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E. O. KOCHANOV, PhD (Military),
Associate Professor of the Department of Environmental Monitoring and Protected Areas Management
e-mail: kochanov@karazin.ua ORCID ID: https://orcid.org/0000-0002-8443-4054
V. N. Karazin Kharkiv National University,
4, Svobody Sq., Kharkiv, 61022, Ukraine

ANALYSIS AND IMPROVEMENT OF CHEMICAL POLLUTION DISPERSION MODELS IN THE ENVIRONMENT

Purpose. To develop and analytically substantiate a model for assessing the chemical situation during accidents at chemically hazardous facilities, taking into account the specific features of the formation of primary and secondary chemical contamination.

Methods. The study uses an integrated analytical approach to modeling chemical contamination scenarios by applying modified atmospheric diffusion equations, formulas for calculating the mass of substance evaporation, the duration of cloud formation, and its spatial dispersion.

Results. Special attention is paid to incorporating the roughness of the underlying surface, which affects the parameters of toxic cloud dispersion, and to determining the depth of impact zones depending on the type of hazardous substance, meteorological conditions, and site characteristics.The surface roughness parameter was introduced to account for terrain heterogeneity. Calculations were performed for various categories of hazardous substances (ammonia, chlorine) under typical conditions for Ukraine. Reference and regulatory data, as well as algorithms and scenarios from practical assessments of chemical situations, were used. Based on the developed model, calculations of the affected area for typical chemically hazardous facilities were performed; the penetration depth of toxic clouds was determined depending on the type of underlying surface, wind speed, and temperature. It was shown that accounting for roughness increases the accuracy of assessments by 12–18%, which is critical for operational decision-making. It was also established that the secondary cloud forms an additional risk zone, which under certain conditions may exceed the area of primary contamination. The model's applicability for use in environmental monitoring and forecasting the consequences of man-made accidents was demonstrated.

Conclusions. The proposed model allows for the consideration of topographic and meteorological factors in assessing chemical contamination. This improves the accuracy of determining the boundaries of affected zones and can be integrated into decision-support systems for rapid response by emergency services, environmental monitoring, and territorial planning under conditions of potential man-made hazards.

KEYWORDS: *chemically hazardous facility, chemical situation, secondary contamination, affected zone, surface roughness, highly toxic substance*

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Introduction

The expansion of chemical production and the intensification of hazardous material transport have led to a growing risk of emergency situations involving the release of toxic inhalation-hazardous substances into the environment. Such events can cause large-scale harm to the population, degradation of ecosystems, and significant economic losses. This problem becomes particularly acute in the context of increasing urban density, infrastructure development, and the concentration of potentially hazardous industrial facilities in close proximity to residential areas. Modern approaches to ensuring environmental and technogenic safety demand the development of reliable methods for predicting the spatiotemporal dynamics of hazardous chemical cloud dispersion, as well as assessing the potential consequences for both human health and the environment. However, the application of existing models is associated with a number of limitations. Classical Gaussian models fail to account for complex terrain and urban structures, engineering models for dense gases often overlook phase transitions and secondary evaporation, and highly detailed computational fluid dynamics (CFD) approaches require significant computational resources, making them impractical for real-time emergency response.

Numerous studies by both domestic and international researchers propose various approaches to the modeling of accidental releases of hazardous substances. Accidental emissions of toxic compounds remain one of the most pressing issues in the fields of ecological and technogenic safety. Contemporary research increasingly focuses not only on the modeling of toxic cloud dispersion but also on the organization of evacuation procedures. For example, Yoo and Choi demonstrated the effectiveness of using GIS tools to develop risk maps and optimize evacuation plans in the event of chemical spills in South Korea [1]. The authors emphasized that geoinformation analysis helps to minimize evacuation time and reduce the risk of cloud exposure to the population; however, their study did not account for the complex physical processes underlying the formation of primary and secondary chemical clouds. Hou et al. conducted a large-scale review of hazardous chemical leakage accidents in China [2]. Their research showed that organizational factors (such as imperfect monitoring systems and delayed responses) play a role as significant as technical factors. Nevertheless, the authors also underscored the lack of scenario-based models capable of predicting the spatiotemporal dynamics of toxic clouds in real time. Lacome et al. examined the discrepancies in atmospheric dispersion modeling approaches used to assess accident consequences in Europe [3]. Their comparison revealed considerable divergence in results depending on the selected models and parameterizations, highlighting the need for harmonization of methods and the development of unified evaluation criteria. However, the article does not propose a universal model suitable for complex urban environments. Significant progress in physically grounded modeling is demonstrated in the work of Weger and colleagues, who developed the LES-based CAIRDIO model for urban-scale applications [4]. This model is capable of accounting for the influence of buildings, vegetation, and complex geometries, resulting in highly realistic transport scenarios. Its primary drawback is computational complexity, which limits its usability in real-time applications. A more applied approach was taken by Lipták et al., who integrated a Lagrangian model into the ESTE system for predicting pollution dispersion in urban environments [5]. The authors demonstrated that it is possible to strike a balance between computational efficiency and modeling accuracy. However, their model remains limited in its ability to simulate turbulent effects. Di Nicola and co-authors proposed a new method for representing surface roughness in urban dispersion models [6]. Their approach enables more accurate accounting of buildings and other obstructions, making the models more realistic. However, the study was not tested against actual accident scenarios involving the release of toxic substances. Field experiments such as Jack Rabbit II are of critical importance, and their results have been published by Gant et al. [7]. This study tested chlorine dispersion modeling and compared several dense gas models with real-world measurements. The authors found that even the most advanced models struggle to accurately reproduce peak concentrations, which highlights the continuing need for improvement in modeling techniques. In general, studies [1 – 7] cover a wide spectrum of approaches—from organizational aspects of emergency response to high-fidelity CFD simulations. Nonetheless, there remains a clear need for the development of a comprehensive model that combines spatiotemporal accuracy with the capability for rapid deployment in civil protection systems.

