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Numerical Evaluation of Wind Speed Influence on Accident Toxic Spill Consequences Scales

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Abstract **– This study aims to evaluate numerically the influence of wind speed on scales of environmental harmful consequences caused by accidentally spilled toxic liquid evaporated from the surface of a free-form outlined spill spot. A coupled problem of the gas-dynamic movement of a toxic air-mixture cloud in the atmosphere's surface layer under the influence of wind and a negative toxic inhalation impact on a human in an accident zone is solved by means of mathematical modelling and computer experiment. A three-dimensional non-stationary mathematical model of the turbulent movement of a gas-air mixture is used for obtaining distribution of relative mass concentration of toxic gas impurities in time and space. A probabilistic impact model based on using a modernized probit analysis method is used to obtain fields of conditional probability of a fatal human injury resulting from toxic gas inhalation. This technique allows environmental safety experts assessing the scale of considered type technogenic accident consequences numerically depending on wind speed conditions and elaborating the means to mitigate them to acceptable levels.**

Keywords **– Accidental toxic spill; evaporation rate; hazardous area; impact probit analysis; inhalation toxic dose; toxic gas concentration.**

Nomenclature		
X, Y, Z	Coordinates of the right Cartesian system	–
G_Σ, G_i	Total spot and individual cell evaporation rates	kg/s
N	Number of discrete spill spot cells	–
τ_1, τ_2	Start and stop times of an evaporation process	s
F	Spill spot total area	m^2
q^e	Total evaporation rate	kg/s
μ	Molar mass of dangerous substance	kg/mol
$u^e_{0\,\mathrm{ef}}$	Initial effective velocity of a secondary cloud	m/s
P_s	Pressure of saturated vapor of dangerous substance	mmHg
ΔH_b	Heat of evaporation of the liquid substance	J/kg

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T_a, T_b	Air temperature and boiling liquid temperature	K
R	Universal gas constant	J/(mol K)
H_1, H_0	Actual and measurement point heights	m
V_1, V_0	Wind speed at actual and measurement heights	m/s
k	Power coefficient in wind speed profile dependency	–
P	Conditional probability of damage to a human	%
Pr	Probit function of lethal injury due to toxic gas inhalation	–
t	Influence integral parameter of the impact factor	–
D	Inhalation toxic dose	–
A, B, n	Toxic substance semi-empirical coefficients	–
Q	Toxic gas mass concentration	ppm
τ_{exp}	Exposure time	s

1. INTRODUCTION

Accidental release of a hazardous gas can be considered as a disturbance of an air normal state which is characterized by a mass concentration. The disturbed chemical composition of the air leads to the formation of dangerous factors: toxic dose (for toxic gases), overpressure and impulse of the explosion wave (for explosive gases) and heat flow density (for flammable gases). All these factors are hazardous for humans in accident zone and can lead to harmful consequences for their health. The environment state parameters (such as wind speed) during the accidents can affect hazardous zones formation. The detection of such influence is an actual scientific and applied problem, the solution of which will allow experts to analyse safety conditions of industrial enterprises, predict the risks of possible environment consequences of accidental emissions, and develop rational measures to eliminate or mitigate the scale of such harmful impact. The purpose of this study is to identify the influence of wind speed on the size of the danger zone, which is formed during an accidental spill of toxic liquid, its evaporation into the air with the formation of a toxic gas-air cloud, which moves downwind from the epicenter of the accident and affects the company's service personnel. The area of the zone, where the probability of lethal toxic poisoning of a person exceeds a given threshold value, is considered as a scale parameter of accident consequences.

