THE ROLE OF SOFTWARE TOOLS IN RISK ASSESSMENT GOT FROM AN ACCIDENT AND EMISSIONS OF HAZARDOUS MATERIALS

Venezija Ilijazi[1]
Ministry of the Interior of the Republic of Serbia

Slobodan Miladinović, PhD[2]
University of Criminal Investigation and Police Studies, Belgrade, Serbia

Abstract: The development of atmospheric dispersion models is an important step in the process of predicting, assessing and managing the risk of potential disasters. They are of particular importance in defining and analyzing risk zones in order to prevent endangering a large number of people, property, the environment and natural resources. Today, making a model is almost unthinkable without the use of appropriate software solutions. Numerous software tools for atmospheric dispersion modeling have been developed, the primary role of which is risk assessment, which includes the analysis of accident and emission pollution models used to simulate the transport and diffusion of various pollutants. As many industrial and development projects potentially cause unwanted consequences in the environment, by applying such tools the harmful consequences could be minimized. The development of sensor and computer technology has enabled the development of complex algorithms for the development of models that can be executed in real time, which enables their active role in managing the process of responding to an incident that has occurred.

This paper presents the possibilities of modelling software tools through the example of the impact of chemicals on the environment in the case of emissions of hazardous gases due to an accident. The characteristics of the mathematical model and the simulation scenario made in the *Aloha* software tool are presented.

Keywords: accident simulation, modelling, risk assessment, ALOHA

INTRODUCTION

Releases of dangerous gases into the atmosphere, whether accidentally due to human negligence, plant failures, transport of dangerous substances, natural disasters, or intentionally in terrorist attacks, pose a great danger to the population and infrastructure. Risk (hazard) is defined as an action that has the potential to cause harm to human health or the environment.

1 venezija.ilijazi@mup.gov.rs
2 slobodan.miladinovic@kpu.edu.rs

Physical, chemical, chemical-physical and electrochemical methods are used to measure the concentration of hazardous gases. The limit value of hazardous gases is the prescribed flow or concentration of harmful and hazardous components at the accident site. The measurement results can be displayed as mass per unit volume of gas or as mass flow per unit time (mg/h, gr/h, etc.). Continuous methods (continuous, for a longer period of time) and discontinuous methods (measurement of gas concentration in a shorter time interval) are used to determine the emission of hazardous gases. Measurement is of great importance for determining the impact of the concentration of hazardous gases on the health of the population and the environment, as well as modelling the emission of hazardous gases in the event of accidents. In case of emissions of hazardous gases into the atmosphere, the expert teams of the Sector for Emergency Situations need to provide the necessary and relevant data in a very short time, in order to take adequate and effective actions to cause as little damage to the population and infrastructure.

Regardless of the fact that the information obtained by the measuring stations maintains the real state of the atmospheric air in the places where the measurement is performed, the causes of air pollution remain unknown. Also, this information shows the level of pollution only at certain points and cannot give an adequate picture of the state of the air in the entire desired territory. To solve these problems, modelling of the spread of air pollution is performed, which enables the assessment of the degree of pollution at the observed point without performing the appropriate measurements. In addition, the use of modelling can predict changes in atmospheric air over time, various hypothetical situations can be modelled (for example, the construction of a new factory that would represent a potential pollutant) and pre-planned measures to prevent air pollution. Modelling requires complex consideration of many factors, such as the parameters of the source of pollution, the current meteorological state of the atmosphere, the conditions of scattering of pollutants at a given place, the properties of pollutants, etc.

Numerous dispersion models have been developed to estimate the motion and propagation of air pollutants after their release into the atmosphere, which are divided into physical models and mathematical models. Physical models simulate the real phenomenon of significantly reduced values in laboratory conditions. They reveal the dispersion mechanism and provide validation of the data obtained by mathematical models. Mathematical models that describe the movement of pollutants in the air under the influence of wind (transmission) and turbulent movement of the atmosphere (diffusion) are called models of atmospheric dispersion. They can be further divided into deterministic and statistical models. Deterministic models are based on a fundamental mathematical description of atmospheric processes and all cause-and-effect relationships that affect the dispersion process. Statistical models are based on semi-empirical statistical relationships derived from the existing data and measurements.

