This study's object is the process of monitoring and managing environmental risks in railroad accidents involving transportation of hazardous goods.

A problem has been identified, related to the absence of a single, holistic approach to risk management during transportation, which would integrate methods of spatial-temporal forecasting with a formal assessment of uncertainty. A mathematical model has been suggested that makes it possible to process and analyze data acquired from a mobile automated air quality monitoring system (MAAQMS). The established dependences laid the foundation for the machine learning and statistical analysis model used in the operation of a simulation model (SM) of monitoring and managing environmental risks.

The simulation model, unlike similar ones, has been developed in the following directions:

1) representation of data and processing of omissions;

2) construction of probabilistic risk maps taking into account uncertainty and calibration of forecasts of the state of environmental pollution at the accident site;

3) adaptation of the model in case of data variability at the accident site;

4) multi-criteria optimization of management decisions.

In summary, the simulation model reported in this study provides decision-makers with the prospect of not only predicting the probability of exceeding the maximum permissible concentrations (MPC) of pollutants on the railroad infrastructure but also forming confidence risk maps.

Unlike similar solutions, the constructed model is ML-oriented. In other words, the prediction of risk level is built in a spatial-temporal statement on a railroad network graph taking into account data received from MAAQMS. The adequacy of the model was confirmed by achieving the area under the ROC curve (AUC = 0.990) and the PR analysis indicator (AP = 0.940)

Keywords: simulation model, environmental risk management, uncertainty, hazardous goods, rail transport

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CONSTRUCTION OF A SIMULATION MODEL FOR MONITORING AND MANAGING ENVIRONMENTAL RISKS IN RAILROAD TRANSPORTATION ACCIDENTS INVOLVING HAZARDOUS GOODS

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1. Introduction

Railroad transport is a key link in the logistics system of many countries [1]. In the post-Soviet countries, railroads provide transportation of huge volumes of cargo, among which a significant share is hazardous goods. Transportation of such substances as ammonia, chlorine, liquefied hydrocarbon gases, and petrochemical products is associated with increased risks [2].

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Accidents on railroads during the transportation of hazardous goods lead to catastrophic consequences. These include chemical pollution of the environment, damage to ecological systems, etc. In addition, such accidents in some cases pose a direct threat to the life and health of people living near the railroad infrastructure [3].

However, existing monitoring and response systems for such incidents face a number of problems and do not provide proper management of environmental risks [4]. Stationary environmental control posts have limited coverage and cannot promptly assess the situation at any point along the vast railroad network. At the same time, standard procedures for responding to accidents with hazardous goods are not flexible enough since they do not take into account changing conditions. The latter include the meteorological situation, topography of the area, and the specific properties of a particular dangerous cargo, etc.

Thus, taking into account the above problems, the task of designing intelligent hardware and software systems capable of monitoring, analyzing, forecasting, and managing environmental risks in railroad transportation becomes relevant. In particular, the use of mobile automated monitoring systems (MAAQMS), equipped with modern sensors and integrated with machine learning (ML) methods, opens up new prospects in this direction [5, 6].

Thus, the relevance of this issue is predetermined by the need to devise an effective model as a tool for monitoring and managing environmental risks in accidents with hazardous goods during railroad transportation. Such a model should allow for multi-criteria optimization of management decisions through processing data from mobile sensors (MAAQMS), risk prediction on the railroad network graph, as well as adaptation to sensor drift. This will make it possible to move from passive registration of consequences to proactive, scientifically based emergency management of railroad transportation.

2. Literature review and problem statement

Risk analysis and management in the transportation of hazardous goods has been the subject of numerous studies. Some of them consider the application of machine learning (ML) methods. In [7], approaches in this area are systematized but the paper did not cover advancements in the field of graph neural networks. In [8], the authors use ML to analyze the severity of the consequences of incidents that have occurred. However, the disadvantage of study [8] is the lack of predictive ability for assessing and managing risks in real time. Similarly, the framework for risk assessment proposed in [9], although methodologically valuable, is a conceptual structure, not an implemented model. A likely reason is, as the authors of [9] note, the insufficient level of model testing for various components of the transportation system.

The desire to design operational response systems has led to the development of models for assessing risks in real time. Thus, in [10], the authors used a hybrid GRU-DNN model for risk assessment. However, they focused on time dependences. Work [10] did not take into account the complex topology of the transportation network. In [11], the authors outlined a methodology for assessing risks in the transportation of hazardous goods. However, study [11] did not take into account the work with data from pollution sensors at the sites of accidents with hazardous goods, which was due to the lack of real source data. In [12], the authors use a fuzzy Bayesian network to describe risks. However, such a model faces difficulties in scaling to large and complex heterogeneous networks in transport since the parameters of this model are more static or cannot take into account the need for rapid data updates. Work [13] describes a platform for optimizing hazardous goods transportation routes but its main function is planning, not dynamic monitoring and risk prediction in the event of incidents. This is due to the adopted initial research objectives [13]. Work [14] focuses directly on railroad transportation. The authors propose models for describing incidents involving the transportation of hazardous goods based on data analysis. The disadvantage of this approach is that study [14] is more focused on the analysis and classification of incidents. That is, the model proposed in work [14] is not focused on building a predictive spatiotemporal model of the spread of pollutants at the scene of an accident involving hazardous goods.

Therefore, some authors have recognized spatiotemporal graph neural networks (STGNN) as a promising tool for solving such problems. Studies [15, 16] confirmed that STGNN is an effective method of predictive analysis in transportation systems. However, those works were of a survey nature, which is associated with the task of theoretical research set by the authors. In [17, 18], the authors demonstrated the potential of this approach for tasks similar to monitoring the spread of hazardous goods. However, the disadvantage of [17, 18] is the assumption about the high quality of input data. And the issues of reliability of the models themselves, information systems, and data sources were ignored, since the researchers conducted testing on a simplified set of time series data.

The key problem of such tasks is the uncertainty of both the data from the scene of an accident with hazardous goods and the model or control system itself. In [19], the authors draw a clear distinction between the aleatory and epistemic components. However, this differentiation has not been reflected in applied models for assessing the risks of transporting hazardous goods.

It is worth noting that the primary source of uncertainty in the data is the measuring devices themselves. Works [20, 21] convincingly showed that low-budget sensors used in mobile environmental monitoring systems are prone to significant drift. Accordingly, they require frequent calibration, demonstrating unstable operation in difficult situations. The authors of [20, 21] considered the problem of sensor calibration, machine learning methods used during calibration, and various ways to assess the effectiveness of calibration models. However, studies [20, 21] were limited only to stating this problem and identifying the most critical research issues in this area, which are associated with the inconsistency of studies, the lack of sufficiently large data sets and effective models.

Our review of the literature [17–21] revealed a significant gap in the considerations regarding models for monitoring and managing environmental risks in railroad transportation accidents involving hazardous goods. On the one hand, there are powerful predictive architectures (STGNN) [15, 16], and on the other hand, researchers face practical problems of uncertainty [17, 18, 20, 21] and sensor degradation [11, 20, 21]. This aspect is completely ignored in most theoretical models of risk prediction at the scene of accidents with hazardous goods. This calls into question their applicability as part of the corresponding simulation models under real operating conditions of railroad transportation when carrying hazardous goods. An option to overcome these difficulties may be the integration of spatiotemporal forecasting methods with formal uncertainty assessment and mechanisms for online adaptation to sensor drift. It is these approaches that are proposed to be used in works [20, 21]; however, the authors did not propose a specific solution tool, appealing to the lack of databases and effective models. In addition, the proposals for solving this problem did not contain mechanisms for taking into account uncertainty [19] when modeling in the process of assessing the risks of transporting hazardous goods. All this directly affects the quality of forecasts at the scene of accidents with hazardous goods.

