Assessment of the size of the danger zone caused by an accident during transportation of a dangerous chemical substance

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Abstract

Air pollution is the central topic of all discussions related to environmental protection. Modelling the spread of pollution is one of the methods used to predict the spread paths and levels of pollution and to act in order to combat this problem. The paper presents modelling of dispersion of ammonia through the air using a software tool ALOHA (Areal Locations of Hazardous Atmospheres) based on the Gaussian model of particle dispersion. Modelling in the work is based on data related to the accident that occurred in December 2022 in the vicinity of the city of Pirot, Serbia, as well as on real meteorological data that were collected during the time of the accident and the spread of pollution. As a result of modelling, zones with increased ammonia concentration are obtained. The zone areas will depend on the ammonia concentration at the source and meteorological conditions during the period of the leakage. The aim of the paper is to point out the need to introduce modelling into the operational centres of the local police or military units in charge of emergency situations, as well as additional safety protocols when transporting dangerous goods.

Keywords: Gaussian model; areal locations of hazardous atmospheres; dispersal; ammonia; Pirot.

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1. INTRODUCTION

The great technological progress of civilization and growth of both the smaller and the leading economies of the world led to the fact that exploitation of chemically hazardous substances experienced a huge expansion, and thus there was a significant increase in the number of chemical accidents. In this case, China could be a very good example [1]. The number of chemical accidents with injured persons in this country in the period between 2006 and 2017 amounted to a total of 3,974 [2]. A significant number of those chemical accidents (in China) occurred during the transport of dangerous chemical substances, amounting to 2,657 [3]. That is not a surprise since from more than a 6,000 existing dangerous goods that are transported, 2,000 of them is transported by public roads in China [4]. A large number of accidents were also recorded in maritime transport amounting to 650 for European ports alone for the period from 1919 to 2019 [5]. Data accessible at the global level show a large number of accidents during the transport, roughly 35 %, while 40 % happen during production and the rest present accidents occurring while in storage [6]. In Serbia on the state level the figures are about the same [6]. All countries in the world have to fight with these problems, Serbia not being an exception [7], given the fact that dangerous chemical substances, such as ammonia, cause serious health consequences in the living organisms [8].

Modelling the spread of pollution is one of the methods used to predict the movement path and level of pollutants in a certain zone [9]. There are many mathematical models used as a base for various software tools, programming codes or entire systems utilized to predict propagation of particles [10,11]. The basic division of mathematical models lies in the area of their application [11], but also software tools and modelling systems (such as AERMOD View, Lakes Software, Canada) are divided according to the field of application. Modelling of particles caused by road traffic [12], is not the same as that for particles originating from industrial zones [13], primarily because the shapes and surfaces of

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the pollution sources themselves are different, as well as dimensions and movement frequency of the particles. Also, different modelling approaches are applied for pollution originating from continuous sources [14] and for that arising due to accidents having a certain "shorter" duration [9,15].

2. MATERIALS AND METHODS

The most commonly used mathematical models for predicting the movement path of pollutant particles are the Gaussian dispersion model and the Euler-Lagrange model. Both models are also used with some modifications [16]. The most commonly used Gaussian dispersion models are the Gaussian Plume Model [17] and the Gaussian "Puff" Model [18].

The Gaussian plume model is a basic model, very simple to implement. Let's assume that the source is continuous with the power *Q* (usually expressed in μg s^{-1} representing the rate at which pollutants are emitted). If the source is located at an effective height (*h*), and the wind speed is constant (*u*) then the concentration of pollutants (usually expressed in μg m^{-3}) can be determined by the Equation (1) [19]:

$$C = \frac{Q}{2\pi\sigma_y\sigma_z u} e^{-\frac{y^2}{2\sigma_y^2}} \left[e^{-\frac{(z-h)^2}{2\sigma_z^2}} + e^{-\frac{(z+h)^2}{2\sigma_z^2}} \right] \tag{1}$$

where the coordinate *y* determines the width of the plume, while the position on *z* axis determines the height of the plume, and the position on *x* axis determines the reach of the plume (Fig. 1). Also, the wind direction is in the direction of the x axis. Parameters σ_y and σ_z represent the standard deviation of pollutant dispersion on the given axis, which are obtained by using models combining experimental data and theoretical considerations. The level of turbulence and, correspondingly, σ_y i σ_z, depend on atmosphere stability and orographic structure. Those parameters are divided into classes according to the levels of atmosphere stability defined as: A (extremely unstable), B (unstable) i C (mildly unstable), neutral class D, and stable E (stable) i F (very stable) [20].