Air pollution by technogenic emissions of harmful chemicals into the atmosphere causes negative impact on the environment [1]. Identification of a specific source of pollution [2], assessment of the scale of the consequences of its impact on the environment [3] in order to mitigate the negative impact on air quality [4] can be considered as a part of the complex work of environmental safety experts during an analysis of main trends in the development of pollution impact on climate change [5], a generation of guidelines for environmental certification of technogenic objects [6]. Wind, as a natural phenomenon, on the one hand, is used to create energy parks [7], which eliminate some of the causes of negative climate change [8], and has a strong potential to save the environment from pollution sources [9]. However, on the other hand, it plays a crucial role in the formation of dangerous zones in the process of accidental release and dispersion of toxic substances at high-risk enterprises, since the scale of the consequences of such accidents depends on the wind speed. Obtaining time-space distributions of the mass concentration of a hazardous chemical substance is the most important when identifying hazardous areas for humans. The most adequate way to do that is a physical experiment, when measurements of the amount of a chemical substance in the air are carried out using specialized equipment [10]. When planning a physical experiment, you can take into account various factors that affect the processes of dispersion of a gaseous impurity in the surface layer of the atmosphere: the density of the impurity relative to the air density [11], the complex topography of the area [12], the nature of the surface from which the spilled liquid evaporates [13], atmospheric conditions [14], etc. But the complexity and variety of scenarios of impurity release into the atmosphere, the impossibility of taking into account all possible factors affecting the processes of impurity distribution, including the impurity's poisonous properties, its flammability or explosiveness, make the physical experiment a valuable research tool that is usually used to validate mathematical models of physical processes. Mathematical modelling eliminates almost all the shortcomings of a physical experiment and opens up endless possibilities for modelling the consequences of accidental emissions of dangerous gases into the atmosphere [15].

In this paper, it is proposed to use mathematical modelling to obtain hazardous zones that are formed during accidental releases of hazardous chemicals, and to investigate the effect of wind speed on the scale of environmental consequences (Fig. 1).

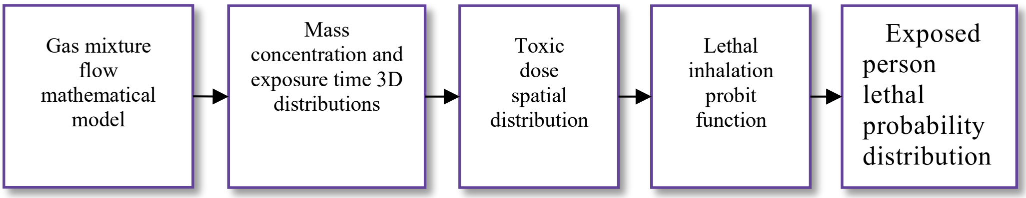

Fig. 1. Toxic spill accident consequences evaluation.

All mathematical models of gas mixture movement in the atmospheric surface layer could be divided into four main groups, which are distinguished by their complexity and mathematical description perfection [15]. The first group includes the simplest models (like [16] and [17]) which use an empirical approach. The second group of models of intermediate complexity includes integral models [18] and shallow layer models [19]. Lagrangian particle trajectory models [20] and Lagrangian puff dispersion models [21] form the third group of advanced mathematical models. The last group includes the most sophisticated Computer Fluid Dynamics (CFD) models which can be divided to Reynolds-Averaged Navier-Stokes (RANS) models [22], Large Eddy Simulation (LES) models [23], and Direct Numerical Simulation (DNS) models [24]. As noted in the review [15] the most adequate description of multicomponent gas mixture movement can be possible only on the base of non-stationary Navier-Stokes equations, but limited capabilities of modern computers do not allow researchers to use direct solvers based on these equations effectively [25]. It is considered that mathematical modelling of turbulent flows can be simplified by solving the Navier-Stokes equations which are averaged over the Reynolds-Favre and complemented by a turbulence model [26]. However, the selection of the turbulence model itself can be very difficult because models adopted to describe adequately only those specific types of flow for which they are designed (that is especially true for flows with intensive separations and temperature sharp gradients). Moreover, some of the modern mathematical models are stationary [27], other models are adopted to estimate air pollution using a deterministic approach [28], other models are risk-oriented with probabilistic approach to determine the environment consequences, but probit analysis is not automated and based on tabular probability dependence on probit function [29]. This does not allow applying this approach in computer systems to obtain non-stationary spatial fields of environment consequences probability during simulation of accidents.

In order to reach the purpose of the work to assess the influence of the wind speed on hazardous zone square, a new approach is suggested and used in this research which integrates two (gas dynamics and safety) models. The first one (mathematical model of multicomponent gas mixture movement based on Euler approach) allows extracting current time value of hazardous factor (toxic inhalation dose) taking to account influence of the wind speed, and the second one (probit analysis model) gives us an opportunity to assess the environmental consequences (human lethal probability, and hazardous zone area) to consider mitigation means [30]. In the future, this approach can allow simulating not only isolated accident scenario of toxic gas release and dispersion but consider more complicated scenarios with flammable or even explosive gas admixtures with other hazardous factors (pressure wave and heat flow).

