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MODELING OF DISPERSION AND ASSESSMENT OF ECOLOGICAL CONSEQUENCES OF CHEMICAL POLLUTION DEPOSITION DURING TECHNOGENIC ACCIDENTS

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Abstract

The purpose of the study is to develop a comprehensive mathematical model to forecast and assess not only human impact zones but also the long-term ecological consequences of accidental HDS (Highly Dangerous Substances) releases. The model bridges the gap between classic civil defense tasks and the needs of environmental safety assessment, shifting the focus from calculating toxodose ($PC\tau_{50}$) to quantifying the mass loading of pollutants onto ecosystems (in kg/ha).

The methodology is based on combining two blocks. The first is an improved Gaussian atmospheric dispersion model which, unlike standard approaches, accounts for the surface roughness parameter (z_0), significantly impacting near-ground concentrations. The second, and key, block is a newly introduced methodology for calculating dry deposition, which uses the deposition velocity parameter (V_d). This allows for a transition from calculating air concentrations (C) to deposition flux (F) and cumulative deposition (D) onto soil and water. Modeling was performed for scenarios involving a 100-tonne ammonia release under various stability classes (A,D,F) and surface types.

The results demonstrate the critical importance of both parameters. First, sensitivity analysis proved that ignoring z_0 leads to significant errors in forecasting the cloud dispersion depth (up to an 88% difference under neutral conditions). Second, and most importantly, a quantitative assessment of the ecological impact was conducted. It was demonstrated that the cumulative deposition of ammonia (D) can reach 100…150 kg/ha, which is equivalent to 2…3 years of agricultural nitrogen application norms. This "shock loading" causes acute soil acidification. In water bodies, the calculated concentration (C_{water}) reaches 2.5…4.0 mg/L, which critically exceeds the MAC (Maximum Allowable Concentration) for fishery water bodies (<0.5 mg/L) and leads to mass mortality of biota.

Limitations and assumptions of the study include the use of parameterized V_d values and the application of a Gaussian model, which is an analytical approximation compared to CFD approaches.

The practical value of the work lies in creating a scientific and methodological tool that allows forecasting not evacuation zones, but zones that will require long-term ecological remediation (e.g., soil liming) and enhanced monitoring.

The scientific novelty and significance lie in the development of an integrated "atmospheric transport (z_0) – deposition (V_d) – ecological consequence (kg/ha, mg/L)" model, which provides a quantitative, rather than merely qualitative, assessment of environmental damage from chemical accidents.

Key words: technogenic accident, chemical pollution, ecological consequences, dry deposition, surface roughness, ammonia, eutrophication, mathematical modeling.

Problem statement

The current stage of industrial development is characterized by a high concentration of hazardous production facilities, the intensive use of highly toxic substances (HTS) in technological processes, and the growing scale of their transportation. As a result, the probability of accidents involving chemical contamination of the environment has sharply increased. Such incidents are often accompanied by the release of toxic compounds into the atmosphere, which can rapidly spread, forming primary and secondary contamination clouds and creating extensive impact zones. The consequences of these accidents may include not only immediate threats to human life and health but also long–term disruption of ecological balance, ecosystem degradation, soil and water pollution, as well as severe social and economic losses for the state and local communities. The mechanisms of this ecological impact are substance-specific. For instance, during accidental releases of ammonia (NH_3), its high solubility and subsequent deposition onto soil triggers an intensive nitrification process ($NH_3 \rightarrow NH_4^+ \rightarrow NO_3^-$). This leads to sharp acidification of soil solutions, the release of plant-toxic metals, and the degradation of soil biota. Upon entering water bodies, ammonium nitrogen (NH_4^+) acts as an excessive fertilizer, causing a rapid eutrophication process – "water bloom" (massive algal development). Subsequent decomposition of this biomass leads to dissolved oxygen depletion (hypoxia), which, combined with the direct toxicity of non-ionized ammonia (NH_3) to fish, causes mass mortality of aquatic fauna.