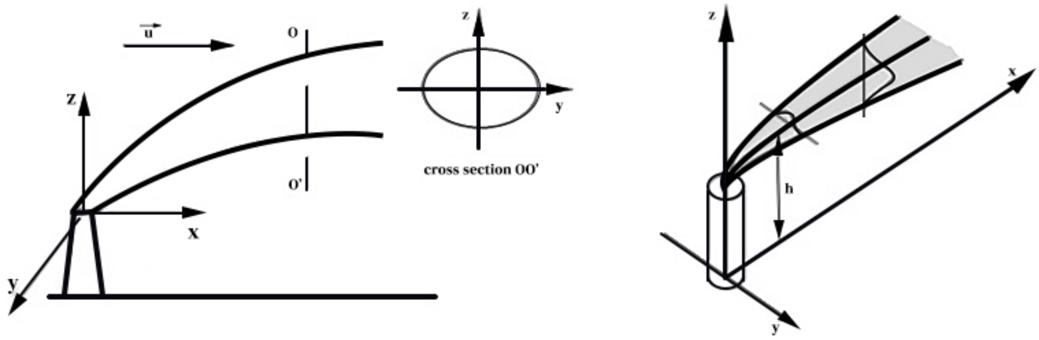

Figure 1. Orientation of the coordinate axes when modelling the smoke plume

There are several models to determine σ_y and σ_z, among which the most common are the Pasquill-Gifford model and Briggs model [20]. Horizontal and vertical dispersions are calculated by this simple Equations (2) and (3) [21]:

$$\sigma_y = ax^b \quad (2); \quad \sigma_z = cx^d \quad (3)$$

The parameters a, b, c, and d from these equations are available in tabular form in many references, including [21].

Areal Locations of Hazardous Atmospheres (ALOHA®) is a software tool introduced by the US Environmental Protection Agency (EPA) and its primary use is for modelling chemical accidents [22] and determination of the pollution level and distribution after an accident. It is very convenient for use in the cases of accidents that are related to transport of dangerous goods primarily of chemical nature [23]. In specific, sizes and shapes of the tank as well as of damage could be chosen with specifying a distance from the bottom. It is possible to model accidents from ground fixed reservoirs [24,25], as the one arising from a chemical puddle that evaporates, and even if the source of pollution is a damaged pipe or a puddle. ALOHA is based on the Gaussian model of dispersion and in the menu “calculation options” it offers to use the Gaussian model or the Heavy Gas Dispersion model or alternatively the option “Let ALOHA to decide (select this if unsure)", and the method will be determined based on the substance involved. This application could be used for damage control and respond, risk assessment and management, or as a quick response in the case of an accident [26]. ALOHA offers even more diversity, so that the accident could be a toxic cloud, area in a blaze, an accident involving explosion and through forming an area of dissipation [27].

3. RESULTS AND DISCUSSION

The accident for which the modelling was done happened on December 25, 2022. between 16:30 and 17:30, near the town of Pirot, Serbia, on the bend of the railway line between Staničenje and Sopot, at coordinates 43°13' N, 22°32'21'' E. According to the reports of some media, the accident happened exactly at 16:36, while others state that it took place at 17:30. The accident occurred when four out of a total of 20 tank wagons derailed. The tankers were transporting ammonia from Bulgaria to the town of Šabac. According to the media and officials from the Department for emergency situations, they were overloaded and carried 45 t each. Figure 2 shows technical characteristics of the tanks with the length of 16.1 m, volume of 95.3 m^3, corresponding to the diameter of 2.75 m. These data are very important presenting input parameters regarding the source of pollution.

Figure 2. Specifications on tanks transporting ammonia

Although there is uncertainty about the initial size and shape of the hole through which ammonia leaked, the hole location and size can still be inferred from published leak data. According to publicly available data, the tankers were returned to the track on January 14, 2023, with the remaining 20 t of ammonia, from the initial 45 t. Based on that fact, it can be assumed that the hole was rectangular, 5 cm long and about 3 cm wide or round shaped equivalent, and it had to be about 90 cm from the bottom, approximately one third of the tank height.

