$ ,  $l = \overline{1, N_c}$  find a point of interest  $p_l^* = \langle t_l^*, x_l^*, y_l^* \rangle$  as the averaging of the values of all points belonging to it:

$$t_l^* = \frac{1}{|c_l|} \sum_{p \in c_l} t, \quad x_l^* = \frac{1}{|c_l|} \sum_{p \in c_l} x, \quad y_l^* = \frac{1}{|c_l|} \sum_{p \in c_l} y.$$

Based on the implemented algorithm for accessing Google Places for more information about each point received, we move from the point of interest to the semantic location.

Having identified all the points of interest of the trajectory, we obtain a sequence of key points (points of interests)  $P^* = \{p_l^*, l = \overline{1, N_{cl}}\}, p_l^* = \langle t_l^*, x_l^*, y_l^* \rangle$  (Fig. 2).

The following algorithm is proposed to detect patterns of object movement within the observation time interval.

1. Based on all the trajectories of the object being moved, identify the sequence of key points (interests) as described above.

2. Determine a hierarchical cluster structure of sequences of interest. By finding groups of similar trajectories, it is possible to draw conclusions about the permanent routes, preferences and habits of the studied object.

3. Using the apriori algorithm, we find associative rules that allow detecting the regularities between related events in the form of "if the object visited point A, then with probability p, it will also visit point B". As related events we consider the points of interest in one trajectory. This app-

| Points of interests        | – – ×   |
|----------------------------|---|
| Drag'n'drop area           | View points on map                                      |
| Select workspace           | -   |
| Radius 100<br>Min points 3 | Show clusters on map<br>Show points of interests on map |
| Time threshold (m) 60      |   |
| Time range:(h) 0 0         | Rules mining  |
| With places                |   |

Fig. 3. The main form

| Load user   | Separator ,  Load custom file   | Support (%):<br>0<br>Confidence(%):<br>0   | 1 1 1<br>25 50 75<br>1 1 1<br>25 50 75                    | 0,04<br>100<br>,0,04<br>100                      |
|---|---|--|---|--|
| ems   | Frequent items  | From   | То  | Suppor   |
| spa   | [spa] : 0,25  | [post_officetravel_a   | [supermarket]   | 0.25   |
| post_officetravel_ac  | [post_officetravel_agency] : 0,0-   | [travel_agency, zoo]   | [post_office]   | 0.16666666666                                    |
| travel_agency   | [travel_agency] : 0,46  | [police, roofing_co  | [post_office]   | 0.16666666666                                    |
|   | S101  |  |   |  |
| university  | [university] : 0,04   | [spatravel_agency,   | [post_office]   | 0.16666666666                                    |
| university<br>post_office   | [university] : 0,04<br>[post_office] : 0,25   | [spatravel_agency,<br>[travel_agency, store]   | [post_office]   | 0.1666666666                                     |
| university<br>post_office<br>store                                      | [university] : 0,04<br>[post_office] : 0,25<br>[store] : 0,04   | [spatravel_agency,<br>[travel_agency, store]<br>[supermarket_trave   | [post_office]<br>[spa]<br>[post_office]                   | 0.16666666666<br>0.166666666666666666666666      |
| university<br>post_office<br>store<br>dentist                           | [university] : 0,04<br>[post_office] : 0,25<br>[store] : 0,04<br>[dentist] : 0,13   | [spatravel_agency,<br>[travel_agency, store]<br>[supermarket, trave<br>[school_dentist]                    | [post_office]<br>[spa]<br>[post_office]                   | 0.16666666666<br>0.166666666666<br>0.16666666666 |
| university<br>post_office<br>store<br>dentist<br>airport                | [university] : 0,04<br>[post_office] : 0,25<br>[store] : 0,04<br>[dentist] : 0,13<br>[airport] : 0,13                         | [spatravel_agency,<br>[travel_agency, store]<br>[supermarket, trave<br>[school, dentist]                   | [post_office]<br>[spa]<br>[post_office]<br>[spa]          | 0.16666666666<br>0.166666666666<br>0.16666666666 |
| university<br>post_office<br>store<br>dentist<br>airport<br>supermarket | [university] : 0,04<br>[post_office] : 0,25<br>[store] : 0,04<br>[dentist] : 0,13<br>[airport] : 0,13<br>[supermarket] : 0,17 | [spatravel_agency,<br>[travel_agency, store]<br>[supermarket, trave<br>[school, dentist]<br>[bank, police] | [post_office]<br>[spa]<br>[post_office]<br>[spa]<br>[spa] | 0.16666666666<br>0.166666666666<br>0.16666666666 |

Fig. 4. Form of searching for associative rules

roach is described in detail in the previous work of the authors [11].

The algorithm for agglomerative hierarchical clustering of trajectories:

1. Consider each trajectory of interest  $P_i^*$ ,  $i = \overline{1, N^k}$  to be a separate cluster  $g_{ij}$   $|g_i| = 1$ . Calculate the distance matrix  $D = \{d_{ij}\}, i, j = \overline{1, N^k}$ , where  $d_{ij}$  – distance between trajectories  $P_i^*$  and  $P_j^*$ , which in this work is calculated by an algorithm DTW, but it is suggested to use the above modified Haversine formula instead of the basic Euclidean metric.

2. In the distance matrix *D* find the minimum element  $d_{ij}$  and clusters  $g_i$  and  $g_j$  unite  $g_{i+j} = g_i \cup g_j$ ,  $|g_{i+j}| = |g_i| + |g_j|$ .

3. From the matrix D remove the distances from  $g_i$  and  $g_j$  to other clusters and add distances corresponding to the new cluster  $g_{i+i}$ .



Fig. 5. Visualization of trajectories



Fig. 6. Visualization of the selected trajectory

To calculate the distance between clusters, there is a general Lance-Williams formula:  $d(g_{i+j}, g_h) = \alpha_1 d(g_i, g_h) + \alpha_1 d(g_j, g_h) + \beta d(g_j, g_j) + \gamma d(g_i, g_h) - d(g_i, g_h)$ . By setting different parameter values  $\alpha_1, \beta_2, \beta, \gamma$ , we will get different types of agglomerative hierarchical methods: single-link, complete-link, average-link and more.

4. Repeat steps 2—3 until we have the required number of clusters or all the objects are combined into one cluster to construct the dendrogram. The optimal number of clusters and other settings has been determined with the use of the multicriteria

quality assessment technology proposed by the authors in [12].

The next step in proposed in this work technology is to identify groups of similar objects based on an analysis of all the trajectories studied over time, as well as finding permanent routes.

Since this problem is more complex than the previous one and the simple application of cluster analysis methods is not possible, an ensemble clustering approach is proposed to solve it [13].

1. Form *M* subsets of data  $U_m = \{P_{mi}^*, i = \overline{1, N_{obj}}\}, p = \overline{1, M}$ , representing the trajectories of interest of all the objects under study in a given day m (M -the number of days in the period under review).