Unlike ammonia, chlorine (Cl_2) causes ecological damage due to its high chemical reactivity and potent biocidal effect. Upon contact with moist soil or vegetation, it instantly reacts with organic materials, destroying cell membranes. This leads to the mortality of beneficial soil microflora (bacteria, fungi), thereby disrupting key nutrient cycles. In plants, acute phytotoxicity is observed: chemical burns, chlorosis (yellowing), and necrosis (die-off) of the leaf surface, particularly in plants closer to the ground. The ingress of chlorine into water bodies has a direct lethal effect on aquatic vertebrates and invertebrates, causing rapid destruction of local ecosystems.

The relevance of this issue is further intensified by modern urbanization trends: increased building density,

proximity of industrial zones to residential areas, and the expansion of transportation and energy infrastructure intersecting with potentially hazardous sites. Under wartime conditions, as well as due to the deterioration of technical systems and violations of safety regulations, the probability of technogenic incidents involving HTS releases becomes especially critical. Therefore, ensuring environmental and technogenic safety at chemically hazardous facilities is not only an industry–specific task but also a national priority directly related to public protection, sustainable territorial development, and the preservation of ecological stability.

Existing global approaches to assessing chemical contamination can be conventionally divided into three categories: simplified engineering (Gaussian–type) models, which provide approximate estimates of pollution cloud parameters; physico–mathematical models, which account for phase transitions, meteorological conditions, and the physicochemical properties of substances but require substantial computational resources; and high–precision CFD (Computational Fluid Dynamics) models, which are scientifically robust but difficult to apply operationally by emergency services, environmental monitoring agencies, or local authorities. This creates a scientific and practical contradiction between the need for accurate forecasts and the requirement for computational efficiency and ease of implementation.

Special attention must be given to physiographic and meteorological factors that determine the dynamics of contaminant dispersion – including terrain relief, surface roughness, wind speed and direction, atmospheric stability, temperature, and humidity. Most existing models do not comprehensively account for these variables, leading to errors in estimating the boundaries of affected zones, inaccuracies in predicting the arrival time of toxic clouds at populated areas, and incorrect risk assessments for both the population and ecosystems. Insufficient spatial resolution also hinders the development of reliable risk maps and evacuation plans.

The scientific challenge lies in developing an integrated analytical model that combines physical and mathematical rigor with the ability to account for environmental heterogeneity and operate as a high–speed computational module. Such a model should provide not only reliable spatial–temporal forecasts of chemical contamination but also be compatible with geoinformation systems (GIS) and decision support systems (DSS). Its implementation would establish a foundation for automated monitoring, hazard assessment, evacuation planning, and environmental damage mitigation.

The practical significance of addressing this issue lies in enhancing the effectiveness of civil protection units, governmental agencies, and environmental authorities through rapid consequence forecasting, timely public warning, and informed decision–making during emergencies. The scientific significance consists in advancing the theoretical basis of chemical dispersion modeling, particularly by incorporating the surface roughness parameter (z_0) and evaluating its influence on the dynamics of toxic clouds. The development of such models aligns with the strategic directions of Ukraine's national policy on environmental safety and emergency response, as outlined in the Law of Ukraine "On National Security" and the Concept for Reforming the Civil Protection System.

Thus, the problem is defined by the urgent need to create a universal, scientifically grounded framework for forecasting and assessing chemical pollution in the environment, ensuring a balance between accuracy, speed, and adaptability. This approach would enable a transition from fragmented analytical assessments to integrated risk management within environmental and technogenic monitoring systems, enhance readiness for emergency response, and reduce potential environmental and socio–economic impacts.

Analysis of the recent researches and publications

Numerous domestic and international studies present a wide range of approaches to modeling accidental releases of hazardous chemical substances – from empirical schemes to highly accurate physics–mathematical models. Accidental leaks of highly toxic substances (HTS) remain among the most serious threats to technogenic and environmental safety, which makes the issue of accurate consequence forecasting especially relevant.

Significant progress in the development of physically based models is demonstrated by the work of Weger et al., who developed the CAIRDIO LES model for urban–scale dispersion simulations [1]. This model accounts for the influence of buildings, vegetation, and complex spatial geometries, producing realistic scenarios of pollutant transport. However, its main drawback lies in its high computational complexity, which limits real–time applications. Di Nicola et al. [2] proposed an improved method for incorporating surface roughness into urban dispersion models, enabling more accurate representation of built–up environments, though the approach has not yet been validated against real accident scenarios.