Modelling was performed for three scenarios. The first scenario includes meteorological data that were reported on that day (December 25, 2022). It is also the most likely scenario for the given event. The other two scenarios are given for meteorological data that were reported on the coldest and the hottest day of the year. These are practically the limit values for the year 2022. Since the range of variables is determined in this manner, it can be presumed that particle dispersion for the studies case falls between those limits.

Scenario 1 (the most probable one)

Meteorological data is adopted from two sources [28,29], which verify that at the given time from 17 till 18 h, temperature was in the interval from 9.3 and 7.7 °C. Thus, the value of 8.5 °C was accepted for the calculation as the arithmetic mean. The substance in the tank was assumed to be at the same temperature, which is ambient temperature. The summary of meteorological data is presented in Table 1. Under these conditions, 45 t of liquid ammonia occupies 68.2 % of the entire tank volume.

Table 1. *Meteorological data (at the moment of incident)*

Parameters	Actual conditions
Temperature	8.5 °C
Wind direction	West
Wind speed	2 m/s
Humidity	70 %
Cloudiness	5/10
Atmospheric stability level	F

The option of ALOHA choosing the appropriate model, Gaussian or Heavy Gas Dispersion model, was used resulting in selection of the second model. The predicted leakage results are as follows – two streams of ammonia as a mixture of liquid and aerosol, leaked initially at the average flow rate of 1,350 kg min^{-1} followed by a sudden drop about 20 min later (Figure 3); the total amount of ammonia that escaped in the environment is 25,718 kg.

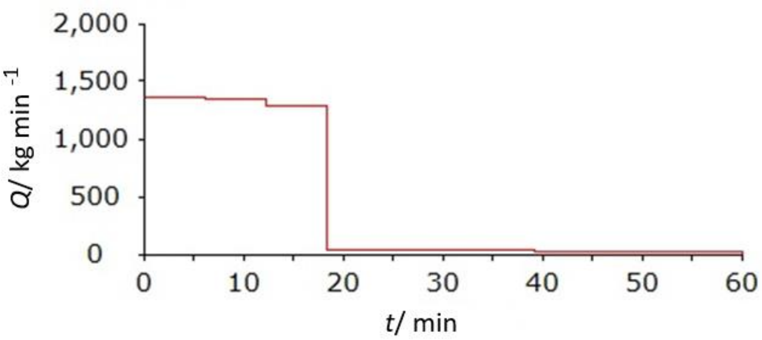

Figure 3. Predicted source strength – flow rate, Q, over time, t, after the start of the accident in Scenario 1

The potential danger zone was about 200 km^2 in size (Fig. 4). The zone of the highest pollution (more than 1,100 ppm, which corresponds to the value of 1.1 kg m^{-3}) extended 2.1 km from the source (red zone in Fig. 4), the zone of significant pollution (more than 160 ppm, *i.e.* 0.16 kg m^{-3}) extended at a distance of 6 km from the source, while the zone of relatively low pollution (more than 30 ppm, *i.e.* 0.03 kg m^{-3}) extended at a distance of 10 km from the source. All concentrations are given for a period of 60 min, although considering the source power diagram (Figure 3), it is clear that the released amounts from the source after 20 min from the initial moment are negligible.

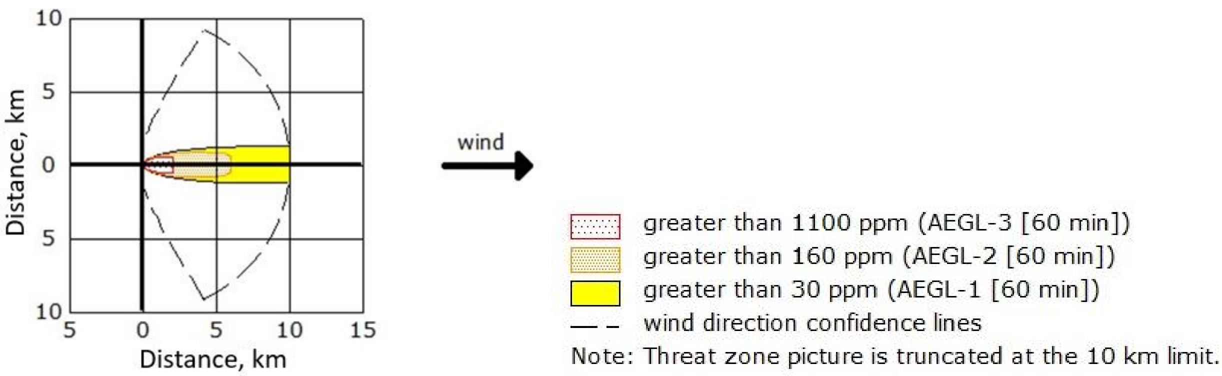

Figure 4. Toxic threat zone - area affected by a certain concentration of ammonia predicted in Scenario 1