Further research has significantly deepened the understanding of dense gas dispersion mechanisms and the advancement of predictive models. For example, Fox et al. summarized the results of the Jack Rabbit II field experiments and the comparative methods used for dispersion modeling [8]. The authors emphasized that experimental data are critically important for validating model performance but also demonstrated significant discrepancies between the results of different approaches, especially under conditions of intense turbulence. Spicer and coauthors proposed a simplified source description for use in the Jack Rabbit II modeling framework [9]. This approach considerably reduces uncertainty in input data yet also revealed that even precise field measurements do not always allow for adequate characterization of the initial cloud formation phase. This highlights the need to develop more flexible initial condition modules within models. In their classical works, Hanna and Chang formulated acceptance criteria for evaluating the performance of urban dispersion models [10]. These criteria (FB, NMSE, FAC2, etc.) are still used today as a benchmark in contemporary studies. However, their application in complex urban settings remains a subject of debate, as real-world dispersion processes may deviate from underlying statistical assumptions. A major contribution to the development of engineering models was made by Fthenakis and colleagues, who reviewed and advanced the HGSYSTEM modeling framework for dense gas scenarios [11]. The model has been widely used in regulatory documents, but it exhibits significant limitations in accounting for complex terrain and urban environments. Earlier, Spicer and Havens validated the DEGADIS model through full-scale field trials [12], which was among the first attempts to use dense gas models for validated impact zone assessment. However, today this model is considered outdated due to its limited ability to reproduce dynamic behavior under complex environmental conditions. More recent CFD-based studies by Bellegoni et al. demonstrated that even small infrastructural barriers such as perimeter walls can substantially alter the trajectory of LNG vapor clouds [13]. This underlines the importance of detailed consideration of infrastructure features in any dispersion forecast.

In Ukrainian research, Amelina et al. examined accidental ammonia leakage scenarios from pipelines [14]. The authors employed a mathematical model to calculate near-surface air concentrations. The significance of this work lies in the adaptation of modeling techniques to the specific conditions of national infrastructure. However, further integration of modern CFD and GIS technologies is required. Thus, studies [8–14] illustrate the evolution from classical empirical approaches to experimentally validated and CFD-based solutions that incorporate complex infrastructural and topographical factors. At the same time, the challenge remains to combine computational efficiency, accuracy, and spatial resolution in a single integrated system.

Contemporary research also highlights the need to consider national and regional specificities. Rusin et al. analyzed the safety of transporting methane–ammonia mixtures through pipelines [15]. The authors demonstrated that even minor leaks can pose significant hazards due to the combined toxic and fire effects. This study emphasizes the importance of comprehensive risk assessment within transportation systems. Significant steps towards the integration of CFD and GIS were made by Wu and colleagues [16], who developed a system combining CFD modeling with geoinformation technologies for rapid prediction of pollution consequences. This approach enables the creation of interactive scenarios for crisis management, although its implementation requires high computational resources. Jiao et al. developed machine learning models for the quantitative assessment of accident consequences [17]. The use of gradient boosting and neural networks allowed for rapid prediction of impact zones and potential casualties. However, the model's accuracy is constrained by its dependence on training datasets, which may not generalize well to atypical conditions. Qian and colleagues demonstrated the application of LSTM networks for the direct prediction of toxic gas dispersion in real-world emergencies [18]. The authors showed that deep learning models are capable of generalizing the dispersion dynamics of various substances; however, the issue of result interpretability remains unresolved. Finally, Viúdez-Moreiras, in his editorial article, summarized recent advances in atmospheric modeling and emphasized the importance of integrating physical and machine learning approaches [19]. The author argued that the future lies in hybrid models that combine CFD, empirical methods, and artificial intelligence algorithms. Overall, studies [15–19] illustrate current trends toward integrating classical and modern approaches, incorporating GIS and AI in forecasting, and adapting modeling techniques to regional contexts. Nonetheless, challenges remain regarding model accuracy, computational performance, and universality.

At the same time, several critical issues remain unresolved. In particular, there is a need to develop a unified approach that combines the precision of physically based models, the ability to account for topographical and meteorological conditions, source parameters, and infrastructural features, while also ensuring sufficient computational speed for real-time use in monitoring and emergency response

The purpose of study is to develop and justify a mathematical model for the dispersion of toxic clouds in the environment during accidental releases at chemically hazardous facilities.

The model accounts for the physicochemical properties of substances, site-specific topographical features, and meteorological conditions, and it is designed to be integrated into environmental and technogenic safety systems.

Methodology

The object of study comprises chemically hazardous facilities (CHFs) where highly toxic substances (HTSs), particularly ammonia and chlorine, are stored or used. The research focuses specifically on assessing the chemical situation (CS) that arises during emergency releases of HTSs, as well as forecasting the spatial extent of contamination zones, taking into account topographical, atmospheric, and physicochemical factors.

The methodology is grounded in a systems analysis of the physical processes that accompany the rupture of HTS storage tanks, the formation of both primary and secondary toxic clouds, their subsequent dispersion, and their environmental impact. To simulate accident scenarios, a formula-based assessment scheme was developed. This scheme includes: the calculation of the spill area for HTSs; estimation of the quantity of substance transitioning into the primary and secondary clouds; determination of the dispersion depth for both primary and secondary clouds; incorporation of surface roughness effects via the introduction of the parameter z_0; calculation of the evaporation time of HTSs from the surface of the spill; and the estimation of the time required for the cloud to reach a specified boundary.

The mathematical modeling is based on atmospheric diffusion equations (modified Gaussian models), adapted to the near-surface air layer, which is especially relevant for localized emergency situations. All formulas were derived or adapted in accordance with [20]. The vertical stability of the atmosphere is described using the Pasquill stability classification (A–F), which influences the dispersion coefficients in the calculations. The model also incorporates an analysis of substance toxicity using the inhalation toxic dose index (PCτ50). It allows for the variation of input parameters for both hypothetical and real-world facilities, including: the quantity of substance (100–200 tons), type of surface (flat, grassy, urban), wind speed, atmospheric conditions, distance to populated areas, and more. Calculations were carried out using analytical modeling tools implemented in Microsoft Excel, followed by validation through comparison with real-life accident data (in particular, the 2007 ammonia release in Lviv Oblast, Ukraine) [21]. The methodology is intended for use in environmental monitoring, technogenic safety management, and the development of automated decision-support systems (DSS) for emergency response.