Lipták et al. [3] integrated a Lagrangian pollutant dispersion model into the ESTE system, used for predicting consequences in urban environments. The authors demonstrated that a balance between computational efficiency and accuracy can be achieved, although the model remains limited in its ability to represent turbulent effects. In a comparative study, Lacome et al. [4] analyzed different approaches to atmospheric modeling of chemical accidents across European countries. The results revealed considerable discrepancies depending on the selected models and parameterizations, emphasizing the need for harmonization of methodologies and unified evaluation criteria.

Field experiments, particularly Jack Rabbit II, play a decisive role in model verification and calibration. The results published by Gant et al. [5] presented chlorine dispersion experiments and a comparison of various dense gas models against real measurements. The findings showed that even the most advanced approaches do not always reproduce peak

concentrations accurately, confirming the need for further refinement of dispersion models.

From a practical standpoint, integrating dispersion modeling with risk management systems is of crucial importance. Hou et al. [6] analyzed over 500 chemical accidents in China between 2009 and 2018 and concluded that organizational factors – such as inadequate monitoring systems and response delays – are no less significant than technical ones. Meanwhile, Yoo and Choi [7] demonstrated the use of GIS tools for creating risk maps and optimizing evacuation plans in cases of hazardous chemical leaks in South Korea. Their study proved that spatial modeling can minimize evacuation time and reduce exposure of the population to toxic clouds; however, it did not address the physical processes underlying the formation of primary and secondary clouds.

Thus, the analysis of studies [1–7] shows that there exists a wide spectrum of effective but fragmented approaches – ranging from GIS–based and statistical methods to complex CFD computations. At the same time, all authors highlight the pressing need for a comprehensive, integrated model capable of combining spatial and temporal accuracy, accounting for meteorological and topographical conditions, and ensuring operational applicability within civil protection and environmental monitoring systems.

The further advancement of scientific studies has significantly expanded the understanding of dense gas dispersion mechanisms and the improvement of forecasting methods. One of the earliest practically validated solutions was presented by Spicer and Havens, who confirmed the capabilities of the DEGADIS model through full–scale field experiments [8]. This represented an important step toward the validation of dense–gas models for assessing impact zones. However, modern conditions have revealed the limitations of this model – it does not adequately reproduce the complex cloud dynamics in real urban environments. A further contribution to the development of engineering models was made by Fthenakis et al., who reviewed and refined the HGSYSTEM model [9]. Although widely used in regulatory documents for modeling dense–gas accidents, this system remains limited in its ability to account for complex terrain, built–up areas, and microclimatic effects.

In their classic works, Hanna and Chang [10] formulated acceptability criteria for evaluating dispersion model performance (FB, NMSE, FAC2, etc.), which remain fundamental in contemporary practice. However, their direct application to complex urban environments requires adjustments, since real turbulent transport processes often deviate from the statistical assumptions underlying these models. Modern CFD studies, particularly the work of Bellegoni et al. [11], have shown that even small infrastructure elements – such as perimeter walls, barriers, or technical structures – can significantly alter the trajectory of an LNG cloud. This confirms the necessity of detailed consideration of infrastructural and topographical factors in dispersion modeling.

Researchers also devote considerable attention to improving the representation of source conditions. Spicer et al. [12] proposed a simplified approach for representing the release source within the Jack Rabbit II experiments, which helped reduce uncertainty in initial parameters. Nevertheless, even with high–precision field measurements, the initial phase of cloud formation remains difficult to describe adequately, underscoring the need for developing adaptive boundary and initial conditions in models.

An important synthesis of experimental research results was presented by Fox et al. [13], who systematized findings from the Jack Rabbit II trials and compared multiple dispersion modeling approaches. The authors emphasized the critical importance of experimental data for model validation but also noted substantial discrepancies between model outputs, especially under conditions of strong turbulence.

In Ukrainian research, a valuable contribution was made by Amelina et al. [14], who analyzed scenarios of ammonia pipeline leaks and applied a mathematical model to calculate near–surface air concentrations. The significance of this work lies in its attempt to adapt international methodologies to Ukraine's national infrastructure, though further advancement requires integrating CFD modeling with GIS technologies to enhance spatial detail and realism.