The above allows us to argue that it is advisable to conduct a study aimed at devising a single, holistic approach that would integrate spatiotemporal forecasting methods with formal uncertainty assessment and mechanisms for online adaptation to sensor drift. This should occur within the framework of a single decision support system at the scene of railroad transportation accidents involving hazardous goods, which could be implemented in the form of an effective simulation model.

3. The aim and objectives of the study

The purpose of our study is to build a simulation model for monitoring and managing the environmental situation that arose as a result of a railroad transportation accident involving hazardous goods. This will make it possible, taking into account the environmental consequences of the accident, available resources, and the purpose of taking actions to eliminate the environmental disaster, to carry out an adaptive interpretation of strategic decisions regarding the response to environmental risks.

Research objectives:

– to build a mathematical model of automated monitoring of environmental risks, based on the formalization of the influence of aleatory and epistemic uncertainty on the process of assessing environmental risks at the scene of railroad transportation accidents;

– to develop a functional model and algorithm of the environmental risk monitoring and management system for multi-criteria decision-making support;

– to perform experimental testing of the proposed simulation model.

4. The study materials and methods

The object of our study is the process of monitoring and managing environmental risks in the event of railroad transportation accidents involving hazardous goods.

The principal hypothesis of the study assumes that constructing and implementing a simulation model of monitoring and managing environmental risks on a railroad network could lead to a prompt response to an emergency with minimal consequences.

The basic assumption of our study is that ROC analysis, PR analysis, and Pareto front evaluation of non-dominant solutions could confirm the study's hypothesis in simulation experiments. The simplification of the study is the adoption of only three mutually contradictory criteria for modeling in the simulation model (time reduction, cost increase, damage increase).

The methodological foundation underlying our simulation model is the relevant works in the field of ML, environmental risk analysis, and intelligent sensor networks [7–18]. However, unlike previous studies reviewed earlier in [5, 6], the proposed model integrates the tasks of calibrating the MAAQMS sensors, constructing pollution maps, and optimizing the observation schedule into a single mathematical model. A prototype of MAAQMS has been proposed, which is a modular device based on Arduino Nano and ESP8266 microcontrollers. MAAQMS contains sensors: CCS811, Si7021, BME280, GP2Y1010AU0F, as well as a Geiger counter for monitoring ionizing radiation. Additionally, meteorological parameter sensors were installed – temperature, humidity, pressure, wind speed. Data transmission is carried out via the MQTT protocol using a Wi-Fi or GPRS module (GSM/GPRS/GNSS/Bluetooth). Classical graph theory was used to construct a mathematical model of automated monitoring of environmental risks in accidents with hazardous goods. The dependence proposed in [22] for describing the modified focal loss function, taking into account temporal consistency and the semi-tutoring technique, was improved by taking into account the weights of sensitive zones. A spatial-temporal machine learning model [23] was used for the purposes of modeling environmental risk management scenarios. In this case, uncertainties that are distributed according to the classical approach into aleatory and epistemic were taken into account. The classical Pareto set approach was used to solve the optimization problem, which determines a set of strategies that cannot be improved according to all accepted criteria simultaneously. The software implementation of the simulation model of environmental risk monitoring and management was carried out on the basis of Python.

Simulation experiments on the performance of the mathematical model were performed using synthetic data. In the task of automated monitoring and analysis of the risks of accidents with hazardous goods, a spatiotemporal grid was used to measure the data. That is, at each time point t, the values of various features are recorded. These features include air quality sensor readings, meteorological characteristics of OKS, cargo parameters, and its hazard class [1]. In addition, the features include binary or categorical information about the fact of exceeding the maximum permissible concentration (MPC) on specific sections of the railroad infrastructure using the example of Ukraine and Kazakhstan. The effectiveness of the results of simulation experiments was assessed by ROC analysis and PR analysis. In particular, the adequacy of the simulation model was confirmed by achieving a high area under the ROC curve ($AUC = 0.990$), PR analysis indicator ($AP = 0.940$). These values confirm that the simulation model is able to effectively identify events and minimize the number of false positives. The Pareto front formed during the experiment has no overlapping points, that is, it consists of a set of non-dominant management decisions.

5. Construction of a simulation model for monitoring and managing environmental risks in accidents involving hazardous goods

5. 1. Construction of a mathematical model for automated monitoring of environmental risks

A mathematical model for automated monitoring of environmental risks in accidents with hazardous goods should be constructed using graph theory as a basis. Let N be the number of spatial nodes in the railroad transport infrastructure, including components for monitoring the state of the environment. Then F is the number of taken into account signs of changes in the state of the environment (exceeding MPC or other). Therefore, for time point t, it is necessary to determine the observation matrix $X_t \in R$^$(N \times F)$, where the rows correspond to spatial nodes, and the columns to attributes. For this purpose, it is necessary to introduce additional variables:

– a vector of binary indicators $y_t \in \{0, 1\}^N$, reflecting the fact of the presence or absence of exceeding MPC at the corresponding points, including places of railroad transportation accidents involving hazardous goods;

– observability mask $M_t \in \{0,1\}^{(N \times F)}$, which registers which specific features, including those obtained from mobile sensors (MAAQMS), are currently available (that is, are registered by the sensor and transmitted to the computing module). Then, using a binary approach: 1 – the observed feature is present, 0 – an omission.

Formally, this process can be represented by the following equation

$$X_t \in R^{N\times F},\ \ y_t \in \{0,1\}^N,\ \ M_t \in \{0,1\}^{N\times F}. \tag{1}$$

The proposed prototype of MAAQMS is a modular device based on the Arduino Nano and ESP8266 microcontrollers. The MAAQMS prototype provides autonomous collection, primary processing, and transmission of telemetry to the server core of the control system. The system contains sensors CCS811, Si7021, BME280, GP2Y1010AU0F, as well as a Geiger counter for monitoring ionizing radiation. Additionally, meteorological parameter sensors are installed – temperature, humidity, pressure, wind speed. Data transmission is carried out via the MQTT protocol using a Wi-Fi or GPRS module (GSM/GPRS/GNSS/Bluetooth).

Since the data from MAAQMS are characterized by incompleteness, the task of correctly processing the gaps arises. For example, incompleteness occurs due to temporary sensor failures or instability of the data transmission channel. Thus, there is a need to introduce the observation operator – $\widehat{X}_t$. This operator combines the actual received data, the recovered values of the missing components, and the additive noise that describes the random perturbations in the data transmission. Then the observation operator model will take the following form

$$\widehat{X}_t^1 = M_t \odot X_t + (1-M_t)\odot \widehat{X}_t + \varepsilon_t, \tag{2}$$

where $\odot$ is the element-wise product of matrices; $\widehat{X}_t$ is the estimate of missing features obtained using specialized imputation algorithms [24] (autoencoders or graph imputators); ε_t is the noise component that models random errors in MAAQMS measurements.

Accordingly, the observation operator (2) provides the basis for further application of machine learning methods. That is, each observed value $X_t \in R^{(N \times F)}$ should be treated either as a real measurement or as an estimate supplemented by probabilistic uncertainty.

Then the next step in such an analysis will be to take into account the spatial structure of the railroad network. It should be assumed that such a structure is naturally described in the form of a graph. The nodes of the graph correspond to spatial objects. These are the locations of sensors, both MAAQMS and stationary ones. And the edges of the network are their topological connections with density (E).