Results and Discussion

For many years, the Incident and Emergency Centre (IEC) has operated within the structure of the International Atomic Energy Agency (IAEA), receiving real-time information from nuclear facilities around the world. Based on incoming data, one of three response modes – "routine readiness," "basic response," or "full response" – is selected, depending on the significance and degree of environmental hazard posed by the event. However, the methodological support and decision-making tools available for the prevention of ecologically hazardous emergencies remain insufficiently developed.

According to the Law of Ukraine “On National Security of Ukraine” (No. 2469-VIII of June 21, 2018), state policy in the fields of national security and defense is aimed at ensuring Ukraine’s military, foreign policy, state, economic, informational, environmental, critical infrastructure, and cyber security, as well as other areas of national interest.

Within the territory of Ukraine, the following categories of chemically hazardous facilities (CHFs) can be identified:

- Plants and complexes in the chemical industry, as well as individual units and installations that manufacture or use highly toxic substances (HTSs);
- Oil refining facilities and associated industrial complexes;

- Enterprises in other industrial sectors that utilize HTSs in their processes;
- Facilities with refrigeration systems, water pumping stations, and treatment plants using chlorine or ammonia;
- Transport vehicles, including rail tankers, road tankers, containers, and river or sea tankers used for transporting chemical products;
- Warehouses and depots storing pesticide reserves for agricultural use, among others.

It has been established that the territorial distribution of potentially hazardous industrial facilities is characterized by different sectoral structures across specific economic regions. For instance, in the Podillia and Central economic regions, potentially hazardous food industry enterprises dominate (according to the Classifier of Potentially Hazardous Objects, 2006, Code 460), including livestock farms, poultry plants, meat-processing plants, and feed antibiotic factories. In contrast, the Dnipro and North-Eastern regions primarily house enterprises of the heavy and chemical industries (Codes 340 and 100).

The situation is further complicated by frequent and irresponsible violations of technogenic safety regulations. The poorest compliance with safety measures has been recorded in the following oblasts: Volyn (only 50% of safety measures implemented), Zaporizhzhia (37%), Lviv (46%), Odesa (25%), Ternopil (45%), Kharkiv (49%), and Chernivtsi (38%). Furthermore, only 3.6% of potentially hazardous facilities are equipped with early detection systems for emergencies and public alert systems. The implementation of early warning systems is further supported by international experience: such systems are deployed at strategically important sites in the United States, as well as chemically hazardous sites in Germany and other EU countries.

Thus, it is necessary to intensify efforts to develop effective national and international mechanisms for the prompt notification and response in cases of incidents or potential threats at critical and potentially hazardous sites.

One way to meet the high demands for timeliness and quality of decision-making in critical situations is to employ automated decision support systems (DSS) or expert systems. Such systems must possess the following core functionalities:

1. The ability to process poorly formalized, vague, and incomplete input information about critical situations;
2. The capacity to accumulate knowledge about past critical incidents for the purpose of learning from past emergency response experience;
3. Ease of working with large datasets, including the ability to synthesize heterogeneous information on emergencies and provide high-speed access to such data.

A general structure of such a decision support system is presented in Figure 1.

The stated requirements must be based on the software framework of the system. For the efficient implementation of operational algorithms, the software should be grounded in a model or a formula-based scheme for chemical environment assessment.

Chemical environment assessment is a sequence of procedures aimed at obtaining values of chemical contamination indicators. These indicators can be classified into several groups:

– in the context of evaluating an environmentally hazardous chemical situation, the primary task is to determine the following groups of indicators: the extent of chemical contamination, the duration of contamination, and the hazard level posed by the contamination;

– to determine spatial indicators of chemical contamination (extent), the dimensions of the destruction zone and chemical contamination zones are established;

– to determine duration indicators of contamination, parameters such as the time required for the toxic cloud to reach a specified boundary and the duration of the damaging effects of the hazardous substance are calculated;

– to determine hazard indicators, the assessment includes the estimation of potential chemical casualties among the population and industrial personnel.

To develop a methodology for assessing the chemical environment, it is necessary to examine the processes occurring during the destruction of a chemically hazardous facility (CHF). This can be done using a combination of existing mathematical models that describe: the contamination source; atmospheric dispersion of pollutants; and the toxic effects of hazardous substances on the population and industrial personnel.