An example of a deterministic model is a diffusion model in which the output (concentration matrix) is calculated on the basis of mathematical operations of specific input parameters (emission rate, atmospheric parameters). An example of a statistical model is a weather forecast for a specific area. Here, the concentration level for the next few hours represents a statistical function of the currently available measurements and the previous correlation between the measurements and the trends of concentration change. Hazardous gas dispersion models can assess the consequences of scenarios, as well as the effectiveness of applied strategies, to reduce pollution. The development of information technologies has contributed to the accelerated development of dispersion models, which have made them increasingly complex, with more input parameters. In the global market, a large number of these systems are available (Stojanović, 2011).

MATHEMATICAL MODELS OF DISPERSION OF POLUTANTS

The atmosphere is a very complex physicochemical system, so the modelling of that system is extremely complex. The process of spreading a fluent and its concentration depends on the movement of atmospheric masses (winds), mixing of air masses in height, chemical reactions of dangerous gases and/or radioactive decay in the atmosphere and the rate of deposition of pollutants (Kovačević, 2003).

Starting from the method of mathematical description of the impurity scattering process, three classes of air pollution analysis models can be distinguished: Lagrange, Euler and Gaussian (Stockie, 2011). In the Lagrange and Euler method, the concentrations of dangerous gases can be obtained by different methods of solving the turbulent diffusion equation. They belong to the class of deterministic models, while the Gaussian model belongs to the class of statistical models. The Gaussian method is most often used and it is implemented in most software applications, which are used in practice today. Therefore, only the Gaussian model will be presented in the paper.

GAUSSIAN MODEL

The simplest model for calculating the ground concentration of pollution is the statistical Gaussian model. Precisely in most countries, models of this type are mostly used in normative documents for the practical realization of air quality. The basis of this model is the assumption that the impurities emitted by a continuous point source form a smoke column in which a symmetrical distribution of the particle concentration in relation to the axis of the smoke column is observed. The basic equation of the statistical Gaussian model is composed of two probability density functions of the normal distribution law and has the following form (Stepanenko, 2009; Lazaridis, 2011):

$$C(x,y,z)=\frac{Q\,f_F\,f_W}{2\pi\sigma_y(x)\sigma_z(x)\bar{u}}\exp\left(-\frac{y^2}{2\sigma_y^2(x)}\right)\left\{\exp\left[-\frac{(z-h)^2}{2\sigma_z^2(x)}\right]+\exp\left[-\frac{(z+h)^2}{2\sigma_z^2(x)}\right]\right\} \quad (1)$$

where Q is the mass flow (source power); C - impurity concentration at a given point in space; $\sigma_y(x)$, $\sigma_z(x)$, diffusion dispersions in the direction of the respective axes, which depend on the meteorological conditions of the distance that the particle travels from the source to the point with the x coordinate, assuming that the direction of the *0X* axis coincides with the direction of the wind vector; $\bar{u}$ - average wind speed at the level of measurement; h - effective height of the source; f_F and f_W - corrections to the reduction of impurity clouds due to dry deposition of impurities.

In equation (2), σ_y, σ_z are the horizontal and vertical dispersion of the impurity distribution. The following relations are used to determine these dispersions (Hanna, 1982):

$$\sigma_y = A\,x^a; \quad \sigma_z = B\,x^b \quad (2)$$

where A, a, B, b are the coefficients that depend on the stability of the atmosphere and the surface relief and they are determined experimentally.