Then, taking into account the introduced adjacency matrices A and D powers, the normalized Laplacian of the railroad network graph L will take the following form

$$L = I - \frac{1}{\sqrt{D}}\cdot A\cdot\frac{1}{\sqrt{D}}, \tag{3}$$

where L is the normalized Laplacian of the railroad network graph; A is the adjacency matrix of the railroad network graph; D is the power matrix (the sum over the rows of matrix A).

Accordingly, the railroad network graph and the smoothness by topology are determined from the following equation

$$L_{graph} = \sum\nolimits_t tr\left(\left(HZ_t\right)^T \cdot L\left(HZ_t\right)\right), \tag{4}$$

where Z_t – hidden embeddings of railroad network nodes at time t; H – training linear projector (H is the head of the model on the embeddings).

Functional (4) should be minimized in the process of training the model. With the help of the obtained value of L_{graph}, the consistency of embeddings of neighboring nodes of the railroad transport graph is "stimulated". The L_{graph} value reflected the natural proximity of environmental conditions on adjacent sections of the railroad infrastructure. After the data structure is formalized and the topology of the railroad network is taken into account, the main task arises – predicting environmental risks at the scene of a railroad transportation accident involving hazardous goods. In other words, under the conditions of an accident with hazardous goods, it is not only necessary to record current MPC exceedances. In addition, as a mandatory element of modeling based on ML methods, to predict the probability of such exceedances on sections of the railroad infrastructure in the future.

To this end, a spatiotemporal machine learning model [23] should be introduced into the training algorithm. Such a model, as shown in [25, 26], is based on the sequence of observations $\tilde{X}_{1:t}$, the topology of graph A, and additional exogenous factors. The latter include weather conditions and the type of cargo being transported. It should be noted that A in the model means the adjacency matrix of the railroad network.

Then the probability of exceeding MPC on horizon τ should be specified as follows

$$\widehat{\rho}_{1:t} = \sigma\left(f_0\left(\tilde{X}_{1:t}, A, \zeta_{1:t}\right)\right),\ \widehat{\rho}_{t+\tau} \in \left[0,1\right]^N, \tag{5}$$

where f_0 is a parameterized model (a graph recurrent neural network predictor is used); $\zeta_{1:t}$ is exogenous factors (that is, weather conditions and type of cargo transported, etc.); σ is a sigmoidal function [26]; $\widehat{\rho}_{t+\tau}$ is a vector reflecting the probability of exceeding MPC for each node of the railroad network graph during monitoring using MAAQMS; τ is the forecast horizon in time.

In the further analysis, a discrete time step is taken as the time point t, counted from the moment of the emergency event ($t = 0$). The time horizon τ in equation (5) corresponds to the forecast of the state of the air environment τ steps ahead, that is, within the response period of the mobile automated air quality monitoring system (MAAQMS) after the event. The time intervals t are formed in accordance with the telemetry update cycle, which in the designed MAAQMS prototype is 30 seconds. For a 10-minute observation interval, 20 discrete observation points are taken. This provides the synthesis of time series of concentrations of harmful substances.

In this problem, for the purposes of modeling using ML, it is necessary to predict the exceedance of MPC at the scene of a railroad accident during the transportation of hazardous goods several steps ahead.

When implementing the model training procedures, it is advisable to take into account the imbalance of classes (*Pr*). That is, it should be assumed that situations with exceeding

MPC as a result of accidents during the transportation of hazardous goods by railroad are quite rare. If we compare them with normal conditions, then according to statistics, their number is relatively small. And, accordingly, different significance of spatial zones will be obtained. Thus, a modified focal loss function should be used. Moreover, this function (6) is supplemented with the weights of sensitive zones $w_v > 0$.

The dependences used further in the model to describe the weighted focal loss function (6), temporal coherence (7), and the semi-tutoring technique were first proposed in [22]. The dependence for describing the modified focal loss function, taking into account [22], which is supplemented by the weights of the sensitive zones, takes the following form

$$L_{cls} = \sum_{t,v} w_v \begin{bmatrix} -\alpha \cdot y_t[v] \cdot (1-\hat{p}_t[v])^{\gamma} \times \\ \times \log \hat{p}_t[v] - (1-\alpha) \cdot (1-y_t[v]) \times \\ \times \hat{p}_t[v]^{\gamma} \cdot \log(1-\hat{p}_t[v]) \end{bmatrix}, \tag{6}$$

where $w_v > 0$ are weighting factors for zones that have ecological or social significance. These can be water protection areas, urban development, etc. In other words, the so-called sanitary zones; α, γ are hyperparameters that regulate the contribution of "positive" examples and the penalty for "difficult" cases for classification. It is assumed that $\alpha \in (0,1)$ and $\gamma \geq 0$.

The novelty in expression (6) is the fact that the parameter $w_v > 0$ for "sensitive zones" from the point of view of ecological monitoring at the site of railroad accidents with hazardous goods is introduced into the model. This allows for further theoretical calculations and simulation experiments when using ML to predict environmental risks for the railroad network.

To increase the stability of forecasts, it is necessary to introduce an additional criterion of temporal consistency L_{temp}. This criterion will reduce the probability of sharp fluctuations in forecasts that are not due to real changes in the environmental situation on the railroad network, unlike [27, 28]. This can be achieved by matching forecasts with predictions from previous steps. The temporal consistency criterion can be calculated from the formula

$$L_{temp} = \sum_{t,v} \left\| \hat{p}_t[v] - q_{\phi}\left(\hat{p}_{t-1}[v]\right), \zeta_t \right\|_2^2, \tag{7}$$

where q_{ϕ} is the regression model of the trend.

However, as with any risk assessment tasks (economic, environmental, informational, etc.), including risks associated with environmental factors, the data may be incomplete. In addition, part of the information is unlabeled in such tasks. Then, according to [28], the consistency criterion under stochastic augmentations can be used in the calculations. In this case, the model predictions for the original and modified data should remain close, that is

$$L_{cons} = \sum_t E_{\tau} \left[\left\| \hat{p}_t - \hat{p}_t^{(\tau)} \right\|_2^2 \right], \tag{8}$$

where T is a set of stochastic data transformations. Or adding noise, a random subsampling of sensors for MAAQMS; E_{τ} is the mathematical expectation – the average value of random transformations from the set T. That is, E_{τ} is the value averaged over different random augmentations of MPC at the accident site; $\hat{p}_t$ – model predictions on "clean" data; $\hat{p}_t^{(\tau)}$ – predictions on data to which random augmentation T was applied during ML.

In order for the MAAQMS sensor readings to be correctly processed during ML, it is advisable to consider the subtask of correct calibration of probabilities. For this purpose, the conformal forecasting method should be used. In particular, the event exclusion should be introduced into the ML model, as well as the quantile estimate for the calibration set

$$s_i = 1 - \hat{p}_t, \; \hat{q}_{1-\alpha} = Quantile_{1-\alpha}\left(\{s_i\}_{j \in C}\right), \tag{9}$$

where C is the calibration buffer, which is a sliding window based on the latest observations of environmental pollution parameters using MAAQMS; s_i is the exclusion of "exceedance".

Next, based on the calibration results, a confidence region for exceeding the MPC is formed for the current time t

$$A_{\alpha}(t) = \left\{ v : \hat{p}_t[v] \geq 1 - \hat{q}_{1-a} \right\}, \; R_t = \sum_v w_v \hat{p}_t[v], \tag{10}$$

where $A_{\alpha}(t)$ is the set of nodes of the railroad network, which are classified as risk zones with a confidence level of $1 - \alpha$; R_t is the integral risk indicator for the entire network, taking into account the weights of the zones.

