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Development of mathematical decision-making support tools for effective response to emergencies during the transportation of dangerous substances by road transport

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Abstract. Every year, the world sees an increase in the volume of hazardous goods transported by road. However, emergencies may arise related to the depressurization of containers (tanks, containers, cylinders, etc.) during the transportation of dangerous goods under various circumstances (traffic accidents, natural disasters, acts of terrorism, etc.). Furthermore, it can cause the ingress of hazardous chemicals into the environment and create significant risks for the population of the surrounding areas and habitat. The existing methods for assessing chemical accident consequences need to be revised. Therefore, they are not practical tools for solving problems of prompt response to emergencies associated with accidents while transporting dangerous substances by road transport. Unlike the existing ones, the authors developed new mathematical tools that consider all the main factors. They allow for determining the area of the affected zone, forecasting changes in its scale, and assessing risks to public health due to such emergencies. Comparison of the simulation results with the field measurements data showed high accuracy of the developed mathematical support.

1. Introduction

Hazardous materials are flammable, explosive, poisonous, corrosive, infectious, or radioactive products, for example, gasoline, fuel oil, oil, and chemicals. The most harmful substances are a



fundamental part of our daily life and industrial development despite the characteristics of these materials [1].

Approximately 4 billion tons of harmful substances are transported worldwide annually, according to [2]. The demand for hazardous materials in the United States is 3 to 4 billion tons each year. These materials are widely used in manufacturing, agriculture, medicine, and other industrial areas. In China, approximately 95% of hazardous substances are transported from manufacturers to customers by road transport [1]. Between 77.000 and 88.000 million tons of dangerous goods were transported by road within the European Union from 2009 to 2013 [3]. The authors [4] investigated 1932 accidents that occurred worldwide while transporting hazardous substances by road and rail from the beginning of the 20th century to July 2004. They showed that more than half of the accidents occurred on roads.

Danhighways traffic accidents are still considered low-probability compared to more frequent and highly unpredictable natural hazards despite the above facts. In addition, this type of accident is classified as an accident with significant consequences which can seriously affect the population and environment.

Analysis of the sources shows that several incidents during the transportation of harmful substances are deficient. Nevertheless, accidents occur, and some of the consequences are very serious. For example, in November 2005, there was an accident in Sinaloa (Mexico) with a truck transporting ammonia. Thirty-nine people died as a result of the accident [5]. More than 30 accidents related to the transportation of dangerous substances by road occur annually in China, according to statistics A truck [6]. Truck with liquefied natural gas crashed on the highway in front of the tunnel and overturned in Hunan Province on October 6, 2012. Five people died, and two more were injured, including three firefighters, due to the explosion. In 2013, a truck carrying fireworks ahead of Chinese New Year celebrations exploded and destroyed part of an overpass in China's Henan province and killed several people.

It is necessary to consider population density, traffic jams, and road closures while transporting harmful substances in urban areas. City traffic accidents can cause catastrophic human losses due to the high population density. Truck with chlorine collided with another vehicle in a metropolitan area of Nanjing, China, on March 29, 2005. It caused the death of 29 people and the evacuation of more than 10000 people. In October 2020, an 18-wheeler with 5000 gallons of sodium hydrosulfide (an extremely corrosive and toxic substance) overturned downtown Birmingham, England [7] (figure 1). In figure 2 shows a tanker truck accident in New Jersey that spilled 3000 gallons of fuel onto the roadway (February 2019).

Therefore, emergencies may arise related to the depressurization of containers (tanks, containers, cylinders, etc.) during the transportation of dangerous goods under various circumstances (traffic accidents, natural disasters, acts of terrorism, etc.). Furthermore, it can cause the ingress of hazardous chemicals into the environment and create significant risks for the population of the surrounding areas and habitat.