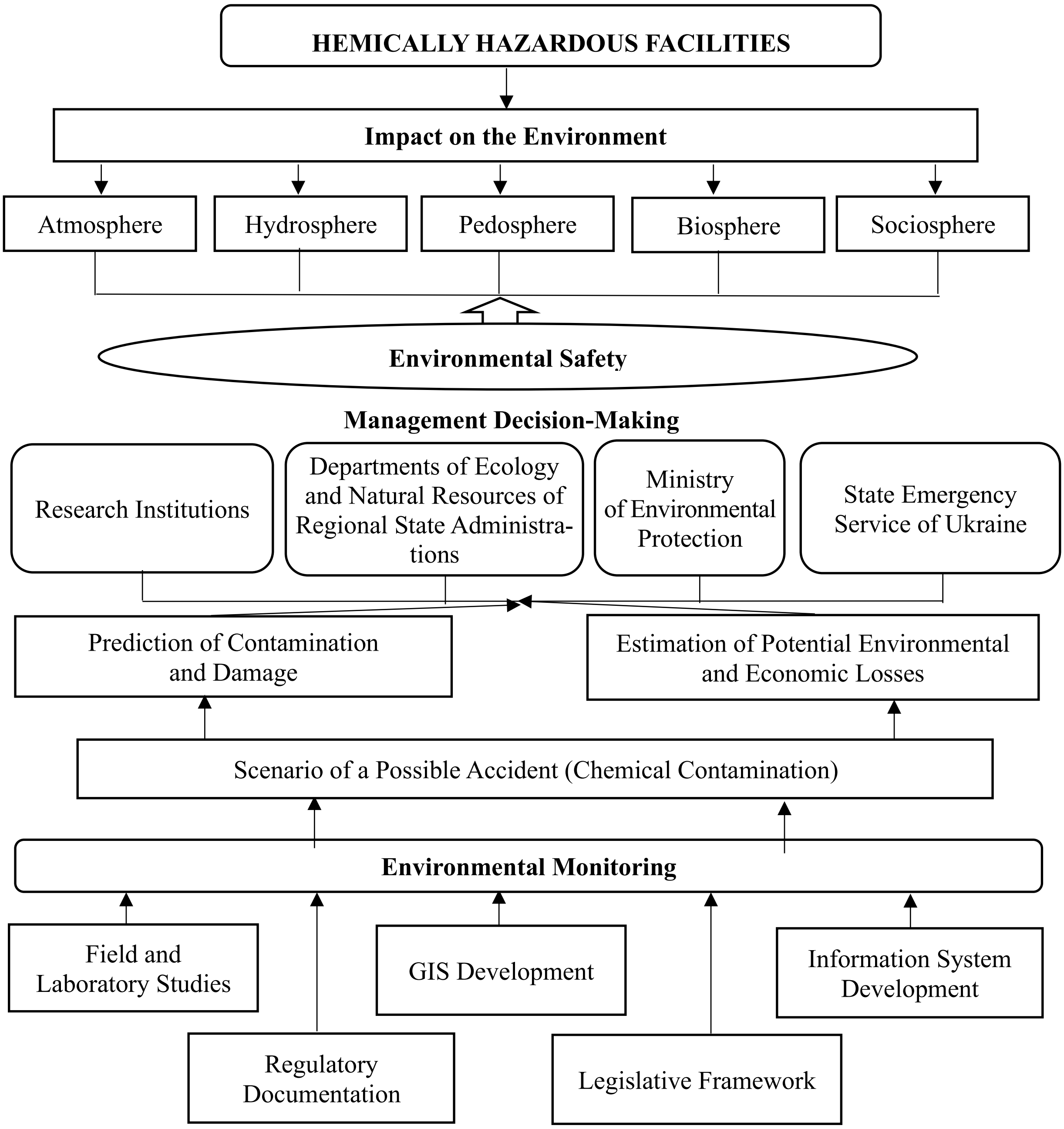

Fig. 1 – Schematic Diagram of Environmental Safety Assurance in the Event of Chemical Contamination Caused by Accidents at Chemically Hazardous Facilities

A preliminary step in developing the appropriate methodology for chemical environment assessment during CHF failure is the construction of a model describing the process of chemical casualties among the population and personnel. The purpose of creating such a model is to estimate the environmental hazard indicators associated with air contamination in the event of an accident at a CHF.

The indicators of chemical contamination scale are determined by:

– the radius ($R_{p}p$) and area ($S_{p}p$) of the destruction zone;

– the depth (G_1) and area (S_1) of the primary toxic cloud dispersion zone;

– the depth (G_2) and area (S_2) of the secondary toxic cloud dispersion zone.

The indicators of chemical contamination duration are determined by:

– the evaporation time of the hazardous substance from the spill surface (τ_{evap});

– the time required for the toxic cloud to reach a designated boundary (t_{arr}).

The hazard indicators of chemical contamination are assessed through the estimation of potential chemical casualties among the population and industrial personnel in environmentally hazardous zones. The primary toxicological characteristic of a hazardous substance is its inhalation toxic dose.

In determining the specifics of the chemical contamination process in various environmental compartments, several hypotheses may be formulated:

1. The formation conditions of the primary and secondary toxic clouds differ. Based on their formation mechanisms, the contamination source for the primary cloud should be considered as an instantaneous point source, while for the secondary cloud, a continuous point source should be assumed.
2. The atmospheric dispersion of toxic clouds can be characterized as follows: first, the distance over which the hazardous substance has a damaging effect typically spans several kilometers; second, the vertical extent of primary and secondary toxic clouds rarely exceeds 150 meters. It is generally accepted that, in cases of isotropic diffusion, the transport of toxic substances occurs horizontally along the x-axis, i.e., within the surface atmospheric layer.

In the event of a spill of highly hazardous toxic substances (HHTS) from damaged storage containers, the liquid typically disperses over a leveled surface within the containment area, forming a shape that closely resembles a circle. This allows for the estimation of the area of the destruction zone (*Sd*) using the following formula:

$$S_d = \pi \cdot R_d^2 \qquad (1)$$

where *Rd* is the radius of the HHTS spill mirror [m].

Alternatively, the area may be expressed through the diameter of the spill mirror (d_d) as:

$$S_d = \pi \cdot \frac{d_d^2}{4} \qquad (2)$$

Here, d_d is the diameter of the spill mirror, which depends on the total amount of HHTS released from the damaged containment. The following equation is used to estimate the diameter based on the volume of the spilled substance:

$$d_d = b \cdot \sqrt{\frac{Q-Q_1}{\rho}} \qquad (3)$$

where:

b is a coefficient depending on the presence of bunding:

- $b = 1.22\ m^{-1/2}$ if bunding is present,
- $b = 5.04\ m^{-1/2}$ if no bunding is provided;

ρ is the density of the HHTS, [kg/m³];

Q is the total mass of HHTS in the storage container, [kg];

Q_1 is the mass of HHTS that transitions into the primary toxic cloud, [kg].

An approximate estimation of the quantity of HHTS (Q_1) that transitions into the primary cloud at the moment of container breach can be performed using the formula presented in [20], which incorporates thermal parameters:

$$Q_1 = \frac{QC_v(t-t_k)}{\lambda}, \qquad (4)$$

where:

Q is the total amount of HHTS in the storage container, [kg];

C_v is the specific heat capacity of the liquid, [kJ/kg·°C];

t is the temperature of the liquid HHTS at the moment of release, [°C];

t_k is the boiling point of the HHTS, [°C];

λ is the specific latent heat of vaporization for the HHTS, [kJ/kg].

The values of C_v and λ are to be obtained from chemical reference data specific to the substance in question.

When determining the depth of dispersion of the primary toxic cloud of hazardous chemicals (HHTS) within the atmospheric boundary layer near the ground surface, the influence of surface roughness on the propagation of the contaminated air mass was not initially considered. To account for the effect of terrain roughness on the dispersion of toxic substances, a standard roughness parameter (z_0) is introduced. This parameter enables the incorporation of surface heterogeneity into the modeling of wind velocity profiles and, consequently, toxic plume behavior. The modified near-surface wind speed (u'), accounting for surface roughness, is calculated using the following logarithmic wind profile expression:

$$u' = u \cdot \ln\left(\frac{z+z_0}{z_0}\right) \qquad (5)$$

where:

u' is the adjusted horizontal component of the wind velocity near the surface, considering terrain roughness, [m/s];
u is the average undisturbed wind speed at reference height, [m/s];
z is the vertical height of the toxic cloud's dispersion, [m];
z_0 is the effective surface roughness length [m], a geometric parameter that reflects the characteristic height of surface irregularities (e.g., vegetation, buildings, terrain features).