Geographical representation of the threat for the city of Pirot and the zones obtained by modelling in ALOHA can be seen in Figure 5. The highest concentration of pollution was at the highway intersection A4, which is why the traffic on this part of the road was stopped. Only due to the favourable meteorological conditions (primarily the wind direction) concentrations in the populated places of Sopot, Staničenje and Pirot were not the highest possible, that is, the red and orange zones bypassed these densely populated places. In this accident, 50 people had injuries to their respiratory organs due to ammonia inhalation, and two people lost their lives.

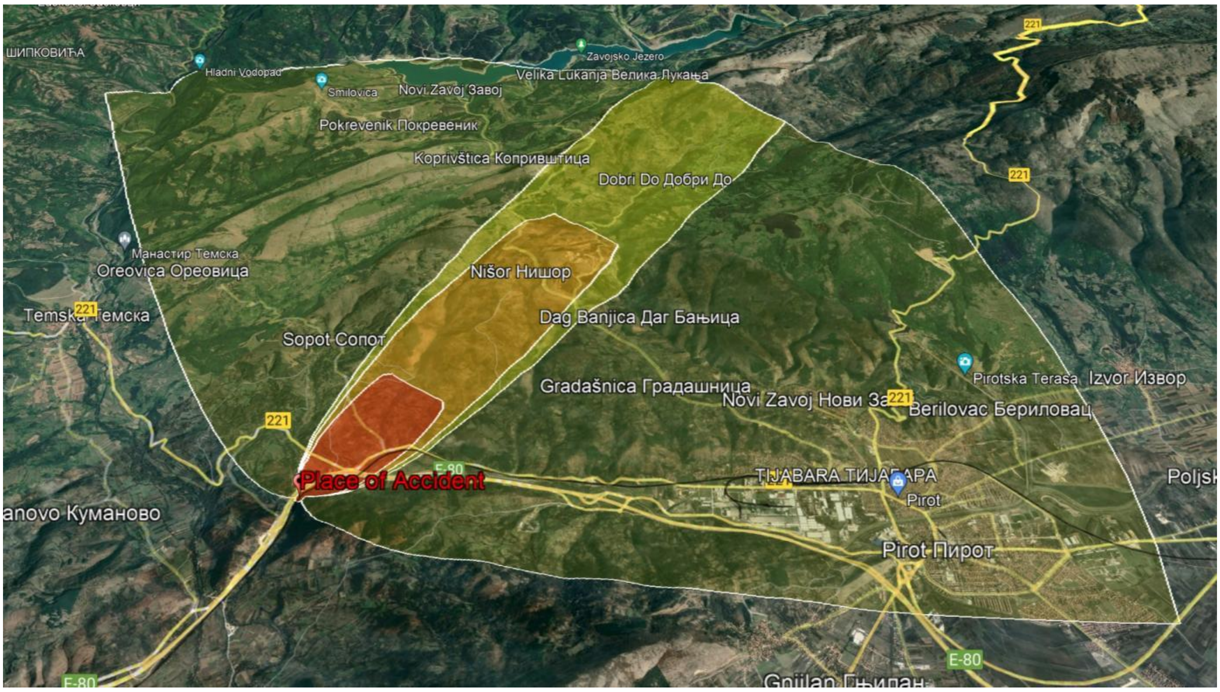

Figure 5. Geographical view of threat zones in Scenario 1

Scenario 2 (extreme winter condition)

Day with the lowest temperature in 2022 was January 25. The complete meteorological data are shown in Table 2 [28,29]. Under these conditions, 45 t of liquid ammonia occupies 64.8 % of the entire tank volume.