The studies [9,10] consider the risk of dangerous substances transportation as a measure of the probability and severity of damage to the population's health and components of the surrounding natural environment due to potential undesirable events. The risk from transporting harmful substances can be divided into two parts: the probability of an accident and the consequences if it occurs. Reniers et al [11] developed a risk assessment methodology for moving hazardous materials. They divided routes into smaller segments using multi-criteria analysis and assessing the likelihood of accidents involving dangerous vehicles leading to fatalities. The work [12] is aimed at determining the impact of hazardous traffic accidents on people with disabilities. It is done to provide the knowledge base necessary for creating competent disaster preparedness procedures. The article [1] contains a model built to reduce risks of transportation of harmful substances and transportation costs, considering several restrictions. This model was tested on a realistic example of transporting hazardous substances in the densely populated metropolitan



Figure 1. Accident in Birmingham (October 2020) [7].



Figure 2. Tanker truck crash in New Jersey [8].

area of Shanghai (China).

Popov et al [13, 14] considered several methods used to assess the situation in the case of accidents related to the spill (emission) of dangerous chemicals from technological containers on road transport. Their shortcomings were identified. It was also established that these methods are not practical decision-making support tools for the prevention and rapid elimination of the consequences of such emergencies. Therefore, developing new mathematical and software tools better than existing analogs in all leading indicators is an urgent and essential scientific problem.

The research aims to develop mathematical tools for assessing the consequences of accidents while transporting dangerous substances by road transport.

2. Development of mathematical means

The developed mathematical means of risk assessment should take into account the realities of the current situation during transporting of chemically hazardous substances (CHS) by road transport, possible types of accidents or partial depressurization, for example, as a result of terrorist acts. We used studies [15–17] to build such tools. Those studies most adequately describe the consequences of forecasting chemical accidents during transportation by road transport of the CHS.

Potential chemical risk in the vicinity of an accident of a mobile chemically hazardous object and the settlement zone near such an object is determined by the formula:

$$R_x = \sum_i^m Q^* \times P_i \times R_i, \tag{1}$$

where,

Q^* – case frequency during the year;

P_i – the probability of a person living in the i -th habitat (tables 1, 2);

R_i – conditional probability of injury to a person in the i -th habitat.

Table 1. Average daily distribution of the urban population by place of residence [16].

Time of day, hour	Residential and public buildings	Production buildings	In transport			Outside		
			Cities with a population (million people)					
			0.25... 0.5	0.5... 1.0	More than 1.0	0.25... 0.5	0.5... 1.0	More than 1.0
1...6	0.94	0.06	-	-	-	-	-	-
6...7	0.74	0.06	0.07	0.09	0.12	0.13	0.11	0.08
7...10	0.22	0.5	0.09	0.11	0.17	0.19	0.17	0.11
10...13	0.28	0.52	0.06	0.07	0.1	0.14	0.13	0.1
13...15	0.45	0.37	0.04	0.04	0.07	0.14	0.14	0.11
15...17	0.27	0.49	0.08	0.09	0.13	0.15	0.15	0.12
17...19	0.45	0.24	0.1	0.12	0.15	0.2	0.18	0.15
19...24	0.77	0.14	0.04	0.04	0.06	0.05	0.05	0.03

Currently, the occurrence frequency of dangerous event Q_j^* is calculated by the methods of risk theory or according to statistical data.

The occurrence frequency of dangerous event Q_j^* can be determined using the theory of expert evaluations. Expert assessments of the frequency of technogenic accidents are carried out taking into account their distribution into five levels:

Table 2. Average daily distribution of the rural population by place of residence [16]

Time of day, hour	Field and agricultural production		Residential buildings	
	During the day	At night	During the day	At night
1...6	0.25	0.1	0.75	0.9
6...7	0.6	0.4	0.4	0.6
7...10	0.75	0.75	0.25	0.25
10...13	0.8	0.8	0.2	0.2
13...15	0.85	0.75	0.15	0.25
15...17	0.85	0.5	0.15	0.5
17...19	0.8	0.4	0.2	0.6
19...24	0.5	0.2	0.5	0.8

- frequent failure: $> 1 \text{ year}^{-1}$;
- probable failure: $1 \dots 10^{-2} \text{ year}^{-1}$;
- possible failure: $10^{-2} \dots 10^{-4} \text{ year}^{-1}$;
- rare failure: $10^{-4} \dots 10^{-6} \text{ year}^{-1}$;
- almost impossible failure – expected frequency of occurrence $< 10^{-6} \text{ year}^{-1}$.