The value of z_0 is selected based on the type of underlying surface and can be found in Table 1 (not included here), which classifies roughness values for various land cover types such as water surfaces, grassy fields, urban areas, forests, and industrial zones.

This correction is essential for improving the accuracy of predictive models used in environmental safety systems, particularly under conditions where local terrain has a significant influence on airflow and toxic plume trajectory.

Table 1

Effective Roughness Height Values (z_0) for Different Types of Surfaces

Surface Type	z_0, [m]
Very flat, snowy or icy surface	$1 \cdot 10^{-5}$
Flat snow over short grass	$5 \cdot 10^{-5}$
Desert	$3 \cdot 10^{-3}$
Snow-covered surface with low shrubbery	$1 \cdot 10^{-3}$
Mowed grass, cut height up to 1.5 cm	$2 \cdot 10^{-3}$
Mowed grass, cut height up to 3 cm	$7 \cdot 10^{-3}$
Mowed grass, cut height up to 4.5 cm	$2.4 \cdot 10^{-2}$
Grass height 60–70 cm:	
– for $0 < u \leq 1.5$ m/s	$9 \cdot 10^{-2}$
– for $1.6 < u \leq 3.5$ m/s	$6.7 \cdot 10^{-2}$
– for $3.6 < u \leq 6.5$ m/s	$3.7 \cdot 10^{-2}$
Heterogeneous surface with predominant areas of grass, shrubbery, and trees	0.1
Forested area with average tree height ~10 m, urban development	0.9

Thus, the expression for determining the depth of propagation of the primary toxic cloud takes the following form:

$$G_1 = b_1 \left(\frac{Q_1 \cdot 10^{-3}}{u' \cdot PC_{\tau 50}} \right)^{a_1} \quad (6)$$

where:
G_1 – depth of propagation of the primary cloud of hazardous chemical substances (HCS) over flat terrain, taking into account the surface roughness, [m];
Q_1 – amount of HCS that transitions into the primary cloud, calculated from expression (4), [kg];
$PC\tau_{50}$ – average threshold value of toxic dose (toxic load), [g·s/m³];
u' – horizontal component of near-surface wind velocity adjusted for the roughness of the underlying surface, [m/s];
a_1, b_1 – dimensionless coefficients depending on the category of vertical atmospheric stability, calculated using the following formulas:

$$b_1 = 15{,}42 \cdot exp(6{,}96 \cdot \varepsilon) \quad (7)$$

$$a_1 = 0{,}57 \cdot exp(0{,}864 \cdot \varepsilon), \quad (8)$$

where (ε) is a parameter of vertical atmospheric stability determined according to the Pasquill stability categories:

- A, B, C (convection): ε = -0.2
- D (isothermal): ε = 0
- E, F (inversion): ε = 0.2

Another indicator characterizing the scale of chemical contamination is the depth of propagation of the secondary cloud of air contaminated with HCS. The amount of HCS transitioning into the secondary cloud is determined by the following expression:

$$Q_2 = Q - Q_1, \quad (9)$$

where:

Q – total quantity of HCS released, [kg];

Q_1 – quantity of HCS that transitioned into the primary cloud, [kg].

The value of Q_2 is associated with the evaporation time of the hazardous chemical substance (HCS). In this context, the minimum evaporation time within which it is reasonable to assess the extent of cloud dispersion should not exceed 24 hours due to the high variability in wind direction.

The following formula is used to estimate the depth of propagation of the secondary cloud, excluding the influence of surface roughness. However, previous assumptions allow the introduction of a parameter to account for the surface roughness effect on the propagation of the contaminated air mass:

$$G_2 = \frac{16.84 \cdot \tau^{-0.51} \cdot b_2 Q_2 \cdot 10^{-3}}{u' \cdot PC\tau_{50}^{a_1}} \qquad (10)$$

where:

G_2 – depth of propagation of the secondary cloud of air contaminated with HCS, [m];

$PC\tau_{50}$) – average threshold toxic dose, [g·s/m³];

Q_2) – amount of HCS entering the secondary cloud, defined by expression (9), [kg];

τ) – evaporation time of HCS from the spill surface, [s];

a_1, b_2) – dimensionless coefficients depending on the vertical atmospheric stability category.

Coefficient a_1 is defined by expressions (7) and (8); Coefficient b_2 is determined by:

$$b_2 = 16.84 \cdot \exp(6.87 \cdot \varepsilon) \qquad (11)$$

where

ε – vertical atmospheric stability parameter, with values as follows:

E, F → ε = 0.2;

D → ε = 0;

A, B, C → ε = -0.2

u' – horizontal component of ground-level wind speed, accounting for surface roughness, [m/s].

The indicators of chemical contamination duration include:

- the evaporation time of the HCS from the spill surface, and
- the time for the contaminated cloud to reach a given boundary.

The toxic effect of the HCS depends significantly on the evaporation time from the surface of the spill. This time is a function of both meteorological conditions and the physicochemical properties of the substances. The parameter is determined using the following formula:

$$\tau_{\text{evap}} = \frac{Q_2}{E \cdot S_{\text{spill}} \cdot 3.6 \cdot 10^3} \qquad (12)$$

where:

τ_{evap} – evaporation time of HCS from the surface of the spill mirror, [s];

E – specific evaporation rate, [kg/m²·s], calculated as:

$$E = 0{,}041 \frac{u \cdot M}{d_{\text{пр}}^{0{,}14} \cdot T_u} \cdot exp\left[\frac{\lambda \cdot M}{R}\left(\frac{1}{T_k} - \frac{1}{T_u}\right)\right], \qquad (13)$$

where:

M – molecular weight of the HCS, [g/mol];

d_{spill} – effective spill diameter from expression (3), [m];

T_u – ambient air temperature, [ºC];

λ – specific latent heat of evaporation, [kJ/kg];

R – universal gas constant, equal to 8.3 [kJ/kmol·K];

0.041 – dimensional consistency coefficient, [s·K·mol / m$^{0.86}$·g];

T_k – boiling point of the HCS, [K].