2. Hazardous Gas Release and Dispersion Problem Statement

In order to determine the influence of wind speed on the scale of the consequences of an accident spill of a toxic liquid for the environment, it is necessary to solve the related problem of the release and dispersion of a hazardous chemical substance and human safety in the area of the accident. The area of the dangerous for humans zone, which is formed under the influence of wind of a given speed, will be considered as a parameter that will be associated with the scale of the consequences of the accident. The spatial computational domain in the Cartesian coordinates system (X, Y, Z) (Fig. 2) is evenly divided into spatial computational cells along the main axes.

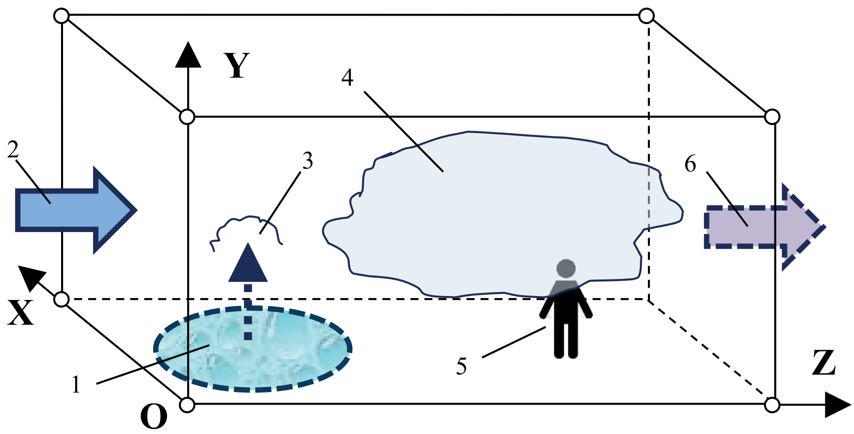

Fig. 2. Accident development scheme: 1 – liquid spill spot; 2 – inlet air flow; 3 – evaporated toxic gas; 4 – gas-air mixture cloud; 5 – exposed person; 6 – outlet flow.

The gas phase is released from the spill surface in the XOZ plane. The spill spot is generally specified by the coordinates of the points of a closed, simply connected contour of arbitrary shape. The gas phase is ejected into the surface layer of the atmosphere with a constant total intensity G_Σ, which is composed of discrete admixture vertical flows $G_i = G_\Sigma / N$ in each of the collection of N computational cells that are adjacent to the earth's surface and fall inside the contour of the strait spot. The release of the gaseous phase of the impurity occurs during the time interval between the moments τ_1 of the start of the evaporation process and τ_2 of its completion, for example, as a result of covering the spill spot with special foam.

Thus, the movement of a gas-air toxic mixture in the surface layer of the atmosphere at a given wind speed is considered in order to determine non-stationary spatial fields of the mass concentration of a hazardous impurity. This dangerous parameter is the basis for determining the inhalation toxic dose at each point in space – a dangerous factor that allows you to determine the conditional probability of fatal toxic damage to a person. Spatial fields of damage probability can be used by safety experts to determine the risks of high danger industrial enterprises. In particular, it is possible to calculate the area of a zone hazardous for humans where the lethal conditional probability is greater than 50 %, and use this parameter as a scale of consequences for comparative computational experiments [30]. By repeating the computational process for different wind speeds, it is possible to achieve the aim of this study to determine the effect of wind speed on the environment consequences of an accidental spill of a toxic chemical.

3. METHODS AND PROCEDURES

3.1. Mathematical Model Basic Equations

Based on a review of mathematical models of the movement of gas mixtures, it was decided to use a spatial non-stationary model of a gaseous admixture dispersion in the surface layer of the atmosphere [30]. The model considers the convective transfer of mass, momentum and energy as the main factor influencing the main physical processes. This assumption allows using the simplified Navier-Stokes equations, which are obtained by dropping the viscous terms (Euler approach with source terms). The complete system of equations describing the non-stationary three-dimensional flow of a two-component gas mixture in this formulation, boundary and initial conditions, numerical solution algorithm, and numerical method are presented in [30]. Moreover, this approach is extended to pressure disturbances of the air during the release and combustion of explosive gases [31], which makes it possible to evaluate the landscape configuration influence on accident consequences [32], assess the safe dimensions of protection devices [33], and consider in future combined scenarios of accident situations. The mathematical model is implemented in a research computer system ‘Toxic Spill Safety’ [34].