2. Applying clustering separately to each of the subsets  $U_m$ , obtain M partitions  $G_m = \{g_1^m, g_2^m, ..., g_{K_m}^m\}$ ,  $m = \overline{1, M, g_i^m} = \{P_j^{*m}, j = 1, |g_i^m|\}$  — the *i*-th cluster in the *m*-th partition,  $i = 1, K_m, \sum_{i=1}^{K_m} |g_i^m| = N_{obj}, \bigcup_{i=1}^{K_m} g_i^m = U_m, g_i^m \cap g_j^m = \emptyset, i, j = 1, K_m.$ 

3. Based on the obtained results, construct adjacency matrices  $A_m = \{a_{ij}^m, i, j = \overline{1, N_{obj}}\}, m = \overline{1, M},$  where

$$a_{ij}^{m} = \left\{ \frac{1, if(P_i^{*m} \in g_k^{m}) \land (P_j^{*m} \in g_k^{m}), k \in [1, K_m]}{0, otherwise} \right\}$$

that is  $a_{ij}^{m} = 1$ , if the trajectories of objects *i* and *j* belong to the same cluster,  $a_{ij}^{m} = 0$  otherwise.

Since the number of clusters  $K_m$  in each of m may be different, the degree of similarity of the objects in this case will not be the same. It is clear that the more clusters in a partition, the more similar are the objects that fall into one cluster. So to account for this difference, multiply each of the matrices  $A_m$  by the number of clusters in m-th partition. So get that

$$a_{ij}^{m} = \left\{ \frac{K_{m}, if(P_{i}^{*m} \in g_{k}^{m}) \land (P_{j}^{*m} \in g_{k}^{m}), k \in [1, K_{m}]}{0, otherwise}, \right.$$

4. Construct an aggregate matrix  $A' = \{a'_{ij}\}, i$ ,  $j = \overline{1, N_{obj}}$ , as follows  $a'_{ij} = \sum_{m=1}^{M} / K'$ , where  $K' = \sum_{m=1}^{M} K_m$ .

The greater the value  $a'_{ij}$ , the more similar the objects *i* and *j* are in their trajectories of interest.

| Points of interests |                    |                                     |   | - 🗆 X                              |
|---------------------|--------------------|-------------------------------------|---|------------------------------------|
| Lat                 | Lng                | Name                                |   |                                    |
| 40.77142527889834   | -73.98214481166782 | The Empire Hotel                    | [night_club, bar, lodging, point_of_interest, esta  | Ми Спутник КУХНЯ                   |
| 40.76537686136595   | -73.98162935928579 | Bruce Berman, PhD, Psychologist     | [health, point_of_interest, establishment]          | S Gershwin Theatre                 |
| 40.75046644607937   | -73.99093909588967 | Sbarro                              | [restaurant, food, store, point_of_interest, establ | 2                                  |
| 40.755007060708856  | -73.97379468258146 | Roger Smith Hotel                   | [bar, lodging, point_of_interest, establishment]    | • запад 12 ва на скве              |
| 40.72673137475076   | -74.00560005386565 | Blood Manor                         | [point_of_interest, establishment]                  | CTDIA, O 00 Times Square           |
| 40.75984021654463   | -73.97233008088493 | Analytic Asset Management           | [finance, point_of_interest, establishment]         | PL /Station Theate                 |
| 40.75549414212696   | -73.97593094867516 | JPMorgan Chase & Co.                | [finance, point_of_interest, establishment]         | P S MIDTOWN                        |
| 40.759302658839154  | -73.97751730213238 | Bill's Bar & Burger                 | [bar, restaurant, food, point_of_interest, establis | The New Yorker                     |
| 40.7560737454129    | -73.97521692875966 | UCC                                 | [point_of_interest, establishment]                  | о <sup>8</sup> А • hdham           |
| 40.74301095662293   | -73.98909382192505 | The 40/40 Club                      | [night_club, bar, restaurant, food, point_of_inter  | Keens Steakhouse                   |
| 40.75719878219422   | -73.97477875075393 | Atlantic Benefits Co Inc            | [insurance_agency, point_of_interest, establishm    | Пенсильвания<br>Hotel Pennsylvania |
| 40.7591056541947    | -73.97323292512169 | Court Square Capital Partners       | [finance, point_of_interest, establishment]         | B Bocrok                           |
| 40.75614812687344   | -73.97189205685622 | Best Western Plus Hospitality House | [lodging, point_of_interest, establishment]         |                                    |
| 40.77148229918757   | -73.96037187820087 | Richard Curtis Associates Inc       | [insurance_agency, point_of_interest, establishm    |                                    |
| 40.74854994194768   | -73.9924673790515  | fresh&co                            | [restaurant, food, point_of_interest, establishme   |                                    |
| 40.748969764925135  | -73.98798383774634 | GameStop                            | [electronics_store, store, point_of_interest, estab |                                    |
| 40.76352746583403   | -73.9777580224236  | Mia Shoes                           | [shoe_store, store, point_of_interest, establishm   | Flatiron Building                  |

Fig. 7. Visualization of points of interest



Fig. 8. Visualization of the received clusters

Value of  $a'_{ij}$  can be considered a measure of closeness, and a matrix A' — a matrix of similarity. Since assigning objects to one cluster on a particular day indicates their closeness across trajectories of interest, and the frequency of their union indicates similarity over time, the measure of similarity thus introduced really reflects the degree of similarity of the two objects along trajectories of interest with regard to time changes.

5. The transition from the similarity matrix  $A' = \{a'_{ij}\}, i, j = \overline{1, N_{obj}}$  to the distance matrix  $D = \{d_{ij}\}, i, j = \overline{1, N_{obj}}$  can be done as follows:  $d_{ij} = 1 - a'_{ij}, i, j = \overline{1, N_{obj}}$ . That is, the more similar objects *i* and *j* in

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the matrix A' the smaller distance between them in the matrix D.

6. Next, we need to get the final solution of the task, namely the division of the objects of the original set  $O = \{O_k, k = \overline{1, N_{obj}}\}$  into clusters. Clustered in one cluster should be those objects that are similar in all trajectories with respect to their temporal changes. Summary partitioning may be gotten by using cluster analysis algorithms that deal with matrix of distances between objects (such as hierarchical, graphical, or fuzzy methods) as input. Hierarchical clustering is used in the work.





Fig. 10. Trajectory visualization

The result of the work is software that implements the above algorithms for analyzing the trajectories of objects and identifying useful patterns in them. The software is written in Java with the use of JavaFX graphical framework.

8 graphical forms have been created for user interaction with the program and easy navigation between them is provided. The main form allows you to download the data and set the parameters of the algorithms (Fig. 3). The form of searching for associative rules is shown in Fig. 4.

The initial data can be viewed on the map by all (Fig. 5) and only the selected (Fig. 6).

Once the points of interest have been identified, they can be viewed on the map, and with the implementation of the algorithm of contacting Google Places service to obtain detailed information about each point (place name, its type, etc) semantic locations cab be obtained. An example is shown in Fig. 7. Each of the obtained clusters can be viewed in detail both on the map and in tabular data (Fig. 8).

The results of hierarchical clustering are also presented as a dendrogram (Fig. 9). In order to abstract from the cartographic representation of information, investigated trajectories can also be viewed on a simple graph (Fig. 10).