Table 2. Meteorological data (under extreme winter conditions reported for January 25, 2022)

Parameters	Winter conditions
Temperature	-16.5 °C
Wind direction	South/South East
Wind speed	1 m/s
Humidity	60 %
Cloudiness	0/10
Atmospheric stability level	F

The predicted leakage results are as follows – two streams of ammonia as a mixture of liquid and aerosol, leaked at the average flow rate of 713 kg min^{-1} initially followed by a sudden drop 35 min later (Fig. 6); the total amount of ammonia that escaped in the environment is 23,935 kg.

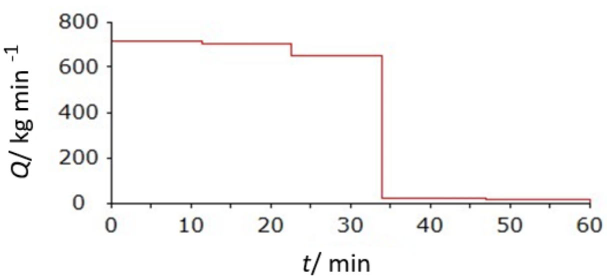

Figure 6. Source strength – flow rate depending of duration from start point

The potential danger zone was a circle about 314 km^2 in size (Fig. 7). The zone of the highest pollution extended 2.2 km from the source (red), the zone of significant pollution extended at a distance of 5.8 km from the source (orange), while the zone of relatively low pollution extended at a distance of more than 10 km from the source (yellow). All concentrations are given for a period of 60 min.

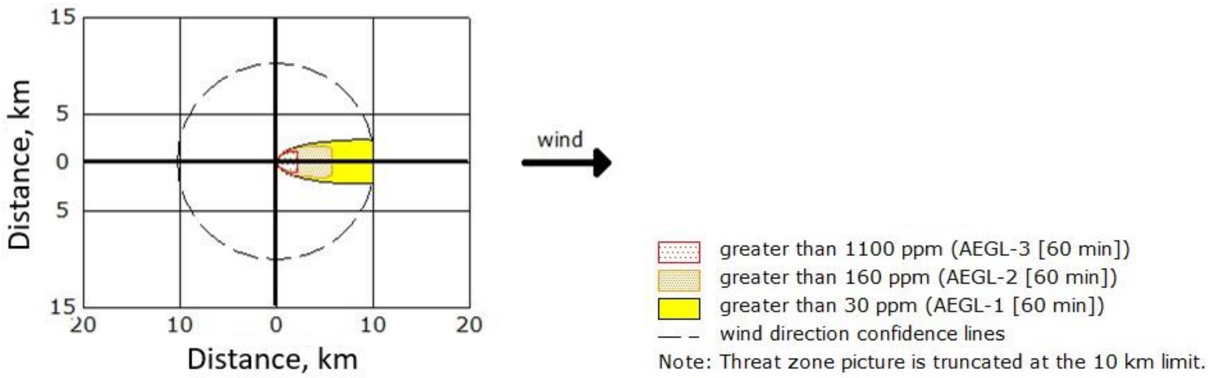

Figure 7. Toxic threat zone - area affected by a certain amount of hazard

Geographical representation of the threat for the city of Pirot and the zones obtained by modelling in ALOHA can be seen in Figure 8.