To ensure timely notification of the population about the onset of chemical contamination and to carry out emergency response measures, it is necessary to determine the time of arrival of the contaminated air cloud at a given facility or populated area. This parameter is calculated using the following formula:

$$t_p = \frac{0.3 \cdot x}{u} \qquad (14)$$

where:

t_p – time of arrival of the HCS-contaminated air cloud at the designated boundary, [hours];

x – distance from the damaged chemically hazardous facility to the assessment object (e.g. settlement), [km];

u – ground-level wind speed, [m/s];

0.3 – conversion coefficient from [m/s] to [km/h].

As an example of a potential threat posed by highly toxic substances to the environment, one can refer to the accident that occurred in Lviv Region on October 3, 2007. During railway transportation of 28 tank cars filled with ammonia (each with a capacity of 20 tons), a leak of 200 kg of ammonia occurred due to a valve failure [21]. While no evacuation was carried out, the smell of ammonia was reportedly noticeable at a distance of more than 10 km.

Thus, the proposed formula-based scheme provides a tool to calculate the indicators of chemical contamination for a hypothetical environmentally hazardous facility. The results of the calculations are presented in Table 2.

The data presented in Table 2 indicate that the risks associated with large-scale storage of hazardous chemical substances can increase by several orders of magnitude in the event of an emergency at environmentally hazardous facilities

Table 2

Calculated indicators of potential chemical contamination for a hypothetical environmentally hazardous facility

Indicators of Chemical Contamination	Type of HCS	Amount of HCS, [t]	Distance to CHO, [km]			
Depth of *primary* cloud spread, [km]	Ammonia	100	13	13	13	13
		200	18	18	18	18
	Chlorine	100	44	44	44	44
		200	62	62	62	62
Depth of secondary cloud spread, [km]	Ammonia	100	29	29	29	29
		200	40	40	40	40
	Chlorine	100	96	96	96	96
		200	133	133	133	133

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Conclusions

A comprehensive formula-based model for assessing the chemical environment has been developed, which takes into account the mechanisms of formation of both primary and secondary contamination clouds. The model is based on the physicochemical properties of substances, local terrain conditions, and meteorological factors. A novel approach has been proposed to incorporate surface roughness (z_0), which enables the model to be adapted to various types of terrain — from open areas to densely built urban zones. This ensures more accurate forecasting of the configuration and parameters of the contamination zone.

The model provides quantitative estimates of the depth, area, and duration of contamination, enabling effective planning of civil protection measures, including the identification of evacuation zones, calculation of response timeframes, and assessment of the level of environmental risk. The mathematical structure of the model allows for algorithmization, making it suitable for integration into information-analytical systems, decision support systems (DSS), and automated modules for emergency monitoring.

Model verification, based on the example of an ammonia leak under different terrain conditions, demonstrated high accuracy and sensitivity to changes in key environmental parameters, confirming its practical applicability.

The results of the study have significant potential for practical application in the fields of civil protection, industrial safety, environmental monitoring, and emergency modeling. The proposed model can be integrated into: automated alert and response systems, operating at national and regional levels of the State Emergency Service of Ukraine (SESU), to forecast impact zones in real-time; decision Support Systems (DSS) to improve response efficiency in case of accidents at chemically hazardous facilities, as well as for planning evacuation routes and determining priority protective measures for the population; training and simulation platforms for preparing emergency response specialists, modeling chemical release scenarios, and practicing response algorithms in contaminated environments; geographic Information Systems (GIS), which will allow spatial data to be combined with simulation results to create interactive chemical hazard maps; normative and methodological frameworks, as a tool for justified assessment of sanitary protection zones and potential evacuation areas for high-risk chemical facilities.

Conflict of Interest

The author declares no conflict of interest regarding the publication of this manuscript. Furthermore, the author has fully adhered to ethical norms, including avoiding plagiarism, data falsification, and duplicate publication.

The work does not use artificial intelligence resources.