Developed algorithms and software were applied to the analysis of real data of the open database of the project «Geolife» (Microsoft Research

Asia) [14], which contains information about the movement of volunteers collected through mobile phones or special trackers; the open database «African Elephant Range (2012)», which contains the locations of elephants according to international organizations reports IUCN, SSC, African Elephant Specialist Group (AfESG) [15], the open database «Taxi & Limousine Commission Trip Record Data», which contains information about boarding and disembarking passengers for the mentioned taxi service in New York [16]. In addition, to test the proposed algorithms in more detail, a web-based JavaScript application was developed, which allows you to create artificial trajectories of moving objects in a convenient mode of interaction with the map.

# Conclusions

The information technology of trajectory data mining has been developed. It allows searching key points and sequences of interest, semantic locations, permanent routes and patterns of behavior as well as identifying patterns of motion of objects in the period of observation. A new approach has been proposed to identify groups of objects by the similarity of their movement routes and the hierarchical structure of all trajectories studied in time based on ensemble clustering. The developed algorithms have been implemented in a modern software complex that may be applied for the intellectual analysis of trajectories in various subject areas.

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## ІНФОРМАЦІЙНА ТЕХНОЛОГІЯ ІНТЕЛЕКТУАЛЬНОГО АНАЛІЗУ ТРАЄКТОРІЙ РУХУ ОБ'ЄКТІВ

**Вступ**. Сучасні технічні досягнення дозволяють майже постійно відслідковувати та фіксувати рух об'єктів у просторі та часі. Виявлення цікавих закономірностей у цих даних, популярних маршрутів, звичок та аномалій у переміщенні об'єктів, розуміння мобільної поведінки є актуальними завданнями у різних сферах застосування, таких як маркетинг, містобудування, транспорт, біологія, екологія тощо.

**Проблематика**. Для отримання корисної інформації з даних траєкторій руху об'єктів важливим є розробка й удосконалення математичних методів просторово-часового аналізу та реалізація їх у вигляді сучасного програмного забезпечення.

Мета. Розробка інформаційної технології інтелектуального аналізу траєкторій руху об'єктів.

Матеріали й методи. Інформаційна технологія містить три основні алгоритми: визначення ключових точок та послідовностей інтересу на основі щільнісної кластеризації траєкторій руху об'єктів дослідження; виявлення закономірностей пересування об'єкта на основі асоціативних правил та ієрархічного кластерного аналізу його траєкторій руху у часовому проміжку спостережень, міру подібності запропоновано обчислювати на основі методу DTW та модифікованої формули гаверсинусів; новий алгоритм пошуку сталих маршрутів та виявлення груп схожих об'єктів за усіма досліджуваними траєкторіями у часі на основі ансамблевої кластеризації. Вибір параметрів кластеризації здійснюється за допомогою багатокритеріальної оцінки якості.

**Результати.** Створено сучасне програмне забезпечення, що реалізовує запропоновані алгоритми, забезпечує зручну взаємодію з користувачем й різноманітні засоби візуалізації. Розроблені алгоритми та програмне забезпечення детально протестовано на штучних траєкторіях рухомих об'єктів та застосовано до аналізу реальних відкритих баз даних.

**Висновки.** Експериментально підтверджено ефективність розробленої інформаційної технології, яку може бути впроваджено на практиці для інтелектуального аналізу траєкторій у різних галузях.

*Ключові слова*: інформаційні технології, виявлення шаблонів, траєкторії руху, точки та послідовності інтересу, кластерний аналіз, міра подібності.



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# CHARACTERISTICS OF NEW PROMISING BENTONITE COAL SORBENTS MODIFIED BY DIFFERENT COMPOUNDS

**Introduction.** Bentonite clays are traditional inexpensive and effective adsorbents that have a high potential for removing heavy metals from wastewater due to their abundance, chemical and mechanical stability, high exchange ability, and unique structural properties.

**Problem Statement.** To obtain activated carbon, high-temperature muffle furnaces are used with the consumption of a large amount of electricity, which is economically unprofitable. In addition, the resulting sorbents must be in the form of granules or tablets, have high strength and the ability to be repeatedly used in technological processes.

**Purpose.** Development of a method for the production of low-cost granular sorbents based on bentonite as a mineral component, activated carbon, as well as natural production waste (sunflower husk, straw, sawdust, etc. as modifiers), which can be removed from the activation process to increase porosity of these materials.

Materials and Methods. Angren brown coal; bentonite of the Navbakhor deposit was used as a sorbent and a basic substance for the granules formation; modifiers were sodium chloride, potassium, chopped straw, sawdust. Methods of thermal decarbonization and activation of the obtained granules under the optimal conditions (950 °C, 45 min) were applied; the bulk density, the specific surface area, pore types and their total volume was determined by optical microscopy and nitrogen adsorption methods.

**Results.** Inexpensive hybrid bentonite-carbon sorbents in the form of high-strength granules were synthesized. The optimal ratio of the main components is Bentonite:Coal = 1 : 2, size (2.5 mm) and strength of granules (83–99%), total pore volume  $0.863-1.01 \text{ cm}^3/\text{g}$ , confirmed the presence of macro-, meso- and micropores. The most promising sample has a specific surface area (Langmuir) 184  $m^2/\text{g}$ .

**Conclusions.** The method for obtaining new effective granular carbon sorbents of low cost, having high sorption capacity relative to organic and inorganic pollutants for purification of industrial process waters has been proposed.

Keywords: coal, bentonite clays, activation, carbonization, microscopic structure, and bentonite-coal sorbents.

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Activated carbon, zeolites, clays, graphene oxides, carbon nanotubes, mesoporous silica, waste biomass and tar have been acknowledged as very effective adsorbents [1]. Bentonite clavs (montmorillonite), kaolinite, biotite, vermiculite, attapulgite (palvgorskite), glauconite are traditional inexpensive and effective adsorbents that have a high potential for removing heavy metals from wastewater due to their abundance, chemical and mechanical stability, high exchange ability and unique structural properties. The prospect of their use is associated, firstly, with the availability and low cost of raw materials, and secondly, with sufficiently high service characteristics: water purification, prevent mechanical stress, can take any form without the use of mechanisms, retain not only toxins, but also moisture, liquefy at rest, become denser in use [2-4].

As an alternative to known adsorbents, granular clay-carbon composites are considered as highly effective materials for removing pollutants [5–8]. Due to their branched porous structure and additional complex adsorption mechanisms, the water treatment process takes place much faster with fairly easy regeneration of the spent adsorbent [9]. Clay-carbon composites consist mainly of bentonite or kaolin clays and activated carbon [10, 11]. The use of activated carbon significantly reduces the cost of such composites, which will allow them to be used effectively in proceedings instead of expensive synthetic sorbents [12].

In this light, the relevant objective is to increase the sorption properties of such clay-carbon composites by applying various modifications, using affordable, inexpensive reagents and simple technological operations [13–16]. In this case, a directed change in the structure of the resulting sorbent occurs, which leads to an increase in the specific surface of the material, its porosity, the number of exchange centers, etc., and as a result, to an increase in its sorption properties. Inorganic and organic natural materials or production wastes can be used as modifying agents — alfalfa seeds, clover, rice husk, sawdust, etc. [13], as well as ther-

mal and electromagnetic processing. Modifying agents during thermal decarbonization and activation should have the ability to be removed from the process and thus increase the sorbent porosity and improve its sorption properties.