The probability of people being in the i -th environment P_i is determined based on the production activity of personnel. Therefore, calculation of the conditional probability of damage or mathematical expectation of injuries from the negative impact of CHS presents specific difficulties. These difficulties are related to the toxic effect on humans of different types of CHS. It is based on their physical and chemical properties and other exposure times depending on the presence in the zone of possible chemical damage.

The conditional probability of damage in the case of being in the zone of chemical injury is mainly determined by the location of damage, considering the height of the cloud rise. The site is formed due to the spread of the affected cloud to the residential part of the settlement in the braking area and the area of the emergency stop of transport from CHS and can be defined as [15]:

$$R = \frac{S_B + S_F}{S_S}, \quad (2)$$

where,

S_B – area of the threshold chemical damage in the braking zone, km^2 ;

S_F – area of the threshold chemical damage in the size of the emergency stop of transport with CHS, km^2 ;

S_S – area of the settlement, km^2 .

The area of the threshold chemical damage in the braking zone and the size of the emergency stop is determined by the depth of the threshold damage in these areas.

The area of chemical damage in the braking zone can be calculated by the following formula taking into account the rise of the affected cloud [15]:

$$S_B = \sum_{i=1}^n S_{B_i} \times \frac{H_C}{H_B}, \quad (3)$$

where,

S_B – an area of chemical damage in the i -th braking zone, It is defined as:

$$S_B = \frac{\pi\varphi}{360^\circ} [D_B + (D_{l_i} - D_B) \times k_m]^2 - D_B^2, \tag{4}$$

where,

D_B – distance from the building beginning to the road, m;

D_{l_i} – depth of the threshold lesion at the i -th braking zone, m;

l – is corresponded to the section of the final braking route to the emergency stop, m;

$l = 1$ – is compared to the braking route area when $D_l = D_B$, m;

k_m – coefficient of spread reduction of the affected cloud depending on the building and number of floors of the buildings. It is defined in the paper [15].

The area of chemical damage in the emergency stop zone can be calculated by the formula taking into account the growth of the affected cloud,

$$S_F = \frac{\pi\varphi}{360^\circ} [D_b + (D_{n_i} - D_b) \times k_m]^2 - D_B^2 \times \frac{H_C}{H_B}, \tag{5}$$

where,

D_{n_i} – depth of the threshold damage in the emergency stop zone;

φ – spread angle of possible chemical damage. It is determined according to table 3.

H_C – the height of the cloud threshold elevation, m;

H_B – the size of buildings in the settlement, m.

Table 3. Angular dimensions of zones of actual chemical damage

Degree of vertical stability	Inversion	Isometry	Convection
φ , degree	Steady wind		
	11.5	14.5	48.5
	Unsteady wind		
	47	48	69

Thus, determining the threshold depth, lethal chemical damage, and height of their cloud rise are essential in calculating the conditional probability of damage during such events.

The formula determines the length of the spill section before the damaged vehicle stops:

$$L_S = V_D t_{rd} + L_{mn}, \tag{6}$$

where,

V_D – speed of transport at the moment of depressurization, km/h;

t_{rd} – driver reaction time (0.3–1.7 sec);

L – braking distance. It is defined as [16]:

$$L_{mn} = V_D t_b + V_D^2 / 2\alpha_{max}, \tag{7}$$

where,

t_b – brake system activation time 0.3-0.5 sec;

α_{max} – maximum acceleration (deceleration) of transport, m/s^2 , $\alpha_{max} = gK_g$ ($g = 9.81 m/s^2$)

K_g – coefficient of tire adhesion of transport with the road surface. For vehicles in dry weather conditions, $K_g \approx 0.5$; during the rain $K_g \approx 0.25$.

Assessment of the reliable width of the CHS spill and its height (thickness) of the spill h_l in the braking zone has great importance. In addition, the amount of CHS will determine if it spilled in this area, ultimately affecting the depth of chemical damage.

The accepted assumption in the existing methods is that determination of the CHS spill width is equivalent to the spill of petroleum products (1 liter of liquid is spilled on 0.15 m² of the road). A statement that $h_l=0.05$ m is incorrect in emergency braking due to the small amount of spilled CHS with a small depressurization on a relatively long braking distance. Based on this, it is necessary to determine the height of the CHS spill on the underlying surface, taking into account the spill area's width and length and the CHS's density. However, this is different based on the various physical and chemical properties of CHS.