References

1. Yoo, B., & Choi, S. D. (2019). Emergency evacuation plan for hazardous chemicals leakage accidents using GIS-based risk analysis techniques in South Korea. *International Journal of Environmental Research and Public Health, 16*(11), 1948. https://doi.org/10.3390/ijerph16111948
2. Hou, J., Gai, W.-M., Cheng, W.-Y., & Deng, Y.-F. (2021). Hazardous chemical leakage accidents and emergency evacuation response from 2009 to 2018 in China: A review. *Safety Science, 135*, 105101. https://doi.org/10.1016/j.ssci.2020.105101
3. Lacome, J.-M., Leroy, G., Joubert, L., & Truchot, B. (2023). Harmonisation in Atmospheric Dispersion Modelling Approaches to Assess Toxic Consequences in the Neighbourhood of Industrial Facilities. *Atmosphere, 14*(11), 1605. https://doi.org/10.3390/atmos14111605
4. Weger, M., Knoth, O., & Heinold, B. (2021). An urban large-eddy-simulation-based dispersion model for marginal grid resolutions: CAIRDIO v1.0. *Geoscientific Model Development, 14*(3), 1469–1493. https://doi.org/10.5194/gmd-14-1469-2021
5. Lipták, Ľ., Cibulka, J., Kucbel, M., & Jurčák, P. (2023). Dispersion and radiation modelling in ESTE system using urban LPM. *Atmosphere, 14*(7), 1077. https://doi.org/10.3390/atmos14071077
6. Di Nicola, F., Brattich, E., & Di Sabatino, S. (2022). A new approach for roughness representation within urban dispersion models. *Atmospheric Environment, 283*, 119181. https://doi.org/10.1016/j.atmosenv.2022.119181
7. Gant, S., Weil, J., Delle Monache, L., Hanna, S., & Chang, J. (2018). Dense gas dispersion model development and testing for the Jack Rabbit II phase 1 chlorine release experiments. *Atmospheric Environment, 192*, 218–240. https://doi.org/10.1016/j.atmosenv.2018.08.009
8. Fox, S., Hanna, S., Mazzola, T., Spicer, T., Chang, J., & Gant, S. (2022). Overview of the Jack Rabbit II (JR II) field experiments and summary of the methods used in the dispersion model comparisons. *Atmospheric Environment, 269*, 118783. https://doi.org/10.1016/j.atmosenv.2021.118783
9. Spicer, Thomas & Tickle, Graham. (2021). Simplified source description for atmospheric dispersion model comparison of the Jack Rabbit II chlorine field experiments. *Atmospheric Environment.* 244. 117866. https://doi.org/10.1016/j.atmosenv.2020.117866
10. Hanna, S., Chang, J. (2012). Acceptance criteria for urban dispersion model evaluation. *Meteorology and Atmospheric Physics.* 116, 133–146. https://doi.org/10.1007/s00703-011-0177-1
11. Fthenakis, V. (1999). HGSYSTEM: a review, critique, and comparison with other models. *Journal of Loss Prevention in the Process Industries, 12*(6), 525-531. https://doi.org/10.1016/S0950-4230(99)00029-7
12. Spicer, T. O., & Havens, J. A. (1987). Field test validation of the degadis model. *Journal of Hazardous Materials, 16*, 231–245. https://doi.org/10.1016/0304-3894(87)80036-5
13. Bellegoni, M., Ovidi, F., Landucci, G., Tognotti, L., & Galletti, C. (2021). CFD analysis of the influence of a perimeter wall on the natural gas dispersion from an LNG pool. *Process Safety and Environmental Protection, 148*, 751–764. https://doi.org/10.1016/j.psep.2021.01.048
14. Amelina, L. V., Biliaiev, M. M., Berlov, O. V., Verhun, O. O., & Rusakova, T. I. (2021). Modeling of Environmental Pollution by Ammonia Emission from a Damaged Pipeline. *Science and Transport Progress*, (1(91), 5–14. https://doi.org/10.15802/stp2021/229167
15. Rusin, A., & Stolecka-Antczak, K. (2023). Assessment of the Safety of Transport of the Natural Gas–Ammonia Mixture. *Energies*, *16*(5), 2472. https://doi.org/10.3390/en16052472
16. Wu, Q., Wang, Y., Sun, H., Lin, H., & Zhao, Z. (2023). A System Coupled GIS and CFD for Atmospheric Pollution Dispersion Simulation in Urban Blocks. *Atmosphere*, *14*(5), 832. https://doi.org/10.3390/atmos14050832
17. Jiao, Z., Zhang, Z., Jung, S., & Wang, Q. (2023). Machine learning based quantitative consequence prediction models for toxic dispersion casualty. *Journal of Loss Prevention in the Process Industries, 81*, 104952. https://doi.org/10.1016/j.jlp.2022.104952
18. Qian, F., Chen, L., Li, J., Ding, C., Chen, X., & Wang, J. (2019). Direct Prediction of the Toxic Gas Diffusion Rule in a Real Environment Based on LSTM. *International Journal of Environmental Research and Public Health*, *16*(12), 2133. https://doi.org/10.3390/ijerph16122133
19. Viúdez-Moreiras, D. (2023). Editorial for the Special Issue "Atmospheric Dispersion and Chemistry Models: Advances and Applications". *Atmosphere, 14*(8), 1275. https://doi.org/10.3390/atmos14081275

20. Brandt M., Becker E., Jöhncke U. A weight-of-evidence approach to assess chemicals: case study on the assessment of persistence of 4,6-substituted phenolic benzotriazoles in the environment. *Environ Sci Eur.* 28, 4, 2016. https://doi.org/10.1186/s12302-016-0072-y
21. Phosphorus accident near Ozhidov. (2007). Retrieved from https://w.wiki/72ff (in Ukrainian)

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Е. О. КОЧАНОВ, канд. військ. наук, доц.,
доцент кафедри екологічного моніторингу та заповідної справи
e-mail: kochanov@karazin.ua ORCID ID: https://orcid.org/0000-0002-8443-4054
Харківський національний університет імені В. Н. Каразіна,
майдан Свободи, 4, м. Харків, 61022, Україна

АНАЛІЗ ТА УДОСКОНАЛЕННЯ МОДЕЛЕЙ ПОШИРЕННЯ ХІМІЧНОГО ЗАБРУДНЕННЯ У НАВКОЛИШНЬОМУ СЕРЕДОВИЩІ

Мета. Розробка та аналітичне обґрунтування моделі оцінки хімічної обстановки при аваріях на хімічно небезпечних об'єктах з урахуванням особливостей формування первинного та вторинного хімічного зараження.

Методи. Використано комплексний аналітичний підхід до моделювання сценаріїв хімічного зараження з використанням модифікованих рівнянь атмосферної дифузії, формул для розрахунку маси випару речовини, тривалості утворення хмари та її просторового поширення.

Результати. Особливу увагу приділено врахуванню шорсткості підстилаючої поверхні, яка впливає на параметри поширення токсичних хмар, та визначенню глибини зон ураження залежно від типу СДОР, метеоумов і властивостей місцевості. Введено параметр шорсткості поверхні для обліку неоднорідностей рельєфу. Розрахунки проведено для різних категорій сильнодіючих отруйних речовин (аміак, хлор), у типових умовах для України. Використано довідкові та нормативні дані, а також алгоритми і сценарії з практики оцінки хімічної обстановки. На основі розробленої моделі проведено розрахунки площі ураження для типових хімічно небезпечних об'єктів, визначено глибину проникнення токсичної хмари в залежності від типу підстилаючої поверхні, швидкості вітру та температури. Показано, що врахування шорсткості підвищує точність оцінки на 12–18 %, що критично для оперативного прийняття рішень. Встановлено, що вторинна хмара формує додаткову зону ризику, яка у певних умовах перевищує за площею первинне зараження. Продемонстровано можливість використання моделі у системах екологічного моніторингу та прогнозування наслідків техногенних аварій.

Висновки. Запропонована модель дозволяє враховувати топографічні та метеорологічні чинники при оцінці хімічного зараження. Це сприяє підвищенню точності визначення меж зон ураження та може бути інтегрована у системи підтримки прийняття рішень для оперативного реагування службами ДСНС, екологічного моніторингу та територіального планування в умовах потенційної техногенної небезпеки.