Another limiting factor in the widespread usage of natural sorbents for the drinking water treatment and industrial effluents is the lack of effective granulation technologies, since clay minerals are exposed to peptization in aqueous media [16–19].

Thus, the purpose of this research is the development of a production method for inexpensive granular sorbents based on bentonite as a mineral component, activated carbon and natural raw materials as a modifier (potassium salts, sodium, fine straw and sawdust), which at high temperatures and in the absence of oxygen can completely burn out and to be removed with exhaust gases from the muffle furnace. Thereat, numerous pores of various sizes appear at the burnout site of these agents, which significantly increases the sorption ability of the obtained granular bentonitecoal sorbents. The performed research work showed that for repeated use, sorbents together with high strength should be in the form of granules or tablets for subsequent extraction from the process, regeneration and further usage.

# 1. Results and Discussion

The method of obtaining hybrid bentonite-coal sorbents is presented in detail in a previous work [20]. The optimal option for the manufacture of bentonite-coal sorbents was selected in the ratio — bentonite: coal = 1: 2. Bentonite was used not only as a sorbent, but also as a binder to shape the granules. The optimal thermal activation of the granules was annealing at a temperature of 950 °C for 45 minutes. Initial parameters for decarbonization and activation were used based on patent sources for coal activation [20–21].

Table 1 shows the results of a decrease in the mass of initial materials and samples of sorbents upon the decarbonization and activation processes. A wide range of samples is presented, including using soot from the methane pyrolysis process provided by JSC *Navoiyazot. Sich* kind of soot is considered a production waste.

The highest degree of mass loss of the organic component during decarbonization and activation can be noted in the initial version with coal, which amounted to 36.9%, with soot -41.2%. For selected variant B: C = 1:2 the degree of decarbonization was 21.5%. BC-12/o-10 variant is modified with sawdust in the amount of 10 g per 100 g of bentonite, 200 g of coal and 500 ml of water. Burning of sawdust during decarbonization led to an increase in the degree of decarbonization to 34.6%. With the possible advantages of this variant in terms of sorption and ion-exchange capacities, as well as strength, this sample will not give an economic effect due to the large consumption of initial material. Variants with soot have showed a lower decarbonization degree from 6.2 to 8.3%. During studying the sorption capacity, the granules isolated soot that stained water in black and therefore variants with soot were excluded from experiments.

Coal, as a flowing substance, is characterized by bulk density, which is a quantitative expression of the ratio of the coal mass to the volume filled freely or uncompressed. Bulk density depends

## *Table 1.* Decrease in the Mass of Sorbents during Decarbonization and Activation in a Muffle Furnace (950 °C, time – 45 min)

| Mass ratio | The initial<br>mass, g | After<br>activation, g | The degree<br>of decrease<br>in the mass,% |
|------------|------------------------|------------------------|--|
|            | Benton                 | ite : Coal             |  |
| Bentonite  | 5                      | 4                      | 20.0                                       |
| Coal       | 10                     | 6.31                   | 36.9                                       |
| 1:1        | 165.37                 | 127.53                 | 22.8                                       |
| 1:2        | 136.71                 | 107.33                 | 21.5                                       |
| BC-12/o-10 | 110.52                 | 72.52                  | 34.6                                       |
|            | Benton                 | ite : Soot             |  |
| Bentonite  | 5                      | 4                      | 20.0                                       |
| Soot       | 8                      | 4.7                    | 41.2                                       |
| 1:1        | 630.01                 | 468.48                 | 25.6                                       |
| 1:2        | 577.05                 | 528.91                 | 8.3  |
| 2:1        | 563.25                 | 528.41                 | 6.2  |

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*Fig. 1.* The image of the granules of bentonite-coal adsorbents BC-12/SN-5: a – increase in ×250 times, b – actual size

on ash content, moisture content, particle size distribution, particle shape and placement. The determination of bulk density was carried out in accordance with the GOST P 54246—2010 methodology [23]. Bulk density X, g/cm<sup>3</sup>, is calculated by the formula:

$$X = \frac{(M_1 - M_2)}{V},$$
 (1)

where  $M_1$  is weight of cylinder with adsorbent, g;  $M_2$  is empty cylinder weight, g; *V* is adsorbent volume, cm<sup>3</sup> (10 cm<sup>3</sup>). According to formula (1), the bulk density of the obtained samples of bentonite-carbon sorbents was determined, which varied in the range from 0.38 to 0.54 g/cm<sup>3</sup> (Table 2).

When studying the size of the granules in variant 1, the diameter of the granules was 4.5 mm, and in variant 2, granules with a diameter of up to 2.5 mm were obtained. With a decrease in the granules size, the total pore volume increases. This leads to an increase in the specific surface area. If



*Fig. 2.* The total pore volume  $(cm^3/g)$  of bentonite-coal sorbents in comparison with the industrial sorbents activated carbon Norit (Holland) and activated carbon (Russia)

in variant 1 with a granule diameter of 4.5 mm, the total pore volume is  $0.478 \text{ cm}^3/\text{g}$ , then a decrease in granule size to 2.5 mm led to an increase in pore volume to  $0.767 \text{ cm}^3/\text{g}$ . Thus, all subsequent studies were carried out to obtain samples having a granule diameter of 2.5 mm (Table 2).

The image of the obtained granules of bentonite-coal adsorbents was taken by Digital Portable Microscope Dino-Lite Special lighting-UV AM4113FVT (Taiwan). The image of the obtained granules of bentonite-coal adsorbents is shown in Fig. 1.

The modification of bentonite-coal sorbents was carried out as follows: per 100 g of bentonite, 200 g of coal and 500 ml of water such modifying reagents were added — NaCl 5 g (BC-12/N-5), finely chopped straw 5 g (BC-12/S-5), a mixture of NaCl 5 g and straw 5 g (BC-12/SN-5), KCl 5 g (BC-12/K-5) as well as a mixture KCl 5 g and sawdust 10 g (BC-12/o-10,K-5). The strength of the granules was determined on a vibrating screen

(80 vibrations per second) for 7 minutes. The total pore volume was determined in accordance with GOST 17219–71 [24].

This method allows us to approximately determine the total pore volume of activated carbons with a diameter of fractions from 0.2 to 5 mm. The calculation of the total porosity  $V_{\Sigma}$  (cm<sup>3</sup>/g) was carried out according to the following formula:

$$V_{\Sigma} = \frac{(m_{w.c.} - m_{d.c.})}{m_{d.c.} r_{w}}, \qquad (2)$$

where  $m_{wc}$  is wet coal weight, g;  $m_{dc}$  is dry coal weight, g;  $\rho_w$  is water density,  $g/cm^3$  (taken equal to 1 g/cm<sup>3</sup> at room temperature not exceeding 35 °C).

Table 2 demonstrates the texture characteristics of bentonite-coal sorbents modified by various reagents. We can see that the granules strength of these samples varies within 83–99%. The most promising three samples with a large total pore volume: BC-12/N-5 –  $0.952 \text{ cm}^3/\text{g}$ , BC-12/SN-5 –  $0.863 \text{ cm}^3/\text{g}$  and BC-12/o-10.K-5 –  $1.01 \text{ cm}^3/\text{g}$ .