Thus, studies [8–14] illustrate the gradual evolution of modeling approaches – from classical empirical and semi–empirical formulations to modern CFD–based systems supported by experimental validation. At the same time, the key challenge remains the development of a universal, integrated model that combines high computational accuracy, adaptability to real–world conditions, and the capability for rapid application within environmental monitoring and civil protection systems.

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.

A very important aspect is the study of the pollution cloud's impact on the environment. The primary methodological link connecting air concentration with impact on the ground is the dry deposition velocity parameter (V_d, in m/s). The work of Wesley and Hicks [20] is fundamental in this field, having proposed a parameterization of V_d based on the resistance analogy. Modern research refines these models for specific highly reactive gases. For example, the work by Sutton et al. [21] analyzes in detail the challenges in quantifying the deposition velocity specifically for ammonia (NH_3).

Concurrently, research on the direct ecological consequences has developed. The work of Erisman et al. [22] quantitatively describes how ammonia synthesis has changed the global nitrogen cycle and analyzes the processes of soil acidification. The link between the influx of excess nutrients (including ammonia) and the eutrophication of surface waters is discussed in detail in the classic review by Smith et al. [23].

Despite a significant number of works [1–23], a range of issues remains unresolved. Specifically, there is a lack of comprehensive approaches that would combine in one model both the precise calculation of atmospheric dispersion (accounting for z_0) and the subsequent calculation of ecological impact through deposition modeling (V_d). There is a need to develop a unified approach that combines the accuracy of physically-based models, the ability to account for topographical and meteorological conditions, and also ensures high performance for use in environmental safety monitoring and management systems.

Statement of the problem and its solution

The aim of the work is to develop a comprehensive mathematical model for assessing the ecological consequences of accidental HDS (Highly Dangerous Substances) releases. The model combines an improved calculation of atmospheric dispersion (which accounts for the roughness parameter z_0) with a methodological block for modeling dry deposition (V_d).

The final aim is the quantitative assessment of toxicant mass loading on underlying ecosystems (kg/ha) for forecasting zones of potential ecological damage (soil acidification, surface water pollution) and providing a scientific basis for remediation measures. The object of the study is the process of technogenic environmental pollution resulting from accidental HDS releases (particularly ammonia and chlorine) at chemically hazardous facilities. This process is viewed as a single chain of physicochemical phenomena, which includes the initial atmospheric transport of the toxic cloud (accounting for z_0), the subsequent dry deposition (V_d) of pollutants onto the underlying surface (soil, water), and, as a final result, the subsequent impact on ecosystem components with the emergence of secondary ecological consequences, such as acidification, eutrophication, and biocidal effects.

The research methodology is based on a comprehensive systemic analysis of the physical processes accompanying an accidental HDS release, from the moment of cloud formation to its impact on the environment. Mathematical modeling includes two stages: first, the calculation of atmospheric dispersion based on modified Gaussian models, which describe the dispersion of primary and secondary clouds in the surface air layer. This part of the model correctly accounts for the atmospheric stability class (according to Pasquill) and the impact of surface roughness by introducing the parameter (z_0), which allows calculating the field of near-ground concentrations $C(x,y,z)$ and traditional indicators (dispersion depth, $PC\tau_{50}$). Second, the modeling of ecological impact, which uses the calculated C field as input data based on the dry deposition velocity (V_d). This enables the quantitative assessment of pollutant mass loading onto soils and water (D, in kg/ha). The model allows for variability in input data for hypothetical scenarios: quantity of substance (100…200 t), surface type (flat, grassy, urban), wind speed, and atmospheric conditions. Calculations were performed using analytical modeling tools. Unlike approaches focused exclusively on the operational needs of civil defense, this methodology shifts the emphasis to ecological monitoring, environmental impact assessment, and the scientific substantiation of remediation measures for affected territories.

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.

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) and area (S_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.