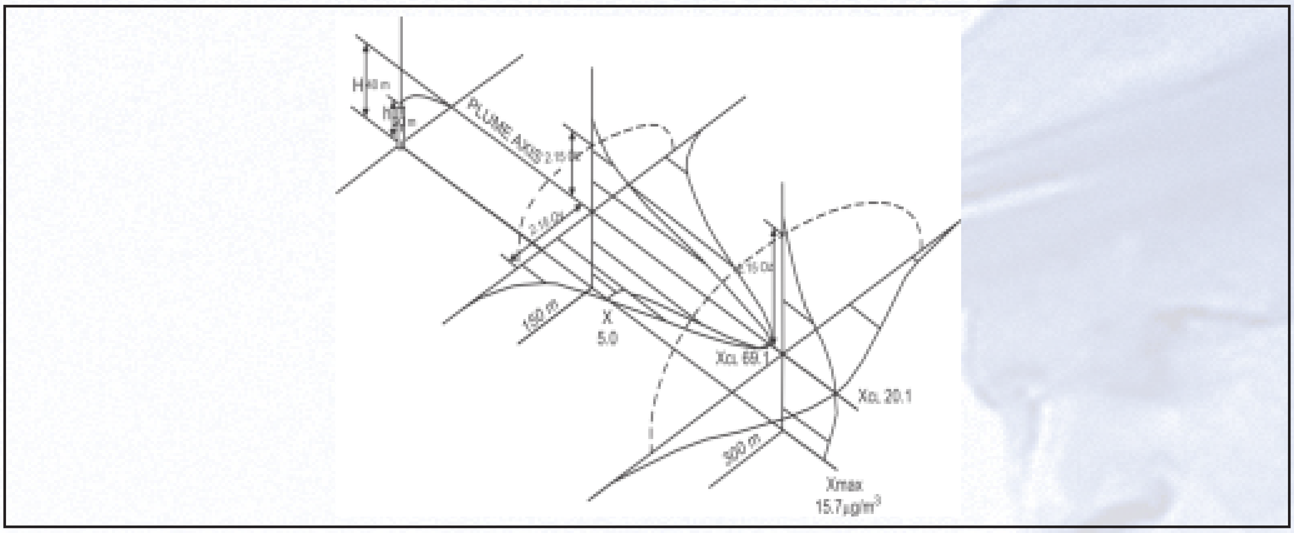

Figure 1 - Graphical representation of air pollution spread assumptions in the Gaussian model (Lazaridis, 2011)

		A	a	B	b
Very unstable	A	0,527	0,865	0,28	0,90
Unstable	B	0,371	0,866	0,23	0,85
Weakly unstable	C	0,209	0,897	0,22	0,80
		A	a	B	b
Neutral	D	0,128	0,905	0,20	0,76
Stable	E	0,098	0,902	0,15	0,73
Very stable	F	0,065	0,902	0,15	0,67

Table 1 - Parameters for calculating the dispersion (Lazaridis, 2011)

HAZARDOUS GAS EMISSION MODELING SOFTWARE

The existing software applications for gas pollution modelling such as MET, ALOHA, SCREEN, BREEZE, TRACE, SAMS provide only a partial solution to the dispersion problem. A large percentage of these software applications do not work in real time, with the simultaneous acquisition and processing of the recorded data, but only analyse the collected data and display the concentration of hazardous substances in two dimensions. Zones of different concentrations of hazardous substances are static and do not take into account the dynamics of the process, the primary change in atmospheric conditions and the change in the strength of pollution sources (Kantar, 2003).

When calculating the danger zones, different types of emission sources (point, surface, volume and pipelines), meteorological conditions at the incident site (wind speed, wind direction and temperature), as well as different types of terrain (urban and rural) are taken into account. The calculated danger zones are displayed on the Web GIS browser from where the danger assessment is performed and actions are taken. As a mechanism for connecting dispersion models and VEB GIS browser, it uses KML (Keyhole Markup Language) protocol which can be accessed via any Internet browser (IE, Opera, Google Chrome, Mozilla Firefox, etc.) and using many devices (smartphone, tablet, desktop and laptop) that have an internet connection.

SOFTWARE APPLICATIONS USED IN THE WORK

The aim of this paper is to present a simple and reliable system for simulation and GIS visualization of accidents caused by the emission of hazardous gases from production, transport and storage facilities based on "open" technologies (Kovačević, 2014). These systems include free modelling software, recommended by relevant global institutions, and widespread and open GIS-based visualization platforms. All this is accompanied by the design of the appropriate software interfaces and "user-friendly" integration (Nikezić, 2016).