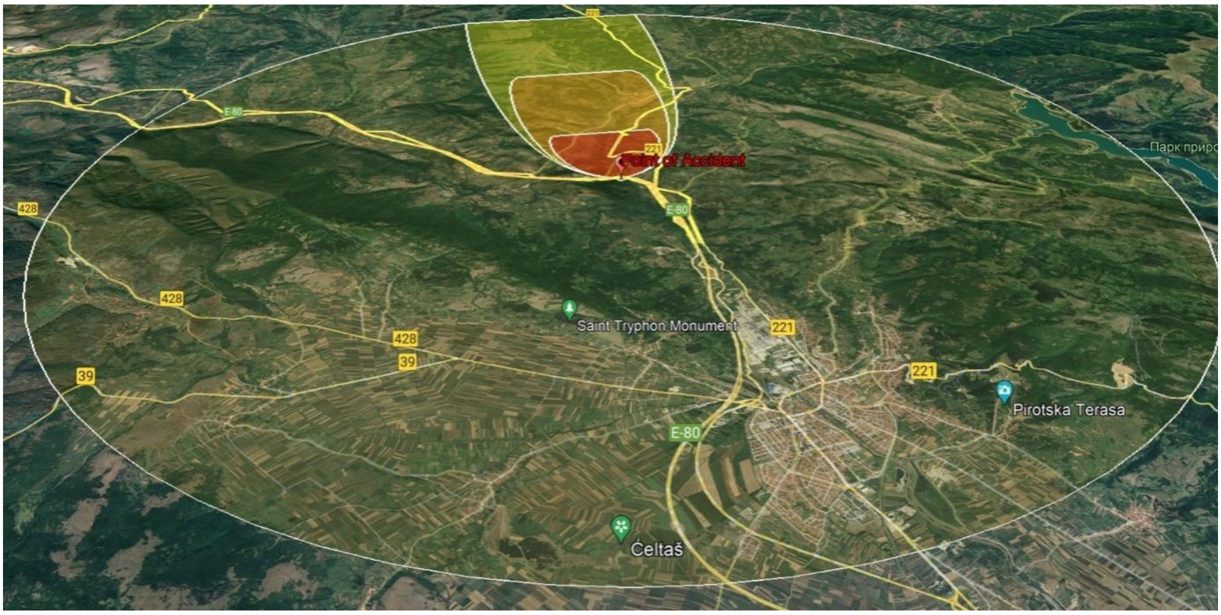

Figure 8. Geographical view of threat zones in Scenario 2

In this scenario the outcome is almost the same as in Scenario 1, but since the wind was blowing from a different direction, dangerous zones are completely away from the populated areas.

Scenario 3 (extreme summer conditions)

The warmest day in 2022 was July 23 for which all meteorological data are provided in Table 3 [28,29]. Under these conditions, 45 t of liquid ammonia occupies 73 % of the entire tank volume.

Table 3. Meteorological data (under extreme summer conditions reported for July 23, 2022)

Parameters	Summer conditions
Temperature	37 °C
Wind direction	North/Northwest
Wind speed	2 m/s
Humidity	30 %
Cloudiness	0/10
Atmospheric stability level	B

The predicted leakage results are as follows – two streams of ammonia as a mixture of liquid and aerosol, leaked at the average flow rate of 2,150 kg min^{-1} initially followed by a sudden drop 12 min later (Fig. 9); the total amount of ammonia that escaped in the environment is 28,002 kg.

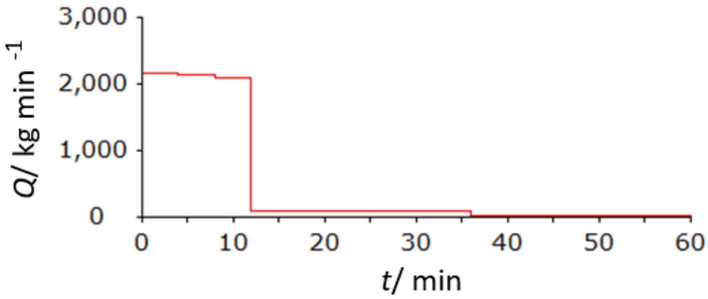

Figure 9. Source strength – flow rate depending of duration from start point

The potential danger zone was about 200 km^2 in size (Fig. 10). The zone of the highest pollution extended 1.6 km from the source (red), the zone of significant pollution extended at a distance of 4.7 km from the source (orange), while the zone of relatively low pollution extended at a distance of more than 10 km from the source (yellow).