One of the main parameters affecting the depth of the secondary damage cloud as an accident result at the chemically hazardous facility with a CHS spill is the area of the spill, the height of the liquid layer (thickness of the spill film), and degree of infiltration of CHS into the underlying surface. However, determining the actual spill area of CHS is somewhat complicated due to the wide range of CHS. In addition, such substances have different physical properties. So, the liquid layer's thickness may differ and depend on the type of underlying surface [18].

The correction coefficients of the spreading surface $K_{n.xy}$ and infiltration K_{in} are one of the ways to solve the problem of the influence of the nature of the CHS spill and the degree of its penetration into the underlying surface. Such coefficients were obtained experimentally.

Prompt determination of the spill area plays a crucial role in the decontamination (disinfection) of the territory in the case of an accident with the CHS spill. The spill area of CHS $S_{l.xy}$ can be defined by the formula taking into account the experimentally determined $K_{n.xy}$:

$$S_{l.xy} = \pi(3.018V_y^{0.393}\vartheta_y^{-0.116}t_l^{0.115}K_{n.xy})^2, \tag{8}$$

where,

V_y – the volume of spilled CHS of y -the type, m³;

ϑ_y – kinematic viscosity coefficient CSH of y -the kind, m²/s;

t_l – fluid spreading time, min.

The height of spilled CHS y -the type on the underlying surface of the x -the type $h_{l.xy}$ (m) can be defined taking into account $S_{l.xy}$ using the formula:

$$h_{l.xy} = \frac{m_y}{\rho_{ly} \cdot S_{l.xy}}, \tag{9}$$

where,

m_y – mass of spilled CHS on the underlying surface of a y -th type, kg;

ρ_{ly} – CHS density y -the type, kg/m³.

The formula determines the evaporation time (striking action) of CHS:

$$T_{\nu d} = \frac{h_l \cdot \rho_l}{K_2 K_4 K_7}, \tag{10}$$

where,

K_2, K_4, K_7 – coefficients according to [15].

The amount of liquid CHS in the braking zone m_b is determined by the formula taking into account the fraction of infiltration during the shedding to stop the damaged transport:

$$m_b = \int_0^{t_{nm}} G(t)dt = K_{in} \left(G_0 \cdot t_{nm} - \frac{\rho_{ly} \cdot g \cdot \mu^2 \cdot S_{ot}^2}{2S_s} \cdot t_{nm}^2 \right), \tag{11}$$

where,

K_{in} – infiltration coefficient;

G_0 – mass consumption at the initial point in time (kg/s) is determined by the formula [19] for small quantities of depressurization area:

$$G_0 = \mu \cdot \rho_l \cdot S_{ot} \sqrt{2g(h_0 - h_{ot})}, \quad (12)$$

$t_{he} = t_{rd} + L_{nm}/V_b$ – CHS spilling time from the moment of depressurization of the capacity to stopping damaged transport;

V_b – averaged braking rate that is defined as $V_D/2$, m/s;

μ – spilling coefficient 0.6 – 0.8;

S_{ot} – hole area, m²;

S_s – cross-sectional area;

h_0 – the initial height of the liquid column in the vessel, m;

h_{ot} – hole height, m.

Stop of transport leads to a spill of CHS rest contained in the tank: or until it is over at $h_{ot} = 0$, or partially (at $h_{ot} > 0$), or up to the time of sealing the hole.