CAMEO (Computer-aided Management of Emergency Operations) is a software product created in cooperation with two American organizations - the Environmental Protection Agency - the Office for Prevention and Preparedness in Emergencies (US Environmental Protection Agency - Chemical Emergency Preparedness and Prevention Office EPA OEP -PR), based in Washington, and the National Oceanic and Atmospheric Administration (NOAA), based in Seattle. CAMEO includes a number of software applications with the basic function of increasing operability in planning and responding to accident situations. The program consists of a set of databases with two accompanying modules - the model for dispersion of toxic gases ALOHA and the program for electronic cartographic support MARPLOT. All programs are supported by Microsoft Windows. CAMEO consists of three integrative compatible components, schematically shown in Figure 2.

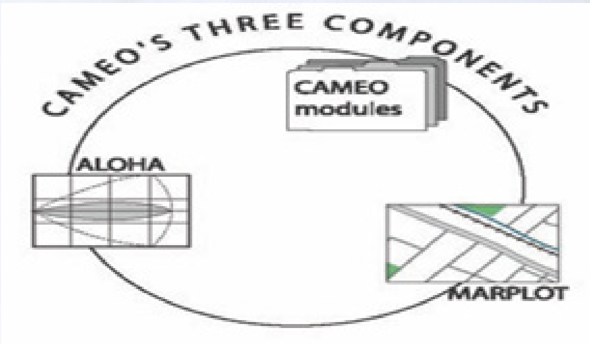

Figure 2 - Basic components of the CAMEO program

CAMEO can be used in cases of quick access to the stored data, and processing of these data to assess the specific accident situation and transmit information to the competent authorities, which are necessary for an adequate response to the accident event, especially in the prevention and preparedness phases. The program is in use in many European countries and has been translated into English, Spanish and French. CAMEO was selected by the United Nations, Environmental Protection Program to support the development of national programs for the preparation and response to chemical accidents and is part of the UNEP program for emergency preparedness at the local level (Pollutant Dispersion in Urban Areas, 2016).

Each defined route can be displayed in electronic form, on a map using the MARPLOT program. Roads, railways and routes in water transport are presented on MARPLOT maps in the form of graphic lines, as shown in Figure 3.

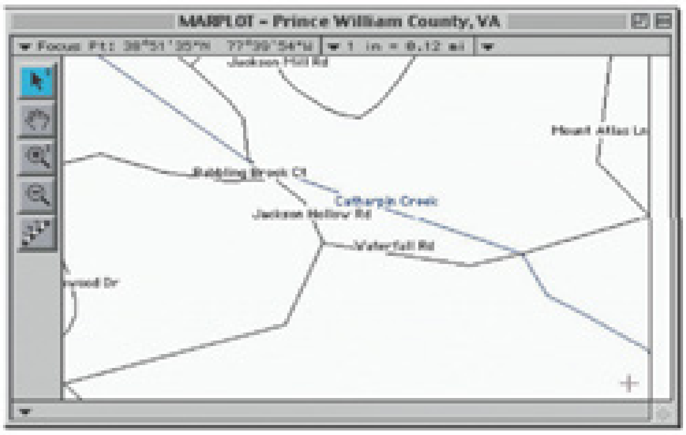

Figure 3 - Demonstration of a routine network for the transport of dangerous goods in the form of the MARPLOT program

All data from the Chemicals in Inventory module can be used and combined with the data from the Routes module. The data on stored hazardous substances in the facilities along it, by which they are transported, can be linked to each route.

When the data on all hazardous substances stored along the transport route are created, the possibility of using the Screening and Scenarios module is opened, in order to investigate the potential danger that may arise in the event of an accident on a certain part of the route.

Figure 4 - Display of the spread of the contamination zone along the transport route using the Screening and Scenarios module

ALOHA (Areal Locations of Hazardous Atmospheres) is a model for displaying the dispersion (expansion) of gases. It is used to estimate the spread (dispersion) of the contamination cloud in the direction of wind blowing. The assessment is based on the physicochemical properties of the substance that caused the accident, the meteorological conditions at the time of the accident and the circumstances under which the uncontrolled emission or release occurred.