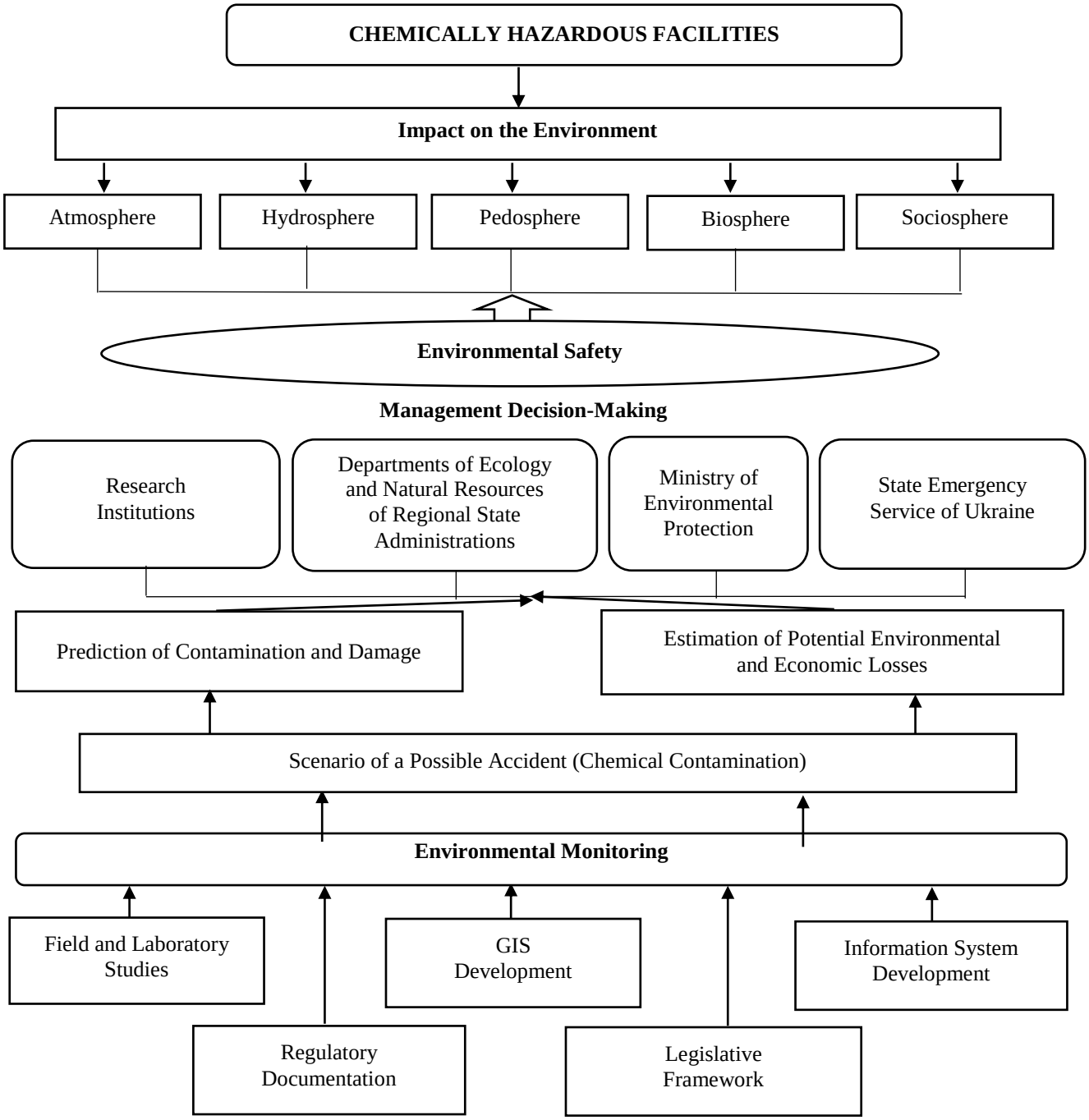

Figure 1 – Structural diagram of the environmental safety assurance system in case of chemical contamination resulting from accidents at chemically hazardous facilities

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 (S_d) using the following formula:

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

where R_d 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:

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

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:

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

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:

$$Q_1 = \frac{Q \cdot C_v \cdot (t - t_k)}{\lambda}, \quad (4)$$

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:

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

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 – for $1.6 < u \leq 3.5$ m/s – for $3.6 < u \leq 6.5$ m/s	 $9 \cdot 10^{-2}$ $6.7 \cdot 10^{-2}$ $3.7 \cdot 10^{-2}$
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:

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

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 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:

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

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:

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

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:

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

where:

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

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

$$E = 0.041 \cdot \frac{u \cdot M}{d_{spill}^{0.14} \cdot T_u} \cdot \exp\left[\frac{\lambda \cdot M}{R}\left(\frac{1}{T_k} - \frac{1}{T_u}\right)\right], \quad (13)$$

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:

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

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].