Table 2. Texture Characteristics of Bentonite-Coal Sorbents Modified by Various Reagents (t = 950 °C)

| Diameter, mm | Sample names B : C | Strength, % | Bulk density, g/cm³ | <i>m</i> <sub><i>d.c</i></sub> , g | <i>m<sub>w.c</sub></i> , g | $V_{\Sigma}$ , cm <sup>3</sup> /g |
|--------------|--------------------|-------------|---------------------|------------------------------------|----------------------------|-----------------------------------|
| 4.5          | 1:2                | 93.5        | 0.42                | 127.53                             | 188.60                     | 0.478                             |
| 2.5          | 1:2                | 98.5        | 0.54                | 44.61                              | 78.83                      | 0.767                             |
| 2.5          | BC-12/N-5          | 83.0        | 0.40                | 102.12                             | 199.44                     | 0.952                             |
| 2.5          | BC-12/S-5          | 98.9        | 0.42                | 168.88                             | 238.57                     | 0.412                             |
| 2.5          | BC-12/SN-5         | 96.5        | 0.38                | 121.87                             | 227.11                     | 0.863                             |
| 2.5          | BC-12/K-5          | 93.0        | 0.46                | 133.97                             | 211.71                     | 0.580                             |
| 2.5          | BC-12/o-10.K-5     | 96.0        | 0.41                | 72.5                               | 110.88                     | 1.01                              |
| 1            |                    | 1           | 1                   | 1                                  | 1                          | 1                                 |



*Fig. 3.* Microphotographs of modified bentonite-carbon sorbents in reflected light: a - BC-12/N-5; b - BC-12/SN-5; c - BC-12/o-10, K-5

In comparison with the reference samples of activated carbons of Dutch and Russian productions, the obtained bentonite-carbon adsorbents (with the exception of sample BC-12/S-5) have a larger total pore volume, which indicates the presence of a developed structure of macro-, mesoand micropores for these adsorbents (Fig. 2) [25]. Therefore, it will allow using them effectively for solving a wide range of tasks in industry, protecting the environment and human life.

Microphotographs of samples of bentonitecoal sorbents modified with NaCl, KCl, straw and sawdust were performed on a Primo Star optical microscope (*Zeiss*, Germany) in transmitted light at ×1000 magnification (Fig. 3).

The macropores indicated by arrows are clearly visible in the figure. The presence of mesopores can be noted by the degree of looseness of the material. Activation at 950 °C for 45 minutes was optimal, in which new, promising samples of sorbents were obtained, characterized by the presence of different types of pores, which are divided into macro-, meso- and micropores. All types of cations and anions are retained in these sorbent pores. Large molecules are able to be retained by macropores, small ones by micropores. [26–28].



*Fig. 4.* Nitrogen adsorption-desorption isotherms by porous adsorbents based on bentonite and coal, taken in the ratio: a - BC-12/SN-5; b - BC-12/o-10, K-5

The pore size and area was determined by the method of low temperature nitrogen adsorption for samples 1. BC-12/N-5, 2. BC-12/SN-5, 3. BC-12/o-10,K-5, with the use of the volumetric method and *Kelvin-1042* (*Costech Microanalytical*) at the boiling point of liquid nitrogen (Fig. 4–5, Table 3). In this case, the sorbents were previously degassed in a helium stream at a temperature of 110–120 °C. The volume of adsorbed gas was determined at the time of quasiequilibrium in the gas stream, which was controlled by a thermal conductivity detector (measurement accuracy  $\pm$  3 %).

Table 3. Structural Characteristics of Bentonite-Coal Absorbents Calculated from Nitrogen Adsorption Isotherms

| Ratio          | $S_{specific}$ , BET m <sup>2</sup> /g | $S_{specific}$ , Langmuir, $m^2/g$ | $V_{micpo}$ , mm <sup>3</sup> /g | Micropore<br>area, m²/g | Non microporous<br>surface area, m²/g | Average diameter,<br><i>D</i> , nm |
|----------------|--|------------------------------------|----------------------------------|-------------------------|---------------------------------------|------------------------------------|
| BC-12/N-5      | 35.142                                 | 45.070                             | 17.93                            | 50.875                  | -5.805                                | _                                  |
| BC-12/SN-5     | 128.85                                 | 184.02                             | 38.01                            | 107.871                 | 20.980                                | 60.21                              |
| ВС-12/о-10.К-5 | 62.90                                  | 86.53                              | 10.90                            | 30.940                  | 31.965                                | 26.77                              |

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*Fig.* **5**. Pore size distributions by porous adsorbents based on bentonite and coal, taken in the ratio: a - BC-12/SN-5; b - BC-12/o-10, K-5

The convenience of this type of equipments is that they operate in automatic mode and allow the study of adsorbents with low specific surface area and have software - both for research and for calculations with the use of various models of adsorption processes [27, 29–33].

The specific surface area  $S_{spesific}$  was determined with the use of the adsorption value when filling the monomolecular layer  $a_m$ . The monolayer capacity was determined by the *BET* method [29– 31]. The specific surface area is calculated by the equation:

$$S = a_m N \omega_0, \tag{3}$$

where *N* is Avogadro number;  $\omega_0$  is area occupied by an adsorbed molecule in a dense monomolecular layer.

The  $a_m$  value was determined from the *BET* equation, a graphical solution of this equation allows us to find am and the constant *C*. The equation can be applied in the field of relative pressure

 $P/P_s = 0.03-0.35$ . Calculations can also be carried out by processing experimental data, for example, by the least squares method, and implemented in the software product of the aforementioned supplier company. The results of just such processing were used in this work.

The shape of the adsorption isotherms is a reflection of the porous structure of an adsorbent. Moreover, different sections of the adsorption isotherm, depending on the pore size and their ratio in the structure of the porous body, have a different effect on its shape. For the studied samples of bentonite-coal adsorbents, the adsorption isotherm in the low-pressure region rises more abruptly. This type of adsorption-desorption nitrogen isotherm indicates that macropores are present in the samples. The type of hysteresis loop (*curve a*) makes it possible to assert that the pores are predominantly cylindrical shape (Fig. 4) [27].

Curves of pore size distribution calculated from nitrogen adsorption-desorption isotherms demonstrate the presence of different types of pores in the samples. According to the pore classification adopted by the International Union of Theoretical and Applied Chemistry (IUPAC) for sample BC-12/ SN-5, three maxima are characteristic that relate to macro- (R = 40-50 nm), meso- (R = 4-40 nm) and micropores (R = 1-4 nm) (Fig. 5, *curve a*). For the sample BC-12/o-10, K-5 is characterized by the presence meso- (R = 5-20 nm) and micropores (R = 2-4 nm) (Fig. 5, *curve b*). The macropores diameter corresponds to the pressure near  $p/p_0 = 1$  [27, 34], usually such pores weakly participate in the adsorption process and, for several reasons, capillary condensation practically does not occur in them, therefore, they play the role of transport pores in the structure of a solid body.