3.2. Liquid Evaporation Process Simulation

The toxic substance gas phase release modelling is implemented by setting the boundary conditions of ‘evaporation’ on the corresponding faces of the finite-difference computational cells that are adjacent to the surface of the strait spot [30]. The simulation of the cessation of evaporation from the spill spot is carried out by replacing the boundary conditions with the ‘non-flow’ condition [35]. An iterative scheme of the computational process, which uses the Godunov method to simulate the flow of a gaseous admixture of a given flow rate, is presented in [30].

3.3. Evaporation Rate Evaluation

When modelling the evaporation of a toxic liquid from a spill spot, we assume that the evaporation rate is a constant value in the considered time interval [30]. It can be found as a gas flow rate in the secondary cloud formed at evaporation stage from Eq. 1 [36].

$$q^e = F\sqrt{\mu}10^{-6}(5.38+4.1\ u_{0\mathrm{ef}}^e)P_\mathrm{s}\,, \tag{1}$$

where

F Spill spot total area, m^2;

q^e Total evaporation rate, kg/s;

μ Substance molar mass, kg/mol;

$u_{0\,\mathrm{ef}}^e$ Initial effective velocity of a secondary cloud formed at evaporation stage, m/s;

P_s Substance saturated vapour pressure at air temperature, mmHg, which can be determined as follows

$$P_s = 760\exp\left[\Delta H_b\mu\left(1/T_b - 1/T_a\right)/R\right], \tag{2}$$

where

ΔH_b Liquid evaporation heat, J/kg;

T_a Air temperature, K;

T_b Liquid boiling temperature under ambient air pressure, K;

R Universal gas constant, J/(mol K).

It is possible to determine the effective speed of air on the evaporation surface using the power law of the profile of the wind speed versus height in the surface layer of the atmosphere [38].

$$V_1 = V_0\left(H_1/H_0\right)^k, \tag{3}$$

where

V_1 Wind speed at the actual height of determining air parameters, m/s;

V_0 Wind speed at the height of air parameters measurement, m/s;

H_1 Actual height of determination of air parameters, m;

H_0 The height of the air parameters measurement point, m.

k Coefficient that depends on the roughness of the earth's surface.

3.4. Probabilistic Method of Safety Assessment

A human in the zone of an accident release of a toxic liquid inhales harmful vapours and becomes an object of the dangerous impact of the accident on the environment. The consequences of such exposure depend on the value of the received inhalation toxic dose which can be calculated during non-stationary modelling of the spatial movement of the gas-air poisonous cloud in the calculation area. According to the results of such modelling, in each spatial cell it is necessary to accumulate and store the value of the toxic dose for the calculation of the probit function and the conditional probability of a lethal injury to a human [30].

$$P = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\mathrm{Pr}} e^{-\frac{1}{2}(t-5)^2}\mathrm{d}t\,, \tag{4}$$

where

P	Conditional probability of damage to a human;
Pr	Probit function of lethal injury due to toxic gas inhalation;
t	Integral parameter of the dangerous influence of the impact factor.

The probit function for a lethal inhalation impact of an exposed human can be determined from the following equation

$$\Pr = A + B\ln(D), \tag{5}$$

where

A, B	Toxic substance semi-empirical coefficients;
D	Inhalation toxic dose.

According to the adopted methodology, the inhalation toxic dose D, as a main damaging factor, can be calculated using the following definite integral.

$$D = \int_0^{\tau_{\exp}} Q^n \mathrm{d}\tau, \tag{6}$$

where

$\tau_{\exp}$	Exposure time, s;
Q	Toxic gas mass concentration, ppm;
n	Toxic gas table coefficient.