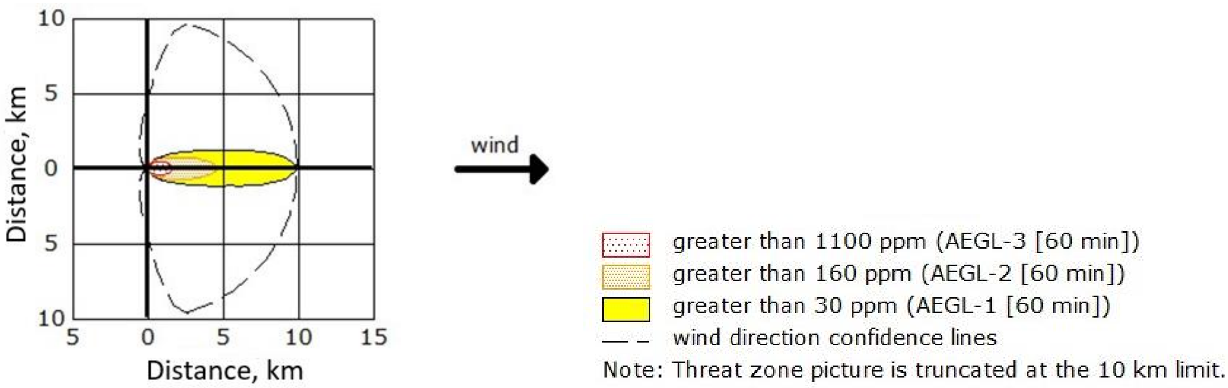

Figure 10. Toxic threat zone - area affected by a certain amount of hazard

Geographical representation of the threat for the city of Pirot and the zones obtained by modelling in ALOHA can be seen in Figure 11.

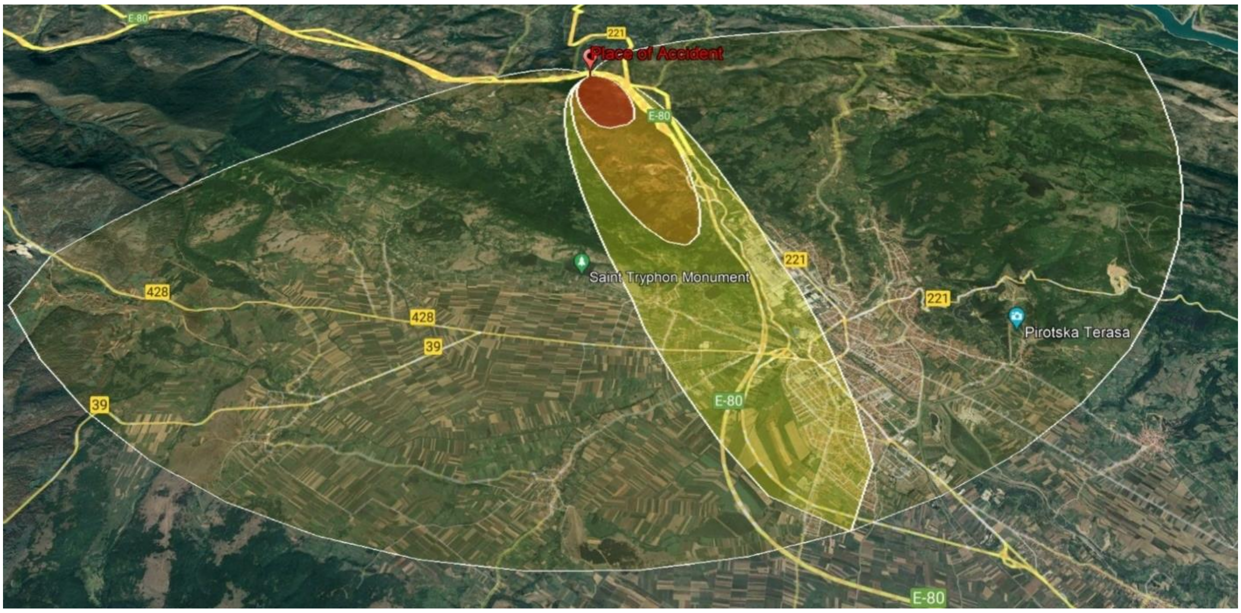

Figure 11. Geographical view of threat zones in Scenario 3

At first glance at the map, this scenario seems the worst of all three scenarios, but that is purely due to the wind direction. If the same wind direction was adopted in the previous two scenarios, it would show a far worse situation in terms of dangerous or lethal concentrations in populated areas. Depending on the conditions at the time of the accident, there is a large difference in the degree of danger. Thus, it could be clearly concluded that wind plays a key role. However, in the case of the city of Pirot, the orography also plays a certain role. In specific, the terrain is such that it would stop further dispersal, but it would also create pockets of higher concentrations.

The fact that it took 20 days to remove the tanks actually indicates how difficult and dangerous it would be to access the site of a more serious accident and how complicated it would be to carry out recovery in a potential severe case. Information circulated in the national media that this is not an isolated case and that there are about 80 of such accidents per year on average. It was announced that this particular place is marked as dangerous, due to derailments often happening there. The tendency to overload wagons is also dangerous. In the present case, the nominal weight was 20 t, but in reality, it was 45 t, which is more than 2-fold higher. By using the same modeling approach in ALOHA the same accident was modelled for a tank carrying 20 t and compared with the modeling results for the real case of 45 t (Table 4).