Table 3 shows the structural adsorption characteristics of the selected bentonite-carbon sorbents calculated from nitrogen adsorption isotherms. Tabular material allows us to select the most promising sample BC-12 / SN-5 with a specific surface area  $S_{specific}$ ,  $(BET) = 128.85 \text{ m}^2/\text{g}$  ( $S_{specific}$ ,  $(Langmuir) = 184.02 \text{ m}^2/\text{g}$ ) micropore area equal to 107.87 m<sup>2</sup>/g. These values are within the mi-

nimum range of  $100-1500 \text{ m}^2/\text{g}$  needed for industrial application and removal of small molecules. [35].

# Conclusions

The experimental studies on the production of hybrid granular bentonite-carbon sorbents have shown the promise of this research area. The optimal ratio of components is bentonite: coal = 1: 2. Samples with bentonite and soot polluted the cleaned medium by the release of finely dispersed organic carbon and therefore were excluded from further studies. When studying the granule size, it was found that a decrease in the diameter of the granules to 2.5 mm leads to an increase in pore volume from 0.478 to 0.767 cm<sup>3</sup>/g. Thus, their optimal sizes were determined.

The selection of such starting materials as bentonite and coal that are natural sorbents with a lower sorption capacity has made it possible to obtain a hybrid version of bentonite-carbon sorbent with a higher sorption capacity. The use of available natural materials from production waste as modifying agents (potassium chloride, sodium chloride, chopped straw and sawdust), capable of being removed from the activation process, leads to an increase in the degree of porosity of the obtained samples.

Thus, there is a high potential for using such inexpensive bentonite-coal sorbents with a developed porous structure in the form of highly durable granules after additional studies to purify industrial process waters from heavy metal ions and other pollutants. Further research is ongoing to identify the best among all these potential adsorbents.

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## ХАРАКТЕРИСТИКИ НОВИХ ПЕРСПЕКТИВНИХ БЕНТОНІТО-ВУГІЛЬНИХ СОРБЕНТІВ, МОДИФІКОВАНИХ РІЗНИМИ СПОЛУКАМИ

**Вступ**. Бентонітові глини — це традиційні недорогі та ефективні адсорбенти, що мають високий потенціал для вилучення важких металів зі стічних вод через їх доступність, хімічну та механічну стійкість, високу здатність до обміну та унікальні структурні властивості.

**Проблематика**. Для отримання активованого вугілля використовуються високотемпературні муфельні печі, які споживають значний обсяг електроенергії, що є економічно невигідним. Крім того, отримані сорбенти повинні бути у вигляді гранул або таблеток, мати високу міцність і можливість багаторазово використовуватися в технологічних процесах.

**Мета.** Розробка способу виробництва низьковартісних гранульованих сорбентів на основі бентоніту як мінерального компонента, активованого вугілля, а також природніх відходів виробництва як модифікаторів, що можуть бути вилучені з процесу активації, з метою підвищення пористості матеріалів.

Матеріали та методи. Ангренське буре вугілля; бентоніт Навбахорського родовища використовувався як сорбент і базова речовина для формування гранул; модифікаторами слугували хлориди натрію, калію, подрібнена солома, тирса. Застосовано методи термічної декарбонізації та активації одержаних гранул, встановлено оптимальні умови (950 °C, 45 хв); визначено насипну щільність, методами оптичної мікроскопії та адсорбції азоту встановлено величину питомої поверхні, види пор та їх сумарний об'єм.

**Результат.** Синтезовано гібридні бентоніто-вуглецевих сорбенти у вигляді високоміцних гранул. Встановлено оптимальне співвідношення Бентоніт:Вугілля = 1 : 2, розмір (2,5 мм) та міцність гранул (83—99%), загальний об'єм пор: 0.863—1.01 см<sup>3</sup>/г, підтверджено наявність макро-, мезо- та мікропор. Виділено найбільш перспективний зразок з питомою поверхнею (по Ленгмюру) 184 м<sup>2</sup>/г.

**Висновки.** Запропоновано методику одержання нових ефективних гранульованих вуглецевих сорбентів низької собівартості, що мають високу сорбційну здатність щодо органічних та неорганічних сполук для очищення промислових технологічних вод.

*Ключові слова*: вугілля, бентонітові глини, активація, карбонізація, мікроскопічна структура, бентоніто-вугільні сорбенти.



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# POSSIBILITIES OF CREATION AND IMPLEMENTATION OF OPEN INNOVATIONS AT R&D ORGANIZATIONS OF THE NAS OF UKRAINE

**Introduction.** The ability of R&D organizations of the NAS of Ukraine to quickly create and implement R&D innovations is crucial for accelerated economic development and is an important factor for raising the competitiveness of Ukraine.

**Problem Statement.** R&D innovation may be created and implemented with the use of closed or open innovation approaches. Recently, the negative impact of several factors on the application of the closed innovation approach to the activities of R&D organizations of the NAS of Ukraine has increased.

**Purpose.** The purpose is to develop and to test improved theoretical and methodological framework for technological audit of R&D works, assessment of organizational maturity and readiness of R&D organizations of the NAS of Ukraine to use open innovations.

*Materials and Methods.* A set of approaches to theoretical generalization, economic analysis and synthesis; mathematical statistics; expert and poll surveys have been used.

**Results.** It has been established that a significant share of R&D products of R&D organizations of the NAS of Ukraine has a low readiness for independent and joint commercialization, which means the use of the closed innovation approach. Only a part of R&D organizations of Ukraine has an average level of organizational maturity, while the vast majority have a low and very low level of organizational maturity and readiness to apply open innovations. The application of this concept may contribute to the accelerated innovative development of R&D organizations of Ukraine. The theoretical and methodological framework for technological audit of R&D works and assessment of organizational maturity and readiness of R&D organizations of the NAS of Ukraine has been developed.

**Conclusions.** The proposed method allows R&D organizations of the NAS of Ukraine to accelerate the creation and commercialization of R&D innovations.

Keywords: open innovations, R & D works, and open innovation approach.

The ability of R&D organizations to quickly create innovative R&D works and to market them is crucial for accelerating the economic development of the country, and is the most important modern factor for raising its competitiveness. The creation and implementa-

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tion of R&D innovations may be realized with the use of the closed innovation or the open innovation approach.

For many years, R&D organizations of the NAS of Ukraine have been relying on the conventional closed innovation and creating developments internally, i.e. focusing mainly on the use of internal resources to create R&D works and to commercialize them.

Traditionally, the assessment of innovation and organizational capacity of R&D institutes of the NAS of Ukraine is based on the use of general indicators of R&D activities, i.e. the number of publications and patents filed by researchers, which, although useful, but provide R&D organizations only a general view of innovation. This evaluation does not show the current innovative efficiency of research results, which affects the productivity of industrial corporations and economic growth in Ukraine.

Recently, the unfavorable impact of several factors on the application of closed innovation approach to the activities of R&D organizations of the NAS of Ukraine has increased. This results in:

- uncontrolled release of disruptive R&D results, or their components into the external environment and their use by other companies that gain high profits, while the major costs for the development of innovation are borne by R&D organizations;
- R&D organizations spend significant resources to solve problems for which there are quite effective solutions that may be available at fairly low prices;
- most products that have been patented are not used by R&D organization for 100% and are unprofitable;
- many projects that, in the opinion of R&D organizations, are impracticable, in fact, are quite valuable, but not implemented by R&D organizations, since they do not fit to the existing organizational system.