Using the probit function value calculated every time at each point in space for a lethal impact to a human, a safety expert can use the tabular dependence of the impact probability on the probit function [29] which is commonly used in industry. But this approach to estimating the value of the integral (4) is unacceptable for the developed methodology of assessing the consequences of an accidental release of a hazardous substance into the environment. Therefore, in order to automate non-stationary calculations of the spatial fields of the impact probability, a piecewise cubic Hermitian spline [37] is used to replace the tabular dependence (Fig. 3).

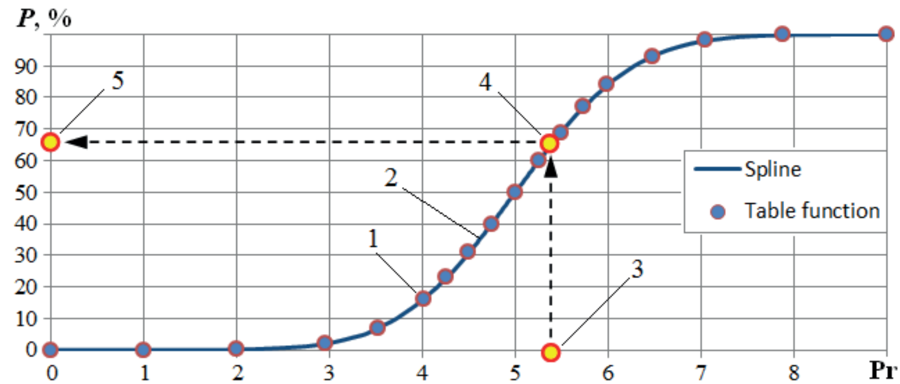

Fig. 3. Spline approximation of conditional probability function: 1 – table function; 2 – cubic Hermitian spline; 3 – calculated probit function Pr; 4 – point on the spline; 5 – calculated conditional probability of damage P.

4. Results

The process of evaporation of 6098 kg of liquefied cyanide hydrogen spilled on 177 m^2 area under the constant wind conditions is simulated (Fig. 4). A wind speed vector makes an angle of 45° with the OZ axis. Cyanide hydrogen is a toxic substance with density 689 kg/m^3, molar mass 0.027 kg/mol, boiling temperature 298.6 K, and evaporation heat 933 kJ/kg. Evaporation takes place from a free form spot described by a collection of points $\{C_i\}$ with coordinates (X_C; Z_C) (Fig. 4). It is assumed that the spilled liquid layer is 0.05 m thick, which can be used as H_1 value in (3). It is also considered that the height of a measurement point H_0 is 0.5 m high. Let the area around the accident meets the 'city outskirts' conditions. Then the coefficient k of the power-law function for the wind speed profile (3), which depends on the roughness of the surface of the earth, is equal to 0.4 [29]. For toxic hydrogen cyanide, the following table coefficients are used when calculating the probit function of the lethal outcome and the inhalation toxic dose [29]: $A = -37.98$, $B = -3.7$, $n = 1$.

The calculation domain width L_x, height L_y, and length L_z are 85, 10, and 85 m long. All calculation cells have the same dimensions and cubic shape with side 1 m long. The computer has the following characteristics: Intel® Core™ i7-360QM CPU @ 2.40 GHz, 16.0 GB RAM, Windows 7. CPU time for each experiment is about 5 min. Five options V1–V5 of wind speed V_1 at a measurement point 0.5 m are considered (Table 1) in order to evaluate the influence of wind conditions on hazardous area value. Using (3) an initial effective velocity of a secondary cloud formed at evaporation stage $u_{0\,\mathrm{ef}}^{e}$ at the spilled liquid layer height H_1 can be calculated (Table 1). Then, using (1), the values of total evaporation rate q^e for each wind option can be calculated (Table 1) taking into account that spill spot total area F equals 177 m^2.