The main characteristics of the program are:

- The program generates a number of specific output scenarios, including the drawings of hazard zones, hazards at a specific point and a graph of source strength.

- It calculates the rate of leakage of chemicals coming out of tanks, pipelines, etc., and predicts how that rate changes over time.
- It assesses different types of hazards (toxicity, flammability).
- It models several release scenarios (cloud of poison gas, fire jet, and steam explosion).
- It minimizes the entry of incorrect data by cross-checking the entered values and warns the user when the value is incorrect or not physically possible.
- It contains its own chemical library with physical characteristics for about 3000 common hazardous chemicals so the user does not have to enter that data.

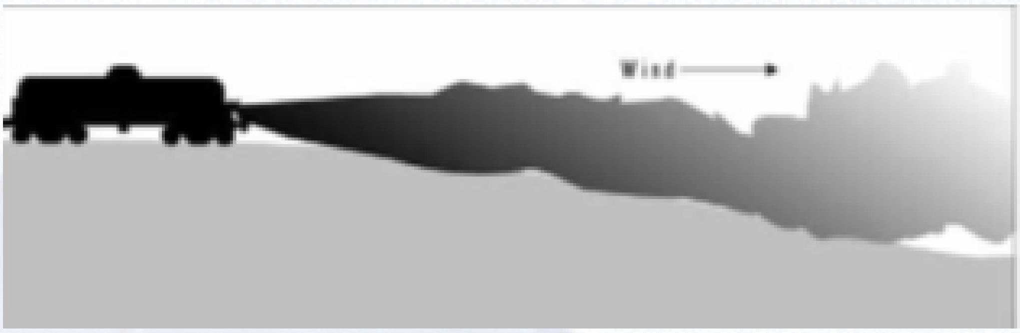

Figure 5 - The spread of clouds of hazardous substances in accidents

RISK MANAGEMENT METHODOLOGY FOR TRANSPORT OF DANGEROUS GOODS

Managing the risk of an accident situation in the transport of dangerous goods is a process that consists of several sub-processes that are interdependent, i.e. making mistakes within one of the sub-processes directly affects the next sub-process, i.e. the quality of the output results (Filipović, 2000).

The methodology for managing the risk of an accident includes identifying possible hazards, determining the mechanisms of its occurrence and development, and considering the possible consequences.

The stages that make up the Accident Risk Management Methodology are:

1. Accident risk analysis;
2. Planning measures for prevention, preparedness and response to the accident situation;
3. Planning measures for elimination of consequences from the accident situation (rehabilitation).

Each of these phases, within the Accident Risk Management Methodology, consists of several steps (phases) aimed at increasing the level of safety, which is achieved by reducing the level of risk and reducing the consequences for the population and the environment.

According to the prescribed methodology, the analysis of the danger of an accident situation (the first phase) takes place through three phases, as follows:

• the first phase - hazard identification,

• the second phase - consequence analysis, and

• the third phase - risk assessment.

The priority in the analysis of the danger of an accident situation should be focused on the identification of the danger (the first phase), which includes the collection of all necessary data and consideration of potentially dangerous factors of all kinds. This phase is the most important element of risk management and the starting point for further work on the implementation of other phases.

In the second phase of accident risk management, preparations are made to eliminate the possibility of an accident (accident) so that the risk of dangerous activities and dangerous substances in a certain area would be acceptable.

Within this phase, the management of the risk of an accident takes place through the following steps:

1. the first step - prevention,
2. the second step - readiness, and
3. the third step - response to an accident.

Planning measures to eliminate the consequences of an accident situation (remediation) is the third (last) phase within the Risk Management Methodology.

Measures to eliminate the consequences of the accident situation (accident) are aimed at monitoring the situation after the accident situation, restoring and rehabilitating the environment, returning to the original state, as well as eliminating the danger of recurrence of the accident situation (Miljuš, 2003).