For the completeness of the analysis, it is necessary to divide uncertainty into alethoric and epistemic. Alethoric refers to uncertainties according to [19], associated with the randomness of observations using MAAQMS. And epistemic uncertainties are those associated with the uncertainty of knowledge of the presented model. Formally, this can be represented as follows:

$$H_t[v] = -\sum_{c \in \{0,1\}} \hat{p}_t^c[v] \log \hat{p}_t^c[v],$$

$$v_t[v] = Var_{m=1,\ldots,M} \hat{p}_t^{(m)}[v], \tag{11}$$

where H_t is the prediction entropy [19]; v_t is the variance over the dropout/ensemble.

Summarizing dependences (5) to (11), it should be noted that they formalize the ML subproblems. Such decomposition provides the prospect of their interpretation into the ML model with subsequent implementation both as a simulation model and as a computational kernel block for MAAQMS.

In other words, the aleatory uncertainty $H_t[v]$, modeled using (11), reflects the natural randomness of the environment in the course of ML. Thus, in the problem of analyzing the parameters of the state of environmental pollution at the accident site, $H_t[v]$ shows that even with completely correct data, there is always a probability of random fluctuations in the concentration of pollutants. In particular, this can occur due to the influence of turbulent air flows or unpredictable wind gusts at the accident site.

Epistemic uncertainty $v_t[v]$ in expression (11) is associated with the lack of knowledge of the ML model. In other words, in this problem it will manifest itself, for example, if the MAAQMS sensor operates unstable. This can occur as a result of the fact that data in a given area is collected extremely rarely, or the ML algorithm is not trained on a similar situation. For example, there is a rare combination of weather conditions and the type of dangerous cargo. The less data for ML and the larger the scale of the unusual situation at the accident site, the higher the epistemic uncertainty.

With the built ML model, two issues can potentially arise during the operation of the MAAQMS:

– the so-called sensor drift occurs due to wear of electrochemical elements and causes an increase in epistemic uncertainty if no correction measures are taken;

– change in data modes – such a problem is a consequence of situations that are not typical for the training sample.

Therefore, further, based on the logic of applying ML methods, the model should be expanded to dependences (12), (13), (15). These dependences describe, respectively:

– sensor drift and online calibration procedure (for modern sensors, a priori is used);

– a mechanism for adapting model parameters when changing the mode;

– statistical functionality for event detection (for example, when an event should be understood as a sudden release of a pollutant from sources other than railroad transport).

These dependences (12), (13), (15) together provide the connection: "uncertainty" → "adaptation" → "detection".

And such a connection is a necessary condition for the operation of the computational core of the simulation model and MAAQMS under conditions of real railroad transportation accidents.

Since one of the main reasons for the growth of the epistemic component $v_t[v]$ is the drift of sensors, then, to formalize the drift in the calculations, a model with additive and multiplicative components should be introduced. Let $\tilde{x}_t^{(i)}$ be the true value of the pollutant impurity in the railroad transport node (i) at time (t). Then the observed value of the MAAQMS sensor can be described by the following formula

$$\tilde{x}_t^{(i)} = \alpha_t^{(i)} + x_t^{(i)} + \beta_t^{(i)} + \varepsilon_t^{(i)}, \tag{12}$$

where $\alpha_t^{(i)}$ – multiplicative drift, that is, change in sensitivity of the MAAQMS sensor; $\beta_t^{(i)}$ – additive drift, that is, zero offset; $\varepsilon_t^{(i)}$ – measurement noise.

The parameter vector $(\alpha_t^{(i)}, \beta_t^{(i)})$ evolves in time as a random process. Typically, the process is modeled as a low-order autoregression. In order for the monitoring system to remain operational, the APS computing core must perform online calibration. Technically, this is usually achieved by applying regular updates of estimates $(\alpha_t^{(i)}, \beta_t^{(i)})$. Online calibration should be based on known "reference" observations.

The vector of drift parameter estimates can be described as follows

$$\hat{\Theta}_t^{(i)} = \hat{\Theta}_{t-1}^{(i)} - \eta \cdot \nabla_{\Theta} \cdot L_{calib}^{i}(t), \tag{13}$$

where η is the learning step; $L_{calib}^{i}(t)$ is the calibration error functional (in the MAAQMS system, the difference between the observations of the sensor and reference sources – stationary sensors monitoring the state of the environment was used); ∇_{Θ} is the gradient (nabla operator), or the vector of partial derivatives of the error function with respect to parameters (α, β) or

$$\nabla_{\Theta} \cdot L_{calib}^{i}(t) = \left(\frac{\partial \cdot L_{calib}^{i}(t)}{\partial a}, \frac{\partial \cdot L_{calib}^{i}(t)}{\partial \beta} \right). \tag{14}$$

In addition, when implementing a simulation model with MAAQMS, in addition to the fact of sensor drift, it is necessary to take into account the change in data modes. In particular, for ML, it is necessary to take into account emergency releases of hazardous goods, sudden changes in weather conditions, and the receipt of data from new types of sensors that are installed stationary. These changes in the ML model must be recorded, so event detection statistics are used for this purpose [2]

$$S_t = \max_{i,N}\left(0, S_{t-1} + l_t - k\right), \tag{15}$$

where l_t is the logarithmic likelihood ratio between the current model and the alternative hypothesis of a "change in mode" of the MAAQMS sensors; k is the regularization threshold.

Then, if the S_t value exceeds the pre-set MPC level of hazardous goods on the railroad network, MAAQMS will record this event. This is either an emergency release or a necessary change in the mode of operation of the MAAQMS sensor.

In other words, in the ML model, expressions (1) to (15) ensure the system's resistance to sensor degradation and unexpected situations. And in the hardware implementation of the MAAQMS structure, expressions (12), (13), (15) connect the ML model with the operation of the hardware part of the system.

Thus, the mathematical model of automated environmental risk monitoring can be formalized as multi-criteria optimization

$$\min_{u_t \in U}\left(j_1(u_t), j_2(u_t), j_3(u_t) \right), \tag{16}$$

where u_t – management strategy (distribution of liquidation resources, choice of evacuation routes, etc. is determined when drawing up the technical task of emergency monitoring and decision-making); U – admissible set of strategies.

The first optimization criterion is the integral environmental damage, which takes into account the spatial-temporal distribution of the pollutant and its weight coefficients in socially significant zones along the railroad transport network

$$j_1(u_t) = \sum_{\tau=0}^{T} \sum_{v} w_v \cdot \hat{p}_{t+\tau}[v] \cdot c_v(u_t, \tau), \tag{17}$$

where w_v – weight of the railroad network node (in terms of consequences for the environment, population activities, etc.); $\hat{p}_{t+\tau}[v]$ – probability of exceeding MPC as a result of a railroad transportation accident involving hazardous goods; $c_v(u_t, \tau)$ – cost of damage with the u_t strategy.

The second optimization criterion is the time to eliminate emissions of hazardous goods to a safe level

$$j_2(u_t) = \min\left\{ \tau : \hat{p}_{t+\tau}[v] < \delta \ \forall v \in V \right\}, \tag{18}$$

where δ – MPC safety threshold (dictated by international and national standards and regulations); V – the set of all nodes of the railroad network, along which hazardous goods are transported.