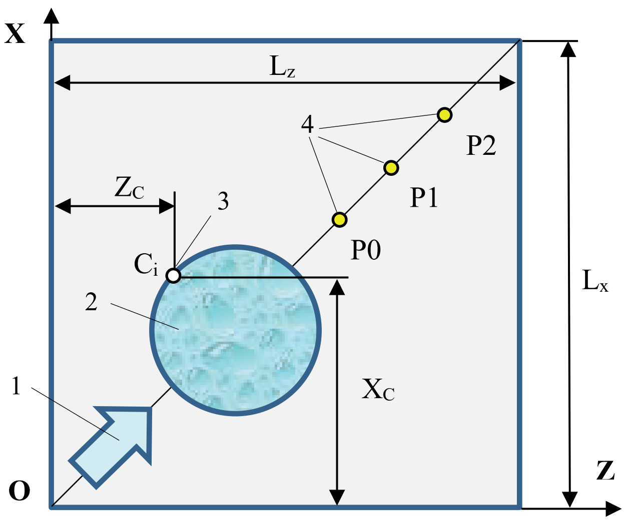

Fig. 4. Map of objects: 1– wind vector; 2 – spill spot; 3 – points collection of a spot outline; 4 – control points.

TABLE 1. SPILL EVAPORATION PARAMETERS

Parameter	Options				
	V1	**V2**	**V3**	**V4**	**V5**
Speed V_1, m/s	3.0	5.0	7.0	9.0	11.0
Speed $u_{0\,\mathrm{ef}}^{e}$, m/s	1.19	1.99	2.79	3.58	4.38
Evaporation rate, kg/(m^2 s)	0.00106	0.00139	0.00173	0.00206	0.00240

In order to analyse the behaviour of admixture dispersion, collect toxic dose values, and evaluate the consequences for human the three control points P0 (34.5 m; 34.5 m), P1 (54.5 m; 54.5 m), and P2 (74.5 m; 74.5 m) are set along the wind vector direction (Fig. 4).

A single-connected free-form spill spot is approximated by finite-differential square cells using the algorithm described in [30] (Fig. 5).

It is assumed that the evaporation process for each wind option takes place during the time between $\tau_1 = 0$ s and $\tau_2 = 5$ s. Each calculation stops after the toxic cloud left the limits of the calculated area (Fig. 6).

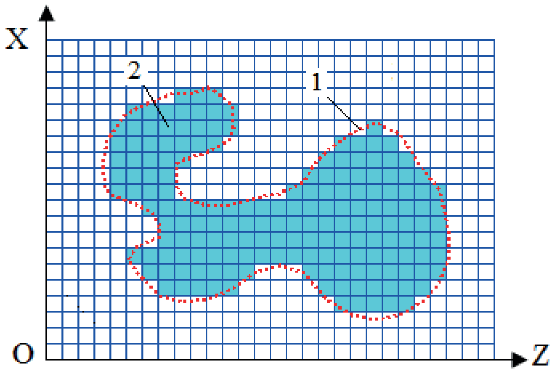

Fig. 5. Discretization of a free-form outlined spill spot: 1 – points collection of the spot; 2 – selected cells with evaporation boundary conditions.

During each computational experiment for each option of wind speed, a history of admixture dispersion is controlled (Fig. 7). It is obvious that with distance from the epicentre of the accident, the concentration of toxic gas gradually decreases due to turbulent diffusion. Therefore, the distribution of the conditional probability of fatal human poisoning indicates a decrease in the risk of death with increasing wind speed (Fig. 8).

The confirmation of the risk reduction is also detected on the diagram of lethal conditional probability at the control points depending on the variant of the wind situation at the industrial site (Fig. 9(a)). If the area of the dangerous zone, where the conditional probability of damage exceeds 50 %, is taken as a characteristic of the scale of the accident consequences, it is obvious that an increase in wind speed significantly affects the consequences of an accidental spill of a poisonous liquid for the environment (Fig. 9(b)).

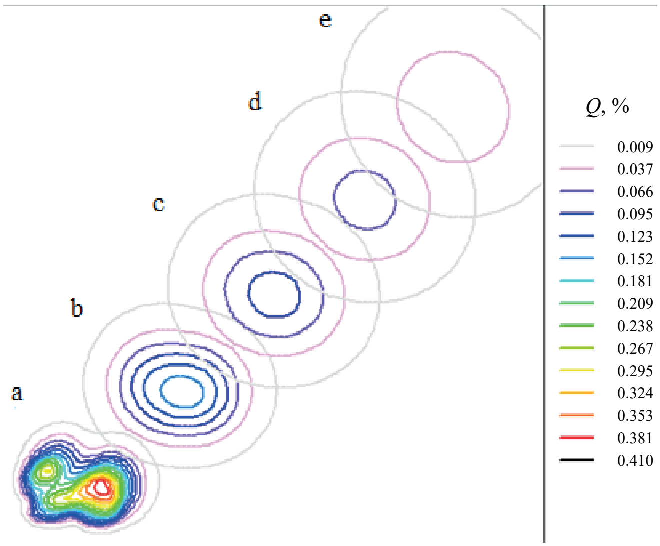

Fig. 6. Admixture mass concentration fields near the ground for V1 option: a–e – after 3, 13, 23, 33, and 43 sec.