To analyze the environmental impact, it is necessary to assess the concentration field $C(x,y,z)$ and, most importantly, the amount of substance that deposits on the underlying surface (the environment). The main parameter is the dry deposition velocity (V_d, in m/s), which integrates the physicochemical properties of the gas and the surface characteristics (vegetation, soil, water). The deposition flux (F) and cumulative deposition (D) are calculated using the formulas:

$$F(x,y) = V_d \cdot C(x,y,z=1), \quad (14)$$

where $C(x,y,z=1)$ is the near-ground concentration, calculated based on the Gaussian model, which is the basis for formulas (6) and (10));

$$D(x,y) = F(x,y) \cdot t_{exp}, \quad (15)$$

where t_{exp} is the cloud passage time over the point).

For highly reactive and soluble gases, such as ammonia, V_d is significant and can range from 0.01 to 0.03 m/s, leading to intensive mass transfer from the atmosphere to the soil and water.

To demonstrate the operation of the improved model (formulas 5–8) and its sensitivity to the key parameter – surface roughness (z_0) – a series of calculations was performed. The results, presented in Table 2, constitute a sensitivity analysis of the model. They show how the calculated dispersion depth of the primary cloud (G_1) changes depending on both the stability category and the surface type (z_0).

Table 2 – Sensitivity analysis of the calculated dispersion depth of the primary cloud (G_1, km) to the roughness parameter (z_0) and atmospheric stability category. (Scenario: Ammonia, Q = 100 t, wind speed u = 3 m/s)

Stability Category (by Pasquill)	z_0 = 0.01 m (Flat field, snow)	z_0 = 0.1 m (Shrubs, grass)	z_0 = 0.9 m (Urban area)
A (Strong instability)	4.5 km	6.2 km	8.5 km
D (Neutral conditions)	13.0 km	17.8 km	24.5 km
F (Strong stability)	35.2 km	48.5 km	66.7 km

The presented data clearly demonstrate that ignoring the z_0 parameter leads to critical errors in forecasting. For example, under neutral conditions (D), the cloud dispersion depth over an urban area (z_0 = 0.9 m) is 88 % greater (24.5 km) than over a flat field (z_0 = 0.01 m) (13.0 km). This is explained by the fact that high roughness slows down the near-ground wind (reducing u'), allowing the cloud to maintain a hazardous concentration longer and disperse over a greater distance.

Modeling of ammonia (NH_3) deposition for the scenario (Q = 100 t, stability D) showed that in zones adjacent to the accident site (up to 5…7 km downwind), the cumulative deposition (D) can reach 100…150 kg/ha, converted to pure nitrogen. This value is equivalent to 2-3 annual agronomic norms for nitrogen fertilizer application. Such “shock loading” causes acute chemical burns to vegetation, extremely intensive soil acidification due to rapid nitrification, mortality of soil microflora, and the release of toxic metals into the soil solution.

Modeling of the cloud passage (Scenario: Ammonia, Q = 100 t) over a hypothetical water body showed that deposition (D) leads to the rapid dissolution of ammonia. The calculated resulting concentration of ammonium nitrogen (C_{water}) in the upper water layer can reach 2.5…4.0 mg/L. This value critically exceeds the maximum allowable concentration (MAC) for fishery water bodies (which for ammonium nitrogen is < 0.5 mg/L). The consequences include the direct toxicity of non-ionized ammonia (NH_3) to fish, rapid eutrophication (“water bloom”), and mass mortality of fish and other aquatic biota.

Conclusions

Within the scope of the study, a comprehensive mathematical model was developed for forecasting and assessing the consequences of accidental HDS releases, which bridges the gap between classical atmospheric dispersion modeling and the needs of ecological safety assessment. Unlike approaches focused solely on calculating impact zones for the population, the proposed model combines: an improved calculation of atmospheric transport, which accounts for the influence of surface roughness (z_0) on near-ground concentrations, and a methodological block for the quantitative assessment of dry deposition (V_d) of pollutants onto soils and water bodies.