As a result, the closed innovation approach becomes ever less effective because, on the one hand, R&D organizations have paced down the commercialization of innovation and profit-making, which limits the development of further research and implementation of R&D works, and, on the other hand, third corporations do not invest funds in basic and applied research. Because of increasing negative impact of several external and internal factors, the application of the closed innovation concept fails and puts limitations on ways of implementation of R&D works, which leads to a reduction and loss of innovative growth potential of the NAS of Ukraine.

The application of the open innovation concept may contribute to the accelerated innovative development of R&D organizations of the NAS of Ukraine with increasing their influence in the international scientific environment.

The open innovation is the use of compatible (internal and external) knowledge and resources to create and to implement innovative R&D works that can be used to address existing and future socio-economic needs of society [1, 2].

The use of open innovation by organizations and companies helps identify the factors of the two-way flow of knowledge and decide on the inclusion of external sources at all or some stages of the innovation process [3]. It has been proved that the open innovation approach has a favorable effect on enhancing knowledge and investment in organizations and companies, giving them three main benefits: sharing knowledge, reducing risks, and accelerating development [4]. The allocation of resources and risks between two or more organizations / companies is one way to reduce the costs of developing open innovation [5] and to respond quickly to market needs [6].

However, the open innovation may not be successfully realized, unless there is sufficient organizational readiness of all parties involved in creating and implementing open innovation [7]. Organizations and companies need to find ways to work more closely with external partners, even competitors, without losing competitive advantage and shall have strategies that allow them to integrate their joint efforts [8]. The effectiveness of open innovation increases due to systemic organi-

zation and implementation of indicators of the innovative approach of open innovation [9]. Especially effective is the use of quantitative indicators to evaluate the implementation of open innovation [10]. The groups of evaluation indicators for measuring open innovation include: search and flows of external knowledge and information (breadth and depth of external knowledge and inormation); dependence of innovation process on knowledge inflow and outflow; level of R&D cooperation with external partners (breadth and depth of cooperation), including R&D outsourcing; indicators that measure the internal innovation capacity of the organization, the R&D intensity, efficiency of R&D cooperation, the degree of openness, HR and internal R&D research group factors [11].

The substantiation of the need to monitor the process of open innovation application [12] has allowed establishing factors and indicators of influence on improving the efficiency of the innovation process of organizations and companies, which use the open innovation approach [13]. However, despite the existing understanding of the need and importance of open innovation, in practice, organizations and companies have been applying an open innovation approach through trials and errors [14].

In Ukraine, one of the main sources of the creation and implementation of R&D projects/innovations is the NAS that carries out 2717 applied research and 2454 fundamental research works financed from various funds (general fund and special fund of the state budget); the number of implemented R&D works (innovations) is 1011 units (based on data for 2017) [18].

Prospects and obstacles to the use of the open innovation approach in R&D organizations of the NAS of Ukraine are closely related to the general situation of the legislative and infrastructural framework in Ukraine [15–16].

The purpose of this research is to develop and test improved theoretical and methodological framework for technological audit of R&D works and assessment of organizational maturity and readiness of R&D organizations of the NAS of Ukraine to implement open innovations.

The improved scientific and methodological approach to the technological audit of R&D works includes evaluating the four capacities: innovation, commercialization, transfer, and the ability to openness. This includes a varied number of parameters and characteristics, which are evaluated by a scoring system and describe the profile of R&D work: *the innovation capacity* that characterizes the uniqueness of development, competitive advantage, non-infringement quality, and sales markets; the commercialization capacity that describes the area of commercialization, the modifiability of the product range, the possibility of industrial production, financial costs and conditions of commercialization; the transfer capacity that characterizes the readiness of the product and personnel for the transfer, the conditions of transfer of R&D product, compliance with regulatory documentation; and *the openness capacity* that shows the possibility of applying the open innovative approach at the stages of the commercialization and the application of outide-in knowledge and information flows, the independent inside-out promotion of R&D product. As a result, the technological audit of profiles of R&D works has not only a qualitative assessment, but also a quantitative evaluation of potentials: innovation, transfer, commercialization, and openness.

The developed scientific and methodological approach has been tested for technological audit of 70 promising R&D works carried out by R&D organizations of the NAS of Ukraine in the field of structural and functional materials technology, which have rich experience in materials science [17].

The distribution of these R&D works by *Eurostat* types of innovations has shown that 28 (40%) R&D works are process innovations and 42 (60%) ones are product innovations.

The results of technological audit of R&D works and comparative assessment of four capacities have shown that most R&D works have a high potential: innovation capacity from 46% to 72%, com-



*Fig. 1.* Comparative evaluation of innovation, commercialization, transfer, and openness capacity of R&D works of R&D organizations of the NAS of Ukraine, which carry out promising R&D works in the field of structural and functional materials technology

Source: developed by the authors.

mercialization capacity from 40% to 85%, and transfer capacity from 30% up to 76% (Fig. 1).

The evaluation of the openness capacity by indicators:

- outside-in process (adsorption of external knowledge): 53 developments have a high level (from 75% to 100%) and 14 developments have a medium level (from 45% to 70%);
- inside-out process (integration or transfer of internal knowledge outside): 45 developments are absolutely unprepared; 21 developments have a low readiness (up to 40%);
- combined process (combination of adsorption and integration processes): 43 R&D works have a low level (up to 40%) and 16 R&D works have a medium level (from 45% to 70%).

Only 4 R&D works have a medium level (from 45% to 70%) of readiness for independent insideout promotion of R&D products and 11 ones have a high level (from 75% to 100%) of readiness for joint promotion of R&D products.

It has been established that the majority of the R&D works of R&D organizations of the NAS of Ukraine is not ready enough for independent or joint promotion of R&D works, which is a result of the widespread use of the traditional closed innovation approach in most R&D organizations of the NAS of Ukraine.

Systematic implementation of an open innovative approach to accelerate the creation and implementation of innovative R&D works at R&D organizations of the NAS of Ukraine requires organizational maturity and readiness of R&D organizations of the NAS of Ukraine to apply the open innovation model.

The advanced scientific and methodological approach to assessing the organizational maturity and readiness of R&D organizations to use open



*Fig. 3.* Comparative evaluation of organizational maturity and readiness of the focus group of some R&D organizations of the NAS of Ukraine to apply open innovations *Source*: developed by the authors.

33.4

39/7

Pysarzhevskyi Institute

for Physical Chemistry

Organizational maturity

2.3

Kukhar Institute for Bioorganic

Chemistry and Petrochemistry

Optimal level

of High-Molecular Compounds

**Bakul** Institute

for Superhard Materials

Kharkiv Physics and Technology Institute

Physics

for General and

Institute of Electrodynamics

Vernadsky Institute

Inorganic Chemistry

innovations includes the assessment of 20 indicators of the three processes of the open innovative approach to the creation and implementation of innovations. This scientific and methodological framework has been used to assess organizational maturity and readiness to use open innovations for 24 R&D organizations of the NAS of Ukraine, which carry out promising R&D works in the field of structural and functional materials technology [17].