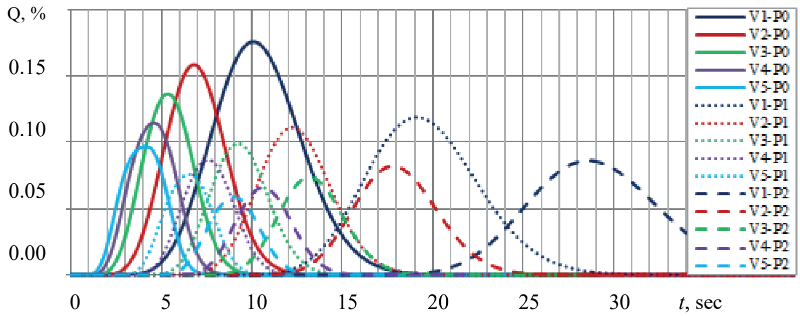

Fig. 7. Mass concentration history for wind options V1–V5 at control points P0, P1, and P2.

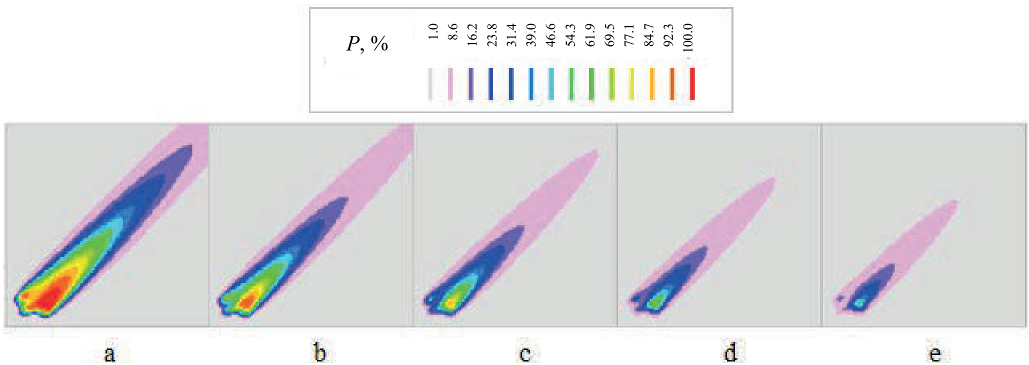

Fig. 8. Lethal conditional probability (%) fields: a–e – wind options V1–V5.

The biggest danger zone is for a weak wind of 3 m/s, a wind of average intensity 5–7 m/s still poses a significant danger to an exposed human, but most likely the consequences of an accident will lead to non-fatal poisoning. A strong wind of 9–11 m/s can be considered safe for a person in the accident zone from the lethal consequences point of view (Fig. 9(b)).

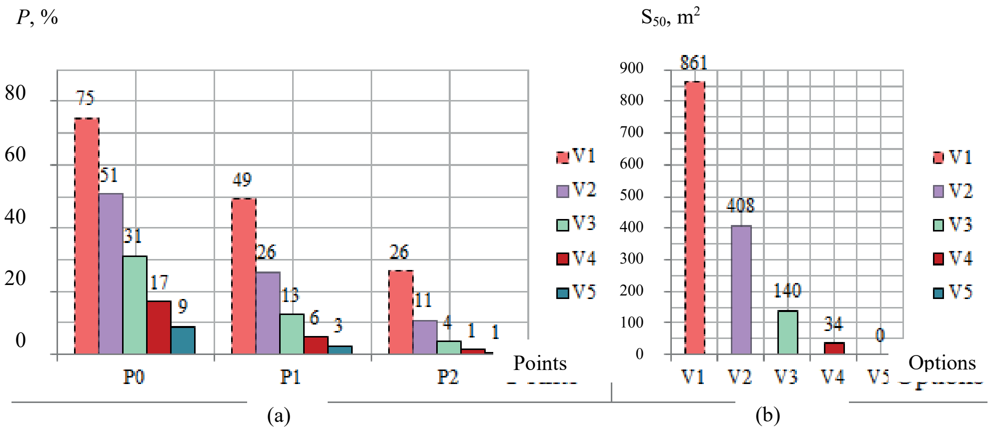

Fig. 9. Lethal impact conditional probability in control points P0–P2 (a) and hazardous area value (b) for different wind options V1–V5.