The third optimization criterion is economic costs, described by a functional that depends on the mobilized resources to overcome the consequences of a railroad accident [29]

$$j_2(u_t) = \sum_{\tau=0}^{T} Cost(u_t, \tau), \tag{19}$$

where $Cost(u_t, \tau)$) – economic costs for liquidation of consequences of accident on railroad transport during transportation of hazardous goods with the corresponding strategy u_t.

Since criteria $J_1(u_t)$, $J_2(u_t)$, $J_3(u_t)$ are contradictory, there is no single "best" solution. Therefore, it should be assumed that this optimization problem can be solved in terms of Pareto set [22]

$$P = \left\{ u_t \in U \middle| \nexists u_t' : j_k(u_t), \forall k \ k(u_t') < j_j(u_t) \right\} \ for\_just\_one \ j. \tag{20}$$

In (20), the set P will define a set of strategies that cannot be improved on all criteria simultaneously.

Therefore, if decision makers want to minimize the elimination time $J_2(u_t)$, they will have to sacrifice economic costs $J_3(u_t)$. On the contrary, if the goal is to minimize damage to the ecosystem $J_1(u_t)$, then the model during the simulation will recommend more expensive and longer-term measures. The latter include the complete closure of the railroad branch on which the accident with hazardous goods occurred.

5. 2. Construction of a functional model and development of an algorithm for the environmental risk monitoring and management system

The functional model of the environmental risk monitoring and management system includes the following levels (Fig. 1):

– the first level is hardware. This level includes sensor modules, that is, sensors, a microcontroller for primary signal processing, a communication module (LTE/LoRa) with support for the MQTT protocol;

– the second level is communication, which includes an MQTT broker and a transport channel that ensure the delivery of telemetry from the MAAQMS to the computing server;

– the third level is computing, which includes a server core that implements machine learning models and the assessment of MPC indicators (that is, detection) and optimization of strategies. The calculation takes place in a program implemented in the Python programming language;

– the fourth level is interface, which includes a module for visualizing pollution risk maps and recommendations for railroad transport dispatching services. Decisions regarding environmental risk management are made at this level.

In the functional model, each level (a specific hardware process) is associated with a corresponding mathematical interpretation from the model of automated environmental risk monitoring. In particular, dependences (1), (2), (4) work on data received from sensors via MQTT. They provide normalization and filtering of telemetry from sensors. Dependences (5) to (11) are processed in the server ML module. They also form pollution risk maps and calibrated probabilities. Dependences (12), (13), (15) perform online correction of MAAQMS sensor readings and detection of emergency events – emissions of hazardous goods. Dependences (16) to (19) are implemented programmatically in a high-level language in the optimization core of the simulation model.

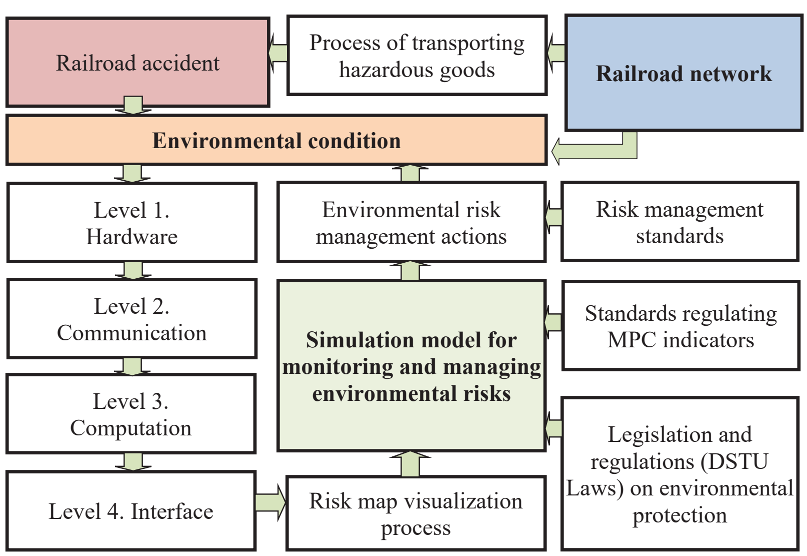

Fig. 1. Functional model of the environmental risk monitoring and management system

Fig. 2 shows a diagram of the algorithm based on the functional model.

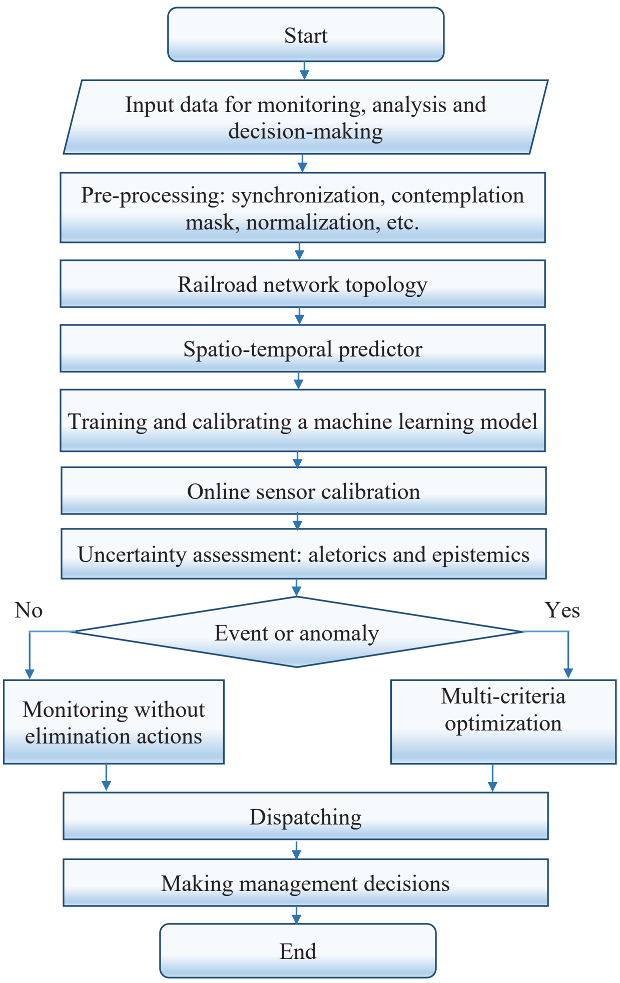

Fig. 2. Algorithm of a simulation model for monitoring and managing environmental risks

The developed algorithm allows for further software implementation of a simulation model of environmental risk monitoring and management based on applied programming languages. In particular, a demo version of the program based on Python was developed on its basis.

5. 3. Testing the proposed simulation model

At this stage of the study, simulation experiments were conducted without using the results of real monitoring of indicators according to MAAQMS, that is, using synthetic data. First of all, the purpose of such a simulation experiment is to check the performance of the models in the demo version of the program, described by expressions (1) to (20). Sensors and, accordingly, the data obtained from them on pollution are not yet used. The use of synthetic data during the computational experiment will allow for a controlled variation of the conditions. These include the intensity of emissions of harmful substances at the site of a hypothetical accident with hazardous goods, the proportion of misses, sensor drift, etc. Additionally, the results of these experiments will allow for the calibration of probabilities and the assessment of the quality of multi-criteria optimization.

The simulation experiment was conducted using a program written in the algorithmic language Python. The procedure for the simulation experiment is given in Table 1, the experimental factors (initial parameters) that were determined by expert means for simulation modeling are given in Table 2. It is assumed that the set of synthetic data for the experiment includes 3000 records that were given empirically (Table 3).