Table 4. Modelling results for 3 studied scenarios with tanks carrying 45 t and 20 t of ammonia

	45 t ammonia		20 t ammonia	
	Release rate, kg min^{-1}	Total released amount, kg	Release rate, kg min^{-1}	Totala released amount, kg
Scenario 1 (25.12.2022.)	1,350	25,718	1,180	3,293
Scenario 2 (25.01.2022.)	713	23,935	484	1,403
Scenario 3 (23.07.2022.)	2,150	28,002	1,990	5,571

As expected, by reducing the amount of ammonia in the tanks, the leaking rate and the total volume of the spill was reduced, so the danger to the environment is significantly smaller. That alone would have a greater impact than any variable being tested. Reducing the total mass of ammonia in the wagons would certainly lead to a more stable ride and lower tendency to derail.

4. CONCLUSION

In this research, modelling using the ALOHA software tool in real-time conditions was applied for the accident that occurred during the transport of ammonia near Pirot, Serbia. At that occasion a significant number of people were injured and two people lost their lives. The modelling results indicate that the situation could have been even much worse in the event of different meteorological conditions (wind direction and intensity, temperature, *etc.*). In the present case, the zones with the greatest pollution "missed" the densely populated places, that is the whole city of Pirot, while the highest concentration of ammonia as a semi-volatile substance (above 1.1 kg m^{-3}) was present exclusively at a distance of 2.1 km from the source, which affected the intersection at the A4 highway near Sopot.

Modelling using ALOHA and similar software tools should become a practice in risk assessment and risk management when dealing with hazardous chemicals and other hazardous substances. As weather conditions play a very important role in the spread of pollution particles, when planning every transport of dangerous goods, analysis and risk assessment in the event of an accident should be carried out with real-time data, read just before the vehicle passes through a certain inhabited zone. In the event that an accident has already occurred, it is necessary to react quickly in order to protect people's lives and health, by monitoring the situation, but also by modelling using the real data, in order to evacuate people from the zones with highest concentrations as soon as possible. This is particularly important since the dispersion is most intense during the first hour after the accident, which is precisely the reason that the ALOHA algorithm was designed to limit the modelling time to 1 h. After that time most sources do not emit hazardous substances any longer. Further spreading of pollutants is exclusively caused by meteorological conditions, primarily by the wind, which eventually lifts the particles and transports them to further places. Places on roads and railways that are marked with a black dot should be additionally secured, while modelling should be performed especially for these places when planning the transport of hazardous materials along these routes. Also, in the cases that those routes are predicted to be too risky, an alternative solution for the transport of the given shipment should be considered.

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Procena veličine zone ugroženosti nastale akcidentom prilikom transportovanja opasne hemijske supstancije

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(Stručni rad)

Izvod

Zagađenje vazduha je centralna tema svih diskusija koje su u vezi sa zaštitom životne sredine. Modelovanje širenja zagađenja je jedan od načina kako možemo da predvidimo putanje širenja i nivoe zagađenja, te da delujemo u cilju suzbijanja ovog problema. U radu je modelovana disperzija amonijaka u vazduhu korišćenjem softverskog alata "ALOHA" (engl. *Areal Locations of Hazardous Atmospheres*) koji se zasniva na Gausovom modelu disperzije čestica. Modelovanje u radu se zasniva na podacima vezanim za akcident koji se dogodio u decembru 2022. godine u okolini grada Pirota, Srbija, kao i na stvarnim meteorološkim podacima koji su bili aktuelni u vremenskom periodu u kom se odigrao akcident i širenje zagađenja. Kao rezultat modelovanja, dobijene su zone sa povećanom koncentracijom amonijaka. Njihova površina zavisi od koncentracije amonijaka na izvorištu i meteoroloških uslova u periodu otpuštanja opasne materije. Cilj rada je da ukaže na potrebu za uvođenjem modelovanja u operativne centre jedinica MUP-a zaduženih za vanredne situacije, kao za i uvođenjem dodatnih bezbednosnih protokola prilikom transporta opasnih materija.

Ključne reči: Gausov model; prostorne lokacije opasnih atmosfera; disperzija; amonijak; Pirot