CASE ANALYSIS

On a bend of the transit road (coordinates 43° 49` 27`` N/20° 35` 12`` E, altitude 211 m), a tanker carrying 18.6 tons of liquid methyl mercamptan overturned on January 17, 2015, at 13:35 (and on July 25, 2015 at 13:49). The paper analyses two simulation scenarios of accidents in different weather conditions and different seasons in the same geographical area. The accident analysis was performed using the Gaussian gas dispersion model, which is used in any similar simulation, when it comes to vapours of liquids or gases.

For the first scenario, the measured current air temperature was -5° C, the humidity was 25%, the clouds were 7/10, and the north wind was blowing at a speed of 7 m/s. During the overturning, an opening 2 cm wide and 40 cm long appeared on the body of the tank, 30 cm from the ground.

In the second scenario, the measured current air temperature was +39° C, the humidity was 75%, the clouds were 7/10, and the northwest wind was blowing at a speed of 3 m/s. During the overturning, an opening 2 cm wide and 40 cm long appeared on the body of the tank, 30 cm from the ground.

Methanethiol (Methyl-mercaptan) is a chemical compound whose formula is CH_4S. It is a colourless gas, very harmful and poisonous, extremely flammable and dangerous to the environment, with a strong smell similar to rotten cabbage.

The expressed power of the source (Figure 6) decreases with time, but the concentration on a relatively small area is significantly increased. Despite the weak influence of the wind, the power of the spring is relatively low with a small concentration on a much larger area.

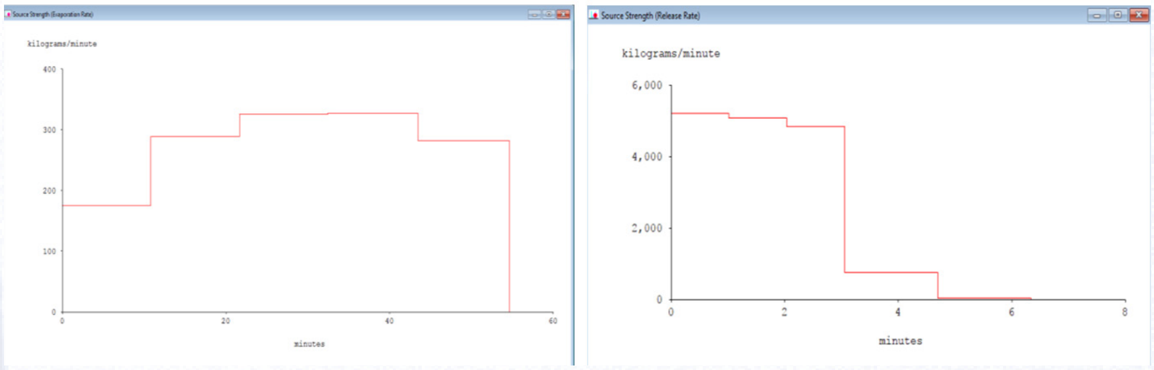

Figure 6 - Source power as a function of time

The spill pressure is 0.64 atm in the first scenario, or 1 atm in the second. Atmospheric stability is determined based on air temperature and wind speed profiles. According to this classification, the stability class is D for both scenarios (neutral). The maximum amount of chemical released is 327 kg/minute in the first scenario and 5200 kg/minute in the second scenario. The total amount of chemical spilled and the duration of the discharge is 15,299 kg for 55 minutes in the first scenario and 16,761 kg for 6 minutes in the second scenario.

Figure 7 - Geographical presentation of population vulnerability on satellite and terrain maps in relation to both scenarios

Figure 7 illustrates the geographical presentation of the vulnerability of the population on the terrain map. Based on the software simulation and analysis, the ground-level pollutant concentrations at different distances were calculated for both scenarios. The analysis was done in accordance with the capabilities of the ALOHA program in relation to the integrated application in the ArcGIS tool used for modelling and spatial display of data analysis results.

Different concentrations of pollution due to accidents are presented in different colours and refer to a time period of 60 minutes.