The results obtained during the simulation experiment are shown in Fig. 3–7, which are displayed by the SM software module.

To assess the quality of the spatial-temporal predictor (for the binary classification task – the presence or absence of exceeding the MPC), the receiver operating characteristic was obtained during the SM testing (Fig. 3). This is the so-called ROC curve (Receiver Operating Characteristic curve).

The plot in Fig. 3 shows for the synthetic data set from Table 3 the obtained ratio between the shares of true positive classifications (True Positive Rate scale) and the shares of false positive classifications (False Positive Rate scale) when varying the decision threshold. As can be seen in Fig. 3, the ROC curve demonstrates high predictive ability for model (1) to (20). The ROC curve (solid blue line in Fig. 3) showed rapid growth and rapid approach to the upper left corner of the coordinate plane. The result indicated the ability of the classifier to provide a high percentage of event detection. In Fig. 3, it can be noted that the value of the indicator was $AUC = 0.990$ (area under the ROC curve or Area Under the Curve, AUC). This is a high result for a simulation experiment. It is close to the ideal value of 1.0. The distance of the ROC curve from the diagonal dotted line (shown by the orange line in Fig. 3 and corresponding to the performance of a random classifier ($AUC = 0.5$)) confirmed the acceptable predictive ability of the model. And the results obtained for the synthetic laboratory data set (Table 3) verified the effectiveness of the proposed ML model (5) to (11) with a high degree of accuracy in distinguishing between states with and without exceeding the MPC at the site of a hypothetical accident with hazardous goods on railroad transport.

Table 1

Step-by-step procedure for a simulation experiment

Step number	Short name of the Step	Actions during the implementation of the simulation experiment Step
1	Initialization	The values are set: N, T, topology G, factor levels according to Table 2
2	Trajectory generation	$\zeta_{1:t}$ is set: weather conditions, emissions of hazardous goods u_t etc.
3	Change calculation	The calculation according to formula (1) is applied and the contemplation mask is determined M_t. $\hat{X}_t$ (2) is derived
4	Preprocessing	Normalization is performed according to (2), and a regularization graph of the railroad network is constructed according to (4)
5	ML model training	Predictor is determined f_0, (5) with losses (6) to (8). Calibration is performed according to (9)
6	Uncertainty assessment	From (11), determine H_t and V_t. Risk maps are built
7	Online correction	From (13), reset the values $(\alpha_t^{(i)}, \beta_t^{(i)})$, and also from (15) statistics are collected for ML
8	ML block for Pareto optimization of strategies	Using (17) to (19), the values are calculated: $j_1(u_t)$, $j_2(u_t)$, $j_3(u_t)$. The Pareto front is built. Determine strategy u_t
9	Metrics and visualizations	PR (Precision-Recall) and ROC (Receiver Operating Characteristic) curves, reliability diagrams, risk heat maps, S_t graphs are constructed (15), Pareto front, summary tables for taking management actions
10	Sensitivity testing	The model is tested and the stability analysis is performed when the variable parameters supplied to the output change
11	Result fixation	Output tables and graphs are generated

Table 2

Experimental factors for simulation modeling

No.	Factor	Designation	Variance level
1	Signal-to-noise ratio	$1/\sigma$	low/medium/high
2	Data gap fraction	r_{miss}	0%, 10%, 30%
3	Intensity of MAAQMS sensor drift	AR for $(\alpha_t^{(i)}, \beta_t^{(i)})$	weak/moderate/strong
4	Size of the railroad network graph	N	20, 50, 100 nodes
5	Density of connections in the graph	E	0–50
6	Pollutant emission capacity	$\|\|u_t\|\|$	low/medium/high
7	Duration of an emergency release of dangerous goods	τ	short-term/medium/long-term
8	Class imbalance (exceeding MPC)	(Pr)	rare/moderate/frequent
9	Regularization coefficient in the loss function	λ	Defined by expert
10	Probability calibration parameters	α	$\alpha = 0.05, 0.1, 0.2$

Table 3

A fragment of the synthetic dataset used in the simulation experiment (11 records out of 3000 are shown)

Indicator and its designation in the simulation modeling module	Railroad network graph node ID – node_id										
	0	1	2	3	4	5	6	7	8	9	2
Discrete step of simulation modeling (t) – time	1	1	1	1	1	1	1	1	1	1	2
Air temperature – temperature	19.36	24.44	15.37	19.75	24.54	12.65	24.36	24.55	22.86	18.47	22.74
Wind speed – wind_speed	3.51	2.15	0.24	4.20	3.61	4.11	3.58	3.92	3.10	2.65	3.37
Moisturize – humidity	63.78	55.29	54.24	41.83	63.73	54.88	67.69	67.98	61.05	49.45	59.78
Type of hazardous goods (categorically) – cargo_type	Toluene	Toluene	Toluene	Toluene	Toluene	Toluene	Toluene	Toluene	Ammonium	Toluene	Formaldehyde
The power of the release of hazardous goods at the accident site – emission_level	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Actual reading, taking into account noise and drift – sensor_value	0.54	0.55	0.32	1.10	0.37	0.65	0.50	0.36	0.11	0.02	0.90
Mask of observation (M_t) – mask_obs	1	1	0	1	1	1	1	1	1	1	1
Binary indicator of exceeding the MPC of hazardous goods – exceed_PDK	0	0	0	0	0	0	0	0	0	0	0

In addition to the ROC analysis, a Precision-Recall curve was constructed to assess the quality of the model (5) to (11), Fig. 4.

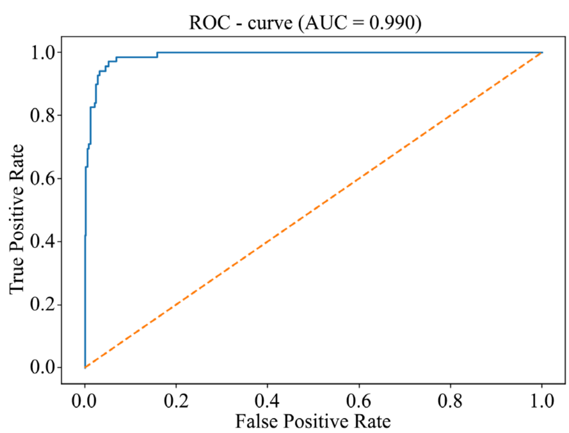

Fig. 3. Visualization of the Receiver Operating Characteristic curve in the simulation model (output from the software module)

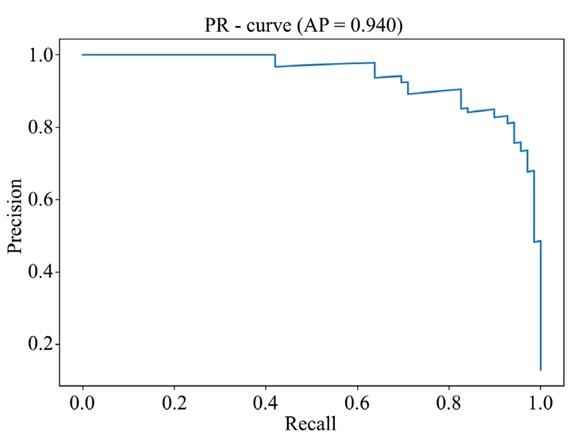

Fig. 4. Visualization of the Precision-Recall curve in the simulation model system (output from the software module)

The curve shown in Fig. 4 demonstrated the effectiveness of the developed predictor f_0 (5). The trajectory of the curve at 4 is located close to the upper right corner of the plot. This confirmed the ability of the model to maintain a high level of accuracy over a significant range of values of the completeness of the data set in Table 3. The model maintained the accuracy of predictions close to 1.0. The *AP* value was *AP* = 0.940. This *AP* value during simulation confirms that the model is able to effectively identify events and at the same time minimize the number of false positives.