5. Discussion

It is unquestionable that experimental values of mass concentration obtained during large-scale field experiments are the most credible data that can be used to reconstruct hazardous zones after accidental release of dangerous substances [10]. Measured concentrations can be used by safety experts to assess the consequences caused by accidents to environment specifically connected to the area of dangerous technogenic objects. Unfortunately, large-scale experiments are very cost-ineffective, time-consuming, depend on specific weather conditions, and cannot really reflect all the circumstances of the accidents. That is the main reason why mathematical modelling of all the physical processes during accidental release and dispersion of dangerous gaseous chemicals into the atmosphere can be reproduced with all the details needed to take into account properties of substances, weather conditions, landscape relief, different release scenarios, etc. in order to evaluate hazardous zones around accident epicentre and assess the risks for human. It is evident from the results of intercomparison exercises on capabilities of different mathematical models to reproduce large-scale gas releases and dispersion in the atmosphere that CFD models are the most adequate tools in the hands of safety experts [12]. It can be noted that different types of CFD models (LES, RANS, and FDS) based on Navier–Stokes equations [39] consume huge computer resources and require careful selection of turbulence models, which depend on flow conditions. That is why, it is reasonable to use alternative CFD models which represent an Euler approach with source terms (simplified Navier–Stokes equations obtained by dropping the viscous terms in the mixture motion equations). Such model [30] is used in this work to investigate the influence of wind speed on environment consequences of accidentally spilled toxic liquid. It is also used in [31] to evaluate safety in mine tunnel during hydrogen explosion. This model is a tool to assess the consequences of gas explosion at refuelling stations [32] and evaluate an efficiency of mitigation measures and selection of the material of protecting wall against overpressure explosion effects [33]. A presented methodology can be used to compare different options of environment circumstances on the consequences for environment that can be extended on evaluating not only the toxic but explosive matters [12].

The boundaries of using the gas-dynamic model are outlined by considering an inviscid flow of a gas mixture, which is acceptable for the main core of the flow, which is explained by the properties of the Euler approach. The used model of liquefied toxic gas evaporation does not take into account the release of the gas phase due to liquid boiling, therefore it is limited to considering cases of ambient temperature, which is below the boiling point of the liquid phase of the toxic substance. It may be questionable also to use hazardous area as a comparing standard for light toxic gases because they rise up during dispersion process, but the methodology can be easily changed to evaluate hazardous volumes instead of hazardous areas in order to compare different environment options.

The next promising steps in the further development of the model of an accidental release of a toxic substance can be considered taking into account the contribution of the boiling of the liquid phase and the temperature of the underlying surface of the spill spot, as well as the consideration of combined accidental scenarios for the release of not only toxic, but also explosive substances.

6. Conclusion

The use of a non-stationary spatial mathematical model of the ingress of a toxic gas admixture into the surface layer of the atmosphere by evaporation of liquid from a spill spot is presented, which, unlike the known ones, uses non-local boundary conditions on the evaporation surface of a free form shape. To identify the influence of wind speed on the scale of the consequences of an accidental release of toxic gas on the environment, a mathematical model of multicomponent gas mixture movement is used together with a probabilistic model of probit analysis. The calculated area of the hazardous zone, where the conditional probability of lethal damage to a human due to a toxic dose inhalation exceeds 50 %, is used as a measure of the accident consequences scale.

Hazardous zones of toxic damage to the facility's personnel are identified, depending on the wind conditions. The results of the study indicate a significant influence of wind speed on the consequences of an accidental spill of a toxic liquid. The developed methodology can be recommended for use by safety experts to assess risk fields around potentially risky enterprises in order to mitigate accident consequences for the environment.

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