The amount of spilled CHS is defined by the formula taking into account the proportion of infiltration m_2 after stopping the damaged transport:

$$m_2 = K_{in} \left(\mu \cdot \rho_l \cdot S_{ot} \sqrt{2g(h'_0 - h_{ot})} \cdot t_F - \frac{\rho_l \cdot g \cdot \mu^2 \cdot S_{ot}^2}{2S_s} \cdot t_F^2 \right), \quad (13)$$

where,

t_0 – time of CHS spill after vehicle stops, min;

h'_0 – the initial height of the liquid column in the tank from the moment of stopping the transport is defined by the formula [20]:

$$h'_0 = h_0 - \frac{\mu \cdot S_{ot}}{S_s} \sqrt{2g(h_0 - h_{ot})} \cdot t_{nm} + \frac{g \cdot \mu^2 \cdot S_{ot}^2}{2S_s^2} \cdot t_{nm}^2, \quad (14)$$

Generally, S_S can be calculated as follows [5]

$$S_S = \int_0^{t_{nm}} 2l \sqrt{h'_0(t) \cdot [D - h'_0(t)]} dt, \quad (15)$$

At short-term spill it can be defined as:

$$S_S = 2l \sqrt{h_0(D - h_0)}, \quad (16)$$

A long-term spill can be defined as:

$$S_S = l \left[\sqrt{h_0(D - h_0)} + \sqrt{h'_0(D - h'_0)} \right], \quad (17)$$

where,

h'_0 – values of the liquid column in the tank for a specific time of the spill, m;

l – tank length, m;

D – tank diameter, m.

The formula defines the time of entire spill through a small hole nm :

$$t_{nm} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (18)$$

The amount of spilled CHS in the emergency stop area with the complete ending (destruction) of the capacity taking into account the fraction of infiltration, is defined as:

$$m_F = K_{in} \cdot (Q_0 - m_b) \tag{19}$$

The following formula calculates the depth of chemical contamination:

$$D_c = \min(D_n(D_D); D_{fr}), \tag{20}$$

where

$$D_n = 0,95 \cdot \sqrt[1+b+d]{\frac{m}{0,13(2\pi)^{\frac{3}{2}} \cdot a \cdot c \cdot C_n}} K_B \cdot K_t, \tag{21}$$

For lethal cases

$$D_D = 0,95 \cdot \sqrt[1+b+d]{\frac{m}{0,13(2\pi)^{\frac{3}{2}} \cdot a \cdot c \cdot C_D}} K_B \cdot K_t, \tag{22}$$

where

- m – CHS mass taking into account the fraction of infiltration, kg;
- C_n, C_D – the value of the threshold and fatal cases for CHS is considered respectively, g/m³;
- K_B, K_t – dependence of depth damage on wind speed and coefficient of exposure to air temperature to the depth;
- a, b, c, d – coefficients of the steppe variance models determined according to [5];
- The formula defines D_{fr} :

$$D_{fr} = U_n \cdot T_{vd}, \tag{23}$$

where

U_n – transfer rate of the cloud front at the given wind speed data and degree of vertical stability of the air, km/h, is determined according to [15];

T_{vd} – time of the dramatic action determined by the formula 10.

The height of the lifting cloud for the limited degree of damage, taking into account sheltering of the population in buildings, is determined by the formula:

$$H_n = c \cdot D_n \sqrt{2 \ln \frac{m \cdot \rho_a (1 - e^{-k_1 \cdot t_{loc}})}{\rho_g \cdot 0,13 \cdot (2\pi)^{\frac{3}{2}} C_n \cdot a \cdot c \cdot D_n^{1+b+d}}, \tag{24}$$

for lethal cases

$$H_D = c \cdot D_D \sqrt{2 \ln \frac{m \cdot \rho_a (1 - e^{-k_1 \cdot t_{loc}})}{\rho_g \cdot 0,13 \cdot (2\pi)^{\frac{3}{2}} C_{cm} \cdot a \cdot c \cdot D_D^{1+b+d}}, \tag{25}$$

where,

- ρ_a, ρ_g – air and gas density of the appropriate type of CHS respectively, kg/m³;
- t_{loc} – time of localization of the accident;
- k_1 – a multiplicity of air exchange in premises of the building, h⁻¹;
- k_2 – coefficient of the wind speed value;
- k_T – ambient air temperature coefficient.

Estimated air temperatures and air exchange requirements in the premises are described in detail in [21].

It should be noted that the disadvantage of the proposed mathematical means is in finding input data. It requires depressurization area to calculate the mass of the spilled CHS by the formula 6.