To visually represent the results of modeling the spatial-temporal distribution of the pollutant, a heat map was constructed (Fig. 5).

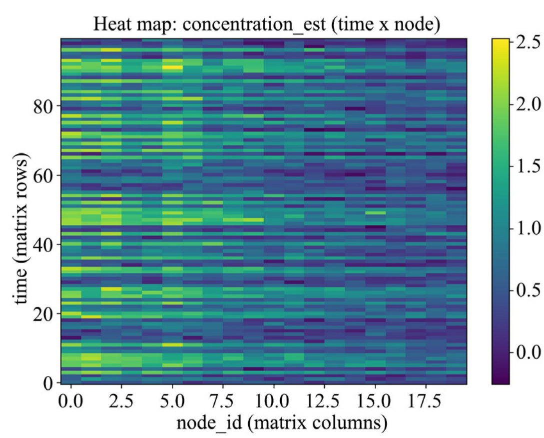

Fig. 5. Concentration estimate (concentration_est) in matrix form (output from the software module)

The visualization in Fig. 5 displays the estimated concentrations (*concentration_est*) in a matrix form. In Fig. 5, the vertical axis is time (*time*). The horizontal axis is the identifiers of the railroad network nodes (*node_id*). The color intensity in each cell in Fig. 5 is proportional to the concentration level in the railroad network node at a time according to the scale shown on the right. Based on the analysis of the heat map, the decision maker or the operator working on the server side concludes that there is a pronounced spatial heterogeneity in the process of leakage and spread of hazardous goods. Figure 5 shows that a limited group of nodes is affected. For the dataset under consideration, these are nodes with indices from 0 to ~ 5. For them, increased levels of concentration of hazardous goods were recorded during the experiment. In Fig. 5, they are shown in green and yellow shades. The rest of the network remains in the zone of low, background values. These are dark blue and purple shades. That is, this result simulates the localized nature of an accidental release of hazardous goods. A development of this form of representation of the results of the simulation experiment was the heat map (Fig. 6).

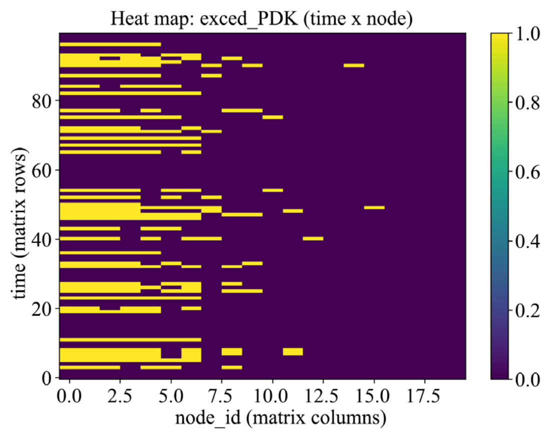

Fig. 6. Visualization of the results of the machine learning model in the form of a heat map (output from the software module)

The map in Fig. 6 visualized the results of the ML model (5) to (11). The axes in Fig. 6 show the states for each node (*node_id*) and the time points (time) when an event was recorded for the simulated data sets during the simulation experiment – exceeding the MPC of hazardous goods. Ultimately, such a result, which is displayed on the server, provides additional tools for prompt decision-making regarding the response to emissions of hazardous goods at the scene of a railroad accident.

But unlike the map of continuous concentrations (Fig. 5), a discrete color scale was used in Fig. 6. In Fig. 6, bright yellow color indicated a recorded exceeding of the MPC. This is an alarm state for the person making management decisions. While dark purple – finding the concentration of hazardous goods within the normal range, that is, it is a safe state. The spatial distribution of risk events for the considered dataset (Table 3) was consistent with previously obtained data. That is, dangerous states are localized in the same limited group of nodes with indices from 0 to ~ 7.

The final stage of the analytical core is the formation of recommendations for decision-makers. Fig. 7 shows a three-dimensional visualization of the results of the multi-criteria optimization block.

Each point in the three-dimensional space in Fig. 7 corresponds to one potential response strategy for the dataset under consideration. The strategy, accordingly, was evaluated during the simulation by three mutually contradictory criteria J_1, J_2, J_3, expressions (17) to (19). The set of presented points for J_1, J_2, J_3 forms a Pareto front. That is, it is a surface consisting of non-dominant solutions for J_1, J_2, J_3. This means that for any point on this surface of the plot in Fig. 7 it is impossible to find another strategy that would be better by all three criteria simultaneously. Improving one indicator, for example, reducing the time J_2, will inevitably lead to a deterioration of at least one other. That is, to an increase in the value of J_3 or a loss of J_1. The graph in Fig. 7 for people making managerial decisions illustrates these compromises. Such visualization of simulation results offers not only the only correct answer but also provides a full range of the most rational and balanced alternatives. That is, the manager makes his/her choice based on substantiated and quantitatively supported data when choosing a strategy using the simulation results since s/he is able to choose a strategy that best meets operational priorities and available resources when eliminating an accident with hazardous goods on railroad transport.

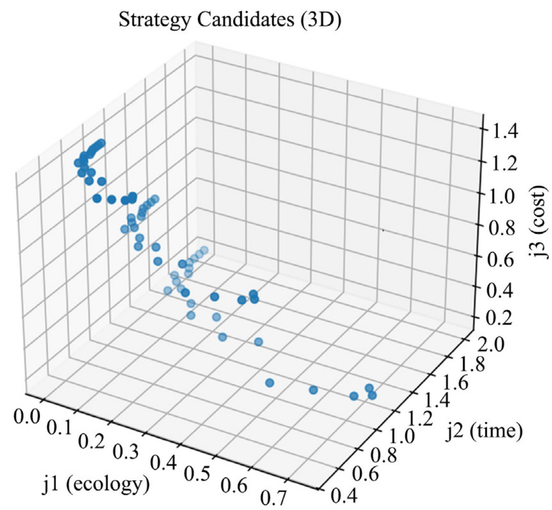

Fig. 7. Visualization of the Pareto front in a simulation model (output from the software module)

For decision-makers, the Pareto set is displayed in 3D format (Fig. 7). It contains candidates for optimal strategies for responding to an emergency situation with hazardous goods at the scene of a railroad accident. In particular, for example, the following strategies can be proposed based on the data provided:

1. Environmental optimization strategy (minimum J_1). This strategy is focused on the least environmental impact at the cost of greater costs or time. According to the plot (Fig. 7), these are the points closest to the beginning of the axis J_1. In this case, the costs will be the highest (about 1.0–1.4) since environmental measures are expensive. The conditional time for eliminating the consequences will be about 1.0–1.5, since the implementation of expensive environmental measures often requires a lot of time.

2. Economic optimization strategy (minimum J_2). This strategy is aimed at minimizing the cost of measures at the cost of greater environmental impact on the environment, while the conditional time for eliminating the consequences will take an average value. According to the plot (Fig. 7), these are the points that are closest to the beginning of the axis J_3. In this case, the J_1 indicator is likely to be the highest (about 0.6–0.7) since cheap solutions are often less environmentally friendly.

3. Compromise (balanced) strategy. This strategy is designed to reflect the best balance between all three criteria, avoiding extreme costs or risks. According to the plot (Fig. 7), these are the points located in the middle part of the Pareto Front. This is approximately the area where J_1 is 0.3–0.4; J_2 – 1.0–1.4; J_3 – 0.4–0.7 (Fig. 7).