КЛЮЧОВІ СЛОВА: *хімічно небезпечний об'єкт, хімічна обстановка, вторинне зараження, зона ураження, шорсткість поверхні, сильнодіюча отруйна речовина*

Конфлікт інтересів

Автор заявляє, що конфлікту інтересів щодо публікації цього рукопису немає. Крім того, автор повністю дотримувався етичних норм, включаючи плагіат, фальсифікацію даних та подвійну публікацію.

В роботі не використано ресурс штучного інтелекту.

Список використаної літератури

1. Yoo B., Choi S. D. Emergency evacuation plan for hazardous chemicals leakage accidents using GIS-based risk analysis techniques in South Korea. *International Journal of Environmental Research and Public Health*. 2019. Vol. 16, No. 11. P. 1948. https://doi.org/10.3390/ijerph16111948
2. Hou J., Gai W.-M., Cheng W.-Y., Deng Y.-F. Hazardous chemical leakage accidents and emergency evacuation response from 2009 to 2018 in China: A review. *Safety Science*. 2021. Vol. 135. Article 105101. https://doi.org/10.1016/j.ssci.2020.105101

3. Lacome J.-M., Leroy G., Joubert L., Truchot B. Harmonisation in Atmospheric Dispersion Modelling Approaches to Assess Toxic Consequences in the Neighbourhood of Industrial Facilities. *Atmosphere*. 2023. Vol. 14, No. 11. P. 1605. https://doi.org/10.3390/atmos14111605
4. Weger M., Knoth O., Heinold B. An urban large-eddy-simulation-based dispersion model for marginal grid resolutions: CAIRDIO v1.0. *Geoscientific Model Development*. 2021. Vol. 14, No. 3. P. 1469–1493. https://doi.org/10.5194/gmd-14-1469-2021
5. Lipták Ľ., Cibulka J., Kucbel M., Jurčák P. Dispersion and radiation modelling in ESTE system using urban LPM. *Atmosphere*. 2023. Vol. 14, No. 7. P. 1077. https://doi.org/10.3390/atmos14071077
6. Di Nicola F., Brattich E., Di Sabatino S. A new approach for roughness representation within urban dispersion models. *Atmospheric Environment*. 2022. Vol. 283. Article 119181. https://doi.org/10.1016/j.atmosenv.2022.119181
7. Gant S., Weil J., Delle Monache L., Hanna S., Chang J. Dense gas dispersion model development and testing for the Jack Rabbit II phase 1 chlorine release experiments. *Atmospheric Environment*. .2018. Vol. 192. P. 218–240. https://doi.org/10.1016/j.atmosenv.2018.08.009
8. Fox S., Hanna S., Mazzola T., Spicer T., Chang J., Gant S. Overview of the Jack Rabbit II (JR II) field experiments and summary of the methods used in the dispersion model comparisons. *Atmospheric Environment*. 2022. Vol. 269. Article 118783. https://doi.org/10.1016/j.atmosenv.2021.118783
9. Spicer T., Tickle G. Simplified source description for atmospheric dispersion model comparison of the Jack Rabbit II chlorine field experiments. *Atmospheric Environment*. 2021. Vol. 244. Article 117866. https://doi.org/10.1016/j.atmosenv.2020.117866
10. Hanna S., Chang J. Acceptance criteria for urban dispersion model evaluation. *Meteorology and Atmospheric Physics*. 2012. Vol. 116. P. 133-146. https://doi.org/10.1007/s00703-011-0177-1
11. Fthenakis V. HGSYSTEM: a review, critique, and comparison with other models. *Journal of Loss Prevention in the Process Industries*. 1999. Vol. 12, No. 6. P. 525–531. https://doi.org/10.1016/S0950-4230(99)00029-7
12. Spicer T. O., Havens J. A. Field test validation of the degadis model. *Journal of Hazardous Materials*. 1987. Vol. 16. P. 231-245. https://doi.org/10.1016/0304-3894(87)80036-5
13. Bellegoni M., Ovidi F., Landucci G., Tognotti L., Galletti C. CFD analysis of the influence of a perimeter wall on the natural gas dispersion from an LNG pool. *Process Safety and Environmental Protection*. 2021. Vol. 148. P. 751-764. https://doi.org/10.1016/j.psep.2021.01.048
14. Amelina L. V., Biliaiev M. M., Berlov O. V., Verhun O. O., Rusakova T. I. Modeling of Environmental Pollution by Ammonia Emission from a Damaged Pipeline. *Science and Transport Progress*. 2021. Vol. 1(91). P. 5–14. https://doi.org/10.15802/stp2021/229167
15. Rusin A., Stolecka-Antczak K. Assessment of the Safety of Transport of the Natural Gas–Ammonia Mixture. *Energies*. 2023. Vol. 16, No. 5. P. 2472. https://doi.org/10.3390/en16052472
16. Wu Q., Wang Y., Sun H., Lin H., Zhao Z. A System Coupled GIS and CFD for Atmospheric Pollution Dispersion Simulation in Urban Blocks. *Atmosphere*. 2023. Vol. 14, No. 5. P. 832. https://doi.org/10.3390/atmos14050832
17. Jiao Z., Zhang Z., Jung S., Wang Q. Machine learning based quantitative consequence prediction models for toxic dispersion casualty. *Journal of Loss Prevention in the Process Industries*. 2023. Vol. 81. Article 104952. https://doi.org/10.1016/j.jlp.2022.104952
18. Qian F., Chen L., Li J., Ding C., Chen X., Wang J. Direct Prediction of the Toxic Gas Diffusion Rule in a Real Environment Based on LSTM . *International Journal of Environmental Research and Public Health*. 2019. Vol. 16, No. 12. P. 2133. https://doi.org/10.3390/ijerph16122133
19. Viúdez-Moreiras D. Editorial for the Special Issue "Atmospheric Dispersion and Chemistry Models: Advances and Applications". *Atmosphere*. 2023. Vol. 14, No. 8. P. 1275. https://doi.org/10.3390/atmos14081275
20. Brandt M., Becker E., Jöhncke U. A weight-of-evidence approach to assess chemicals: case study on the assessment of persistence of 4,6-substituted phenolic benzotriazoles in the environment. *Environmental Sciences Europe*. 2016. Vol. 28, No. 4. https://doi.org/10.1186/s12302-016-0072-y
21. Фосфорна аварія під Ожидовом.2007. URL: https://w.wiki/72ff

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