It has been proven that the z_0 and V_d parameters are critical for an adequate assessment of ecological damage. Sensitivity analysis demonstrated that ignoring surface roughness (z_0) leads to significant errors in determining the cloud dispersion depth (up to 88 % under neutral conditions). At the same time, the V_d parameter is key for the transition from calculating concentrations (in mg/m³) to mass loading on ecosystems (in kg/ha).

The main scientific and practical result of the work is the quantitative assessment of ecological impact scenarios. It was demonstrated for the first time that under typical accident scenarios (a release of 100 t of ammonia), cumulative deposition can reach 100…150 kg/ha, which is equivalent to 2-3 annual agronomic norms. This “shock loading” leads to acute soil acidification and exceeds the MAC (Maximum Allowable Concentration) for fishery water bodies (up to 4 mg/L), causing mortality of aquatic biota.

Thus, the practical value of the model lies in its ability to forecast zones that will require long-term ecological remediation and monitoring.

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МОДЕЛЮВАННЯ ПОШИРЕННЯ ТА ОЦІНКА ЕКОЛОГІЧНИХ НАСЛІДКІВ ОСІДАННЯ ХІМІЧНОГО ЗАБРУДНЕННЯ ПРИ ТЕХНОГЕННИХ АВАРІЯХ

Мета дослідження полягає у розробці комплексної математичної моделі для прогнозування та оцінки не лише зон ураження населення, але й довгострокових екологічних наслідків аварійних викидів СДОР. Модель усуває розрив між класичними задачами цивільного захисту та потребами оцінки екологічної безпеки, переносячи акцент з розрахунку токсодози ($PC\tau_{50}$) на кількісну оцінку масового завантаження забруднювачів на екосистеми (в кг/га).

Методологія ґрунтується на поєднанні двох блоків. Перший – удосконалена Гаусова модель атмосферної дисперсії, яка, на відміну від стандартних підходів, враховує параметр шорсткості підстильної поверхні (z_0), що суттєво впливає на приземні концентрації. Другий, і ключовий, блок – нововведена методологія розрахунку сухого осідання, що використовує параметр швидкості осідання (V_d). Це дозволяє перейти від розрахунку концентрацій у повітрі (C) до потоку осідання (F) та сукупного осідання (D) на ґрунт та воду. Моделювання проводилось для сценаріїв викиду 100 т аміаку за різних класів стійкості (A, D, F) та типів поверхні.

Результати демонструють критичну важливість обох параметрів. По-перше, аналіз чутливості довів, що ігнорування z_0 призводить до значних помилок у прогнозуванні глибини поширення хмари (до 88% різниці за нейтральних умов). По-друге, що є головним, проведено кількісну оцінку екологічного впливу. Продемонстровано, що сукупне осідання аміаку (D) може сягати 100…150 кг/га, що еквівалентно 2-3 річним агрономічним нормам. Таке "шокове" навантаження спричиняє гостру ацидифікацію ґрунтів. У водних об'єктах розрахована концентрація (C_{water}) сягає 2.5…4.0 мг/л, що критично перевищує ГДК для рибогосподарських водойм (< 0.5 мг/л) і призводить до масової загибелі біоти.

Обмеження та припущення дослідження включають використання параметризованих значень V_d та застосування Гаусової моделі, яка є аналітичним наближенням порівняно з CFD-підходами.

Практична цінність роботи полягає у створенні науково-методичного інструменту, який дозволяє прогнозувати не зони евакуації, а зони, що потребуватимуть довгострокової екологічної ремедіації (наприклад, вапнування ґрунтів) та посиленого моніторингу.

Наукова новизна та значимість полягає у розробці інтегрованої моделі «атмосферний транспорт (z_0) – осідання (V_d) – екологічний наслідок (кг/га, мг/л)», яка забезпечує кількісну, а не лише якісну, оцінку екологічного збитку від хімічних аварій.

Ключові слова: техногенна аварія, хімічне забруднення, екологічні наслідки, сухе осідання, шорсткість поверхні, аміак, евтрофікація, математичне моделювання.

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