The most dangerous pollution (marked in red) in the first scenario extends up to 400 m from the source, and in the second up to 3 km. Very large polluted (marked in orange) range is up to 500 m in the first scenario, and up to 4 km in the second scenario. Relatively low pollution (marked in yellow) extends up to 600 m in the first scenario, and up to 5 km in the second scenario. All pollution marked in red leaves serious consequences on the health of all residents. Pollution represented by orange is a problem for certain populations such as children, the elderly and chronic lung and heart patients. The population will probably not be endangered by the degree of pollution marked in yellow.

The maximum value of methanethiol concentration is 65.6% (656,317 ppm^3) in the first scenario and 100% in the second. The limit values for the concentration of chemical pollution are 21.8% (218,000 ppm) for the red area, 13.08% (130,800 ppm) for the orange area and 2.18% for the yellow area in the first scenario. In the second scenario, the concentration limit is 3.9% (39,000 ppm) for the red, 2.34% (23,400 ppm) for the orange and 0.39% (3,900 ppm) for the yellow area.

Figure 8 presents the threat diagrams for scenarios I and II. According to the first scenario (winter conditions - low temperatures), very high concentrations of pollution due to accidents are noticeable at a maximum distance of about 500 m in the wind direction and an accident zone width of 100 to 150 m. According to the second scenario (summer conditions - high temperatures), lower concentrations of pollution are noticeable at a maximum distance of about 6 km in the direction of wind action and an accident zone width of 3 km. Therefore, the potential terrain endangerment area in the first scenario is about 0.075 km^2, while in the second it is about 8 km^2.

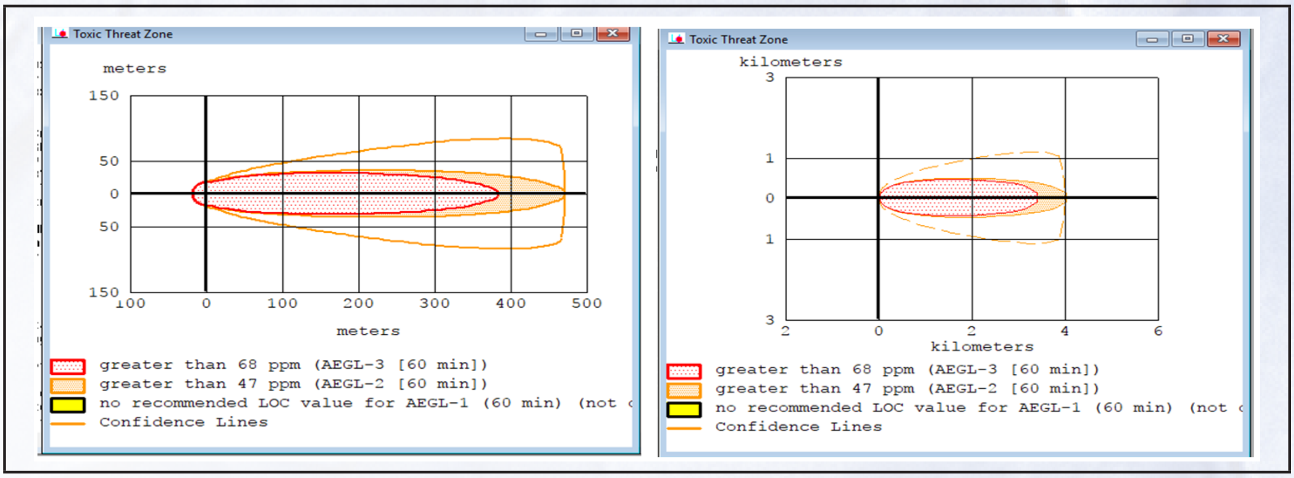

Figure 8 - Population vulnerability diagram for scenario I (left), and scenario II (right)

CONCLUSION

The paper presents the important role of software tools for modelling atmospheric dispersion through adequate presentation of the problem, i.e. approaching the situation to the real scenario, in order to better and more successfully manage risk in crisis situations and accidents. The analysis of mathematical-physical models of dispersion of hazardous substances affects the perception of the severity and magnitude of the problem as well as potentially negative consequences for the environment, both for the population and for plant and animal species.