The decision maker's choice of the final strategy depends on the priorities and goals of environmental risk management. If the priority is ecology, solutions closer to 0 on the J_1 axis are chosen; if the cost of the measures is closer to 0 on the J_3 axis. If there is no clear priority, the decision maker chooses a compromise strategy. Thus, the plot in Fig. 7 is a key tool in choosing the final action plan for the elimination of accidents with hazardous goods.

6. Results of testing the proposed simulation model for monitoring and management of environmental risks: discussion and summary

A simulation model of monitoring and management of environmental risks in accidents with hazardous goods on railroad transport has been built. It is based on the model of automated monitoring of environmental risks (1) to (20). The model built differs from existing solutions by integrating drift correction of sensors of the mobile automated air quality monitoring system (MAAQMS) with differentiation of data into multiplicative and additive components. A functional model (Fig. 1) and an algorithm of the environmental risk monitoring and management system (Fig. 2) have been proposed. The functional model includes 4 levels, each of which corresponds to separate dependences of the automated environmental risk monitoring model. In particular, dependences (1), (2), (4) are implemented at the hardware level, which operate on data received from sensors via MQTT. Dependences (5) to (11) are processed at the communication (second) level of the functional model. Dependences (12), (13), (15) perform online correction of the readings of MAAQMS sensors and detection of emergency events – emissions of hazardous goods at the third level – computational. Dependences (16) to (19) are implemented programmatically in the Python programming language in the optimization kernel at the fourth level of the model. This makes it possible to make informed decisions on managing environmental risks in transport.

Unlike [17, 18, 20, 21], in which researchers encountered practical problems of uncertainty, in our study this is taken into account in dependence (11). For this purpose, uncertainty is divided into alethoric, associated with the randomness of observations using MAAQMS, and epistemic, associated with the uncertainty of knowledge of the presented model. The issues of sensor degradation [11, 20, 21] are taken into account by online correction of indicators in the SM algorithm (Fig. 2), dependences (12), (13), (15). Based on the logic of using ML methods, these dependences, unlike [11, 20, 21], take into account sensor drift and online calibration (12); adaptation of model parameters when changing the mode (13); type of emergency event and its consideration in modeling (15). In particular, for ML, accidental releases of hazardous goods, sudden changes in weather conditions, and data from new types of sensors that are installed stationary are taken into account. Spatial-temporal forecasting methods are taken into account in the optimization kernel of the simulation model and dependences (16) to (19). They adopted three optimization criteria: integral environmental damage, time to eliminate emissions of hazardous goods to a safe level, economic costs of overcoming the consequences of a railroad accident. As a result, it was proposed to apply the Pareto set approach to solving the optimization problem, taking into account the contradictions of its criteria.

Simulation experiments were conducted without using the results of real monitoring of indicators according to MAAQMS, that is, using synthetic data. The results of visual analytics are reported, which were obtained after the final processing of data in the optimization kernel of the model. The results of simulation experiments were evaluated by ROC analysis and PR analysis. The adequacy of the mathematical model was confirmed by achieving a high indicator of the area under the ROC curve ($AUC = 0.990$), the indicator of PR analysis ($AP = 0.940$). Pareto maps of alternatives for responding to environmental risks were determined, which make it possible to make management decisions depending on the priority goals.

A limitation regarding the use of the constructed simulation model is the fact that its demo version involves the use of up to 3 criteria simultaneously in the optimization kernel. Therefore, in the future development of research, it is envisaged to expand the parameters for optimization and determine the Pareto front. The disadvantage of the study is that at the moment the testing was not carried out on real but on synthetic data. In the advancement of this study in the future, it is planned to test the simulation model on information about emergency situations in railroad transport, available in statistical sources.

The results obtained during the study will further serve to implement the simulation model in the activities of railroad transport units for monitoring and managing environmental risks in the transportation of hazardous goods. Such units operate in each country, as a rule, in the structure of the main railroad transport operator for the purpose of implementing environmental management and environmental risk management.

Possible directions for the development of this research, taking into account the above shortcomings and limitations, may be the calibration of the mathematical model of automated environmental risk monitoring by expanding the criteria in the optimization kernel. This will be possible based on the results of testing the simulation model using information on emergency situations in rail transport available in statistical sources.

7. Conclusions

1. A mathematical model of automated environmental risk monitoring has been constructed, which differs from existing solutions by integrating drift correction of sensors of the mobile automated air quality monitoring system (MAAQMS) with data differentiation into multiplicative and additive components, as well as with ML-detection of MPC exceedances, implemented in a single architecture of the simulation model of environmental risk monitoring and management. This together makes it possible to compensate for systematic measurement biases and stabilize the triggering of early warning under conditions of missed observations from MAAQMS sensors, based on machine learning methods. It is shown that the combination of alethoric and epistemic uncertainties in the tasks of assessing environmental risks at the scene of accidents with hazardous goods gives an effect in assessing risks in real time. This occurs due to the formalization of uncertainty channels of MAAQMS sensor readings and ML models, as well as their influence on risk assessment metrics. This is due to the subsequent choice of strategies through a simulation model by decision-makers at the scene of accidents involving railroad transport carrying hazardous goods. A multi-criteria decision support model is proposed based on Pareto optimality with explicit criteria of environmental damage, time to bring to a safe state, and the cost of responding to the consequences of accidents involving hazardous goods.

2. A functional model and algorithm of the environmental risk monitoring and management system have been developed. The functional model of environmental risk monitoring

and management includes four levels: hardware, communication, computing, and interface. At the last level, pollution risk maps are visualized, and recommendations are made for railroad transport dispatching services, as well as decision-making on environmental risk management. The proposed algorithm was used as the basis for the development of modules of the simulation model of environmental risk monitoring and management based on Python.

3. During the simulation experiments, it was demonstrated that it is advisable to build the assessment of such criteria on the data of environmental monitoring and use them in the future for ranking strategies. The results of visual analytics obtained at the output for decision-makers are presented. The results of the simulation experiments were evaluated by ROC analysis, PR analysis. The adequacy of the model was confirmed by achieving a high indicator of the area under the ROC curve ($AUC = 0.990$), the indicator of PR analysis ($AP = 0.940$). Such values of the indicators confirm that the simulation model is able to effectively identify events and minimize the number of false positives. The heat maps "time × node", the drift tracing of MAAQMS sensors, and the Pareto maps of response alternatives have been described and analyzed. In practice, this ultimately contributes to the prompt selection of uncertainty-resistant strategies, including under conditions of limited resources at the scene of an accident involving hazardous goods on railroad transport.

Conflicts of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study, as well as the results reported in this paper.

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Data availability

The data will be provided upon reasonable request.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating the current work.

Authors' contributions

Olena Kryvoruchko: Supervision; Project administration; Conceptualization; Methodology; Investigation; **Maira Shalabayeva**: Methodology; Formal analysis; Validation; **Svitlana Tsiutsiura**: Investigation; Data Curation; Writing – original draft; **Mykola Tsiutsiura**: Data Curation; Formal analysis; **Valentyna Makoiedova**: Investigation; Validation; **Valerii Lakhno**: Methodology; Software; Investigation; Writing – original draft; **Oleksandr Alieksieienko**: Writing – review & editing; Visualization; Project administration; **Yaroslav Shestak**: Investigation; Resources; **Alina Korchevska**: Visualization; Validation; Resources.

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