Calculations were made and compared with full-time measurements to evaluate the accuracy of the proposed mathematical means with the results of other techniques used on the example of an accident occurring in October 2020 at the Birmingham Center (England) [7,22]. Input: there was a tanker depressurization with sodium hydrosulfide, 5000 gallons = 22.73 m³, the hole was 0.04 m² in the bottom, the initial height of the liquid column was 1.5 m, the speed of movement of vehicles was 60 km/h, there was no precipitation inversion, the air temperature was +15°C, the wind speed was one m/s, elimination time was 450 min. Results of calculations of the CHS spilled area on the underlying surface and depth of chemical damage are presented in table 4.

Table 4. Comparison of the calculations results of the CHS spilled area on the underlying surface and the depths of chemical levels defined in various ways.

	Method [23]	Method [24]	Method [25]	Model [15]	Model [16]	Author model	Field measurement
Spill area, m ²	268	280	482	436	323	347	370
δ, %	28	24	30	18	13	6	-
Depth of chemical damage, m	952	985	1476	1347	1130	1158	1246
δ, %	24	21	18	8	9	7	-

The table shows that mathematical models of pollution of the earth’s surface and air as a result of the accident during CHS transport by road allow us to determine the necessary parameters of the damage zone with high accuracy. A significant advantage of such models is that, unlike other methods, they take into account: the nature of the underlying surface; the absorption of hazardous chemicals in case of an accident; the parameters of the spill area for various hazardous chemicals.

Subsequently, it is planned to develop a software-modeling complex based on the results obtained. The complex will become an effective tool for supporting management decisions on a prompt response to such situations to ensure a high level of protection of the population and environment, minimize the extent of damage, and ensure the effective elimination of appropriate consequences.

3. Author contributions

The research results presented in this publication are a collective effort of the individual authors:

- **Andrii V. Iatsyshyn** contributed to the conception and design of the study, analyzed the literature, reviewed incidents in Birmingham (October 2020) and New Jersey (February 2019), determined the quantity of chemically hazardous substances in the braking area, and assessed the reliability of the proposed mathematical tools.
- **Liudmyla M. Markina** evaluated the potential chemical risk in the vicinity of the accident and settlement zone, determined the average daily distribution of urban and rural population by place of stay, and assessed the reliability of the proposed mathematical tools.
- **Olha O. Tiutiunyk** determined the main parameters affecting the depth of secondary damage cloud as a result of an accident at a chemically hazardous facility, determined the initial height of liquid column in the tank at the moment of transport stoppage, and assessed the reliability of the proposed mathematical tools.
- **Vadym V. Tiutiunyk** determined the area and extent of chemical damage in the braking area, analyzed the angular dimensions of actual chemical damage zones, and determined the depth of chemical damage and height of striking cloud rise for limiting degree of damage.

- **Elnur Shukurlu** determined the spill area of chemically hazardous substances, determined the height of spill on underlying surface, determined evaporation time (impact effect) of chemically hazardous substances, and determined quantity of spilt chemically dangerous substances in emergency stop area.

4. Conclusions

Every year there is an increase in the transportation of dangerous materials by road worldwide. It is accompanied by emergencies related to the depressurization of containers (tanks, containers, cylinders, etc.) in various circumstances (road accidents, natural cataclysms, terrorist acts, etc.). In such cases, dangerous chemicals can get into the environment and create significant risks to the population of surrounding areas and the environment.

Existing methods of effects evaluating chemical accidents cannot be used to solve the task due to their significant disadvantages (non-considering nature of the underlying surface; CHS absorption; parameters of spilling area of different CHS; use of mathematical apparatus obtained only empirically; use stationary chemically hazardous objects; they do not allow calculate risks of such emergency events for the population health).

New mathematical means of accident assessment were developed to transport hazardous substances in road transport. They, unlike existing ones, take into account the parameters of the car, speed of the driver's reaction, parameters of the depressurization of the tank, nature of the underlying surface, and parameters of construction in the area place of stay. The high accuracy of the proposed mathematical means is confirmed by comparing it with data from field measurements and results of calculations by other techniques.

Further implementation of the developed mathematical support in the form of software will be an effective tool for solving problems of preventive forecasting and prompt response to emergencies related to the entry of such substances into the environment while transporting them by road.

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