The results of the assessment of 24 R&D organizations of the NAS of Ukraine have shown that: the average level of indicators that characterize the adsorption capacity for the application of external knowledge and information is 30.16% (the outside-in process); the average level of indicators that describe the ability to independently create and promote the results of R&D activities outside the R&D organization is 25.45% (the inside-out process); and the average level of indicators characterizing the organizational readiness to jointly create and promote innovations is 28.93% (the combined process) (Fig. 2).

The assessment of organizational maturity and readiness to apply open innovations in relation to specific R&D organizations of the NAS of Ukraine has shown that: 7 (29% of the studied) research organizations of the NAS of Ukraine) have a medium level of organizational readiness (from 40% to 50%); 4 (16%) R&D organizations of the NAS of Ukraine have lower than medium level of organizational readiness (30–40%); 6 (25%) R&D

| Evaluation of Organizational Maturity and Readiness of R&D Institutes              |
|--|
| of the NAS of Ukraine, Which Do Research in the Field of Structural and Functional |
| Materials Technology to the Application of the Open Innovation Approach            |

| Institute of the NAS of Ukraine                              | Outside-in<br>process, % | Inside-out<br>process, % | Combined<br>process, % | Average, % |
|--|--------------------------|--------------------------|------------------------|------------|
| Kurdyumov Institute of Physics of Metals                     | 45                       | 18                       | 14                     | 25.7       |
| Nekrasov Institute of Non-Ferrous Metallurgy                 | 28                       | 20                       | 34                     | 27.3       |
| Institute for Engineering Thermophysics                      | 40                       | 16                       | 36                     | 30.7       |
| Frantsevych Institute for Problems of Materials Science      | 38                       | 36                       | 36                     | 36.7       |
| Physics and Technology Institute for Metals and Alloys       | 45                       | 48                       | 42                     | 45         |
| Institute for Chemistry of High-Molecular Compounds          | 31.7                     | 22.2                     | 25.3                   | 26.4       |
| Bakul Institute for Superhard Materials                      | 30                       | 53                       | 44                     | 42.3       |
| Kharkiv Physics and Technology Institute                     | 30.9                     | 36.7                     | 32.6                   | 33.4       |
| Kukhar Institute for Bioorganic Chemistry and Petrochemistry | 42.8                     | 20.4                     | 20.4                   | 27.9       |
| Pysarzhevskyi Institute for Physical Chemistry               | 1.9                      | 0.81                     | 1.63                   | 14.5       |
| Institute of Electrodynamics                                 | 3.33                     | 4.08                     | 4.49                   | 39.7       |
| Vernadsky Institute for General and Inorganic Chemistry      | 19                       | 8.1                      | 16.3                   | 14.5       |
| Institute of Applied Physics                                 | 14.2                     | 4                        | 12.2                   | 10.1       |
| Institute of Physics   | 28.5                     | 24.4                     | 16.3                   | 23.1       |
| Lashkariov Institute of Semiconductors                       | 19                       | 14.2                     | 16.3                   | 16.5       |
| Hryshko National Botanical Garden                            | 19                       | 12.2                     | 16.3                   | 15.8       |
| Institute for Nuclear Research                               | 19                       | 8.1                      | 12.2                   | 13.1       |
| Bohatskyi Physics and Chemistry Institute                    | 14.2                     | 8.1                      | 0                      | 7.4        |
| Institute of Single Crystals                                 | 40.4                     | 44.8                     | 36.6                   | 40.6       |
| Galkin Donetsk Physico-Technical Institute                   | 35.7                     | 14.2                     | 18.3                   | 22.7       |
| Karpenko Physico-Mechanical Institute                        | 45.2                     | 51                       | 40.8                   | 45.7       |
| Institute of Gas   | 42.8                     | 44.8                     | 38.7                   | 42.1       |
| Paton Electric Welding Institute                             | 40.4                     | 59.1                     | 44.8                   | 48.1       |
| R&D Institute for Microdevices                               | 50                       | 42.8                     | 42.8                   | 45.2       |

organizations of the NAS of Ukraine have a low level of organizational readiness (20-30%); and 7 (30%) R&D organizations have a very low level of organizational readiness to use open innovations (10-20%) (Table).

It has been found that a smaller part (46%) R&D organizations of the NAS of Ukraine have a medium and low medium level of organizational readiness for open innovations, while the majority (54%) has a low and very low level of organizational readiness for application of the open innovation approach.

The comparative evaluation of organizational maturity and readiness of the focus group of some

R&D organizations of the NAS of Ukraine to apply open innovations in different areas is shown in Fig. 3.

The research has shown that many R&D organizations of the NAS of Ukraine of those studied prefer the traditional closed innovation approach based on their clear desire to preserve the value of innovation and ideas using only internal resources. One of the ways to increase the ability of R&D organizations of the NAS of Ukraine to speed up the creation of innovative R&D works and to quickly market them is the open innovative approach to the creation and implementation of innovations.

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## МОЖЛИВОСТІ СТВОРЕННЯ ТА ВПРОВАДЖЕННЯ ВІДКРИТИХ ІННОВАЦІЙ НАУКОВИМИ ОРГАНІЗАЦІЯМИ НАН УКРАЇНИ

**Вступ**. Здатність наукових організацій НАН України швидко створювати й впроваджувати інноваційні науково-технічні розробки має вирішальне значення для прискореного економічного розвитку та є важливим фактором підвищення конкурентоспроможності України.

**Проблематика**. Створення та впровадження інноваційних науково-технологічних розробок може здійснюватися шляхом використання концепції закритих чи відкритих інновацій. Останнім часом посилився негативний вплив низки чинників використання концепції закритих інновацій в діяльності наукових організацій НАН України.

**Мета.** Розробка та апробація удосконалених теоретико-методологічних засад технологічного аудиту науковотехнологічних розробок, оцінки організаційної зрілості та готовності наукових організацій НАН України до застосування відкритих інновацій.

**Матеріали й методи.** Використано підходи теоретичного узагальнення; економічного аналізу та синтезу, математичної статистики, експертного та анкетного дослідження.

**Результати.** Встановлено, що значна частка науково-технологічних розробок наукових організацій НАН України має низьку готовність до самостійної та спільної комерціалізації, що характеризує застосування концепції закритих інновацій. Лише частина наукових організацій України має середній рівень організаційної зрілості, а переважна більшість має низький та дуже низький рівень організаційної зрілості та готовності до застосування відкритих інновацій. Натомість застосування зазначеної концепції може сприяти прискореному інноваційному розвитку наукових організацій НАН України. Розроблено теоретико-методологічний підхід технологічного аудиту науково-технологічних розробок та оцінки організаційної зрілості та готовності наукових організацій НАН України до застосування відкритих тих інновацій.

**Висновки.** Запропонований метод дозволить науковим організаціям НАН України пришвидшити виведення їх на ринки інноваційних науково-технічних розробок.

Ключові слова: відкриті інновації, науково-технологічні розробки, відкритий інноваційний підхід.



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