Chemical accidents are probably the most dangerous of all accidents. They cannot be predicted in advance, and can lead to very serious consequences. Therefore, it is necessary to analyse all places in the technological process of production, transport and technological process of exploitation and, based on the analysis, work on prevention. Prevention can reduce the consequences, but there is always a risk of an accident. It is never possible to predict absolutely all cases and scenarios of accidents.

The results tell us that the number of victims in the cases described in the simulations would be large if the evacuation did not begin immediately after the accident. The final results show that at least 70% of the inhabited observed area would be exposed to a lethal dose of the chemical. Also, in the first simulation, a toxic cloud is seen, where an increased amount of methanethiol would be registered and evacuation of up to 30% of the population would be required. The second simulation shows that an increased amount of methyl mercaptan would be registered in the surrounding areas, which would cause the need to evacuate up to 60% of the population. When we talk about methyl mercaptan, it must be said that it is an extremely toxic gas, and deadly if monitoring, evacuation and remediation are not started in time.

All actions that are carried out must have only one single goal, and that is to reduce the long-term consequences for the environment to a minimum. Man, as a part of nature, must understand that this is his priority and not cut the branch on which he is sitting.

When it comes to accident prevention, it is not enough just to prepare so that the accident does not happen, but it is also necessary to practice all segments of the defence before the accident. A good team for solving such situations is always well-coordinated. You need to be prepared for everything, because every accident is a new challenge.

When all the facts are taken into account, a person can be recognized as a direct or indirect factor causing the accident. For that reason, it is necessary to educate people, the employees (those who manipulate dangerous substances and those who can influence their movement), as well as ordinary citizens. They need to be educated as dangerous substances are not called that for any reason. Sometimes it is just one breath that separates a person from death. Therefore, it is necessary to explain to people that they have to take care of the environment, because in that way they take care of themselves.

REFERENCES

1. Filipović D. (2000), Geoprostorno modelovanje rizika u životnoj sredini, doktorska disertacija, Geografski fakultet, Beograd.
2. Hanna, S.R., Briggs, G.A., Hosker, R.P., (1982), Handbook on Atmospheric Diffusion. DOE/TIC 11223, Department of Energy)
3. Harvey D. (2000), Modern Analytical Chemistry, McGraw Hill.
4. Kantar S. (2003), Akcidenti pri transportu opasnih materija - primeri iz prakse i pouke, Beograd.

5. Kovačević J., Stojanović R., Karadaglić D., Ašanin B, Kovačević Ž, Bundalo Z., Softić F., (2014), FPGA low-power implementation of QRS detectors, 3rd Mediterranean Conference on Embedded Computing (MECO), pp: 98- 101.
6. Kovačević Ž, Stojanović R, Nikolić G. (2003), Modelling and Simulation of Accidental Air, Beograd.
7. Lazaridis M. (2011), First principles of Meteorology and Air Pollutant, Springer, pp.201-232, New York.
8. Miljuš, M., Vidović M. (2003), Rizik u transportu opasnih materija, Beograd.
9. Nikezić, D.P. (2016), Matematičko modelovanje rasprostiranja zagađujućih materija u vazduhu u okolini nuklearnih i industrijskih objekata, Doktorska disertacija, Tehnološko-metalurški fakultet Univerziteta u Beogradu, Beograd
10. Pollutant Dispersion in Urban Areas – an Approach Suitable for Developing Countries, Works in Progress in Embedded Computing, Vol 2, No 1, June 2016, ISSN 2337-0343.
11. Stockie, J. M. (2011), The Mathematics of Atmospheric Dispersion Modeling. SIAM Review, 53(2), pp. 349–372.
12. Степаненко С.Н., Волошин В.Г., Типцов С.В. (2009), Новая формула оценки уровня загрязнения атмосфры промышленными выбросами, Украинский гидрометеорологический журнал, Но 4, ст. 227-237.