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MODELLING OF CLOUD EFFECTS OF FLAMMABLE GASES AND FUMES

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Predrag Stanković, Ivan Krstić, Emina Mihajlović

Faculty of Occupational Safety, University of Nis, Serbia

Abstract. *During a technological process, either during regular work or in case of an accident, there is a possibility of a fire and explosion owing to hazardous liquids leaking and, flammable and explosive gases being produced. The impact on people and the environment is particularly emphasized when flammable and toxic fumes are formed. In this sense, the subject of the paper is the modelling and simulation of the effects occurring in those conditions with the purpose of designating a safe zone. Based on possible accident scenarios and using a mathematical model, it is possible to assess the ecological risk, where real-time models generate an image of dangerous areas.*

Key Words: *flammable gases and fumes, mathematical model, simulation, safe zone*

1. Introductory Remarks

A cloud consisting of flammable gases and fumes can appear after a sufficient leak duration, when gases and fumes leak continuously for a certain period, or as a result of instant leaking caused by damage of the facility and flammable liquid evaporation.

Depending on the speed and formation of the mixture consisting of air and gases (or fumes), a primary and secondary cloud can be distinguished.

The primary cloud develops when the complete amount of fumes or gases, or their significant part, transfer into the atmosphere as foam or aerosol in about 1-3 minutes during an accident.

The secondary cloud develops due to subsequent evaporation caused by liquid spilling on the ground.

Simultaneous or separate occurrences of the primary and secondary cloud depend on the liquid boiling temperature and pressure in the vessel.

For instance, liquids with a higher boiling temperature than the surrounding air temperature do not produce a primary cloud.

A fume and gas cloud can burn at a certain mixture concentration, the flammability limits of which are specific for any matter, with the possibility of either deflagration and detonation combustion.

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Detonation combustion is characterized by a shock wave, and deflagration combustion by heat radiation, whereas toxic agents are featured in both processes [1].

Effects of flammable gases and fume combustion in unbounded atmosphere space exceed the action scale of regular fires. Dangerous factors of detonation and deflagration combustion spread beyond the safe distance specified for this fire category, thus changing the ecosystem structure and its function dynamics.

All of the aforementioned pose ecological threats for buildings endangered by flammable gases and fumes and, consequently, by heat radiation and a detonation wave.

In this sense, software packages based on the Gaussian dispersion model are used to determine the impact area of the effects of flammable gases and fume combustion, as well as to determine the heat radiation of the detonation wave and toxic products of combustion.

2. Software Packages for Gas and Fume Explosion Process Effects Modelling

Various software packages can be used for possible accident effects modelling:

- CAMEO (Computer-aided Management of Emergency Operations),
- ALOHA (Areal Locations of Hazardous Atmospheres),
- ALOFT-FTTM (A Large Outdoor Fire cloud Trajectory model - Flat Terrain),
- ARCHIE (Automated Resource for Chemical Hazard Evaluation),
- as well as many packages intended only for field fire and explosion protection [2, 3].

These packages, based on emission, corresponding meteorological parameter data sets, and topographic terrain maps, provide a space-time view of fire and explosion products distribution, heat flux density, and detonation wave intensity.

ALOHA is the most frequently used model for gas dispersion representation and it is part of the CAMEO package. It is used for the assessment of wind-direction-oriented contamination cloud dispersion. The assessment is based on physical-chemical properties of matter causing the accident, on meteorological conditions at the moment of accident, and uncontrolled emission circumstances.

The pre-processing phase of the simulation model requires the input of the following:

- the geographical location of the accident - as the software package contains only locations of large cities in the USA, it is necessary to add a desired location, by entering its altitude, latitude and longitude;
- hazardous chemical matter from the database, which caused the accident;
- atmosphere condition indicators at the accident location, for example wind speed, course and direction, clouds, open water area, settlement or forest, air temperature, stability type, humidity and inversion;
- location and type of hazardous matter source (whether it is instant or continuous leakage), as well as probable amount of hazardous matter and source height;
- type of tank from which the leak originated, as well as its width and length;
- state of matter, temperature and quantity of hazardous matter in the tank;
- shape, size, and position of damage on the tank.

One of the most important steps is the selection of scenario type: whether it is an accident with evaporation, fire, or an explosion.

After all the parameters needed for a possible accident scenario have been entered, the next phase is the simulation model processing, where implementation of the pollutant dispersion model using numerical algorithms is used to compute the desired dynamical variables in the space-time continuum. The post-processing phase of this software package includes simulation results, visualization and textual description of the accident. Zones are marked by red, orange and yellow according to toxic risk level.

Depending on accident scenario, in the post-processing phase, simulation results include variables pertaining to:

- pollutants evaporation - pollutant concentration changing over time and graphical representation of toxic hazard zones;
- fire and/or explosion - heat radiation energy change in a considered point during the counted time, source power change during the counted time and graphical representation of heat radiation zones.

Results of visualization scenarios of evaporating pollutants and fire and/or explosion in the post-processing phase, are shown in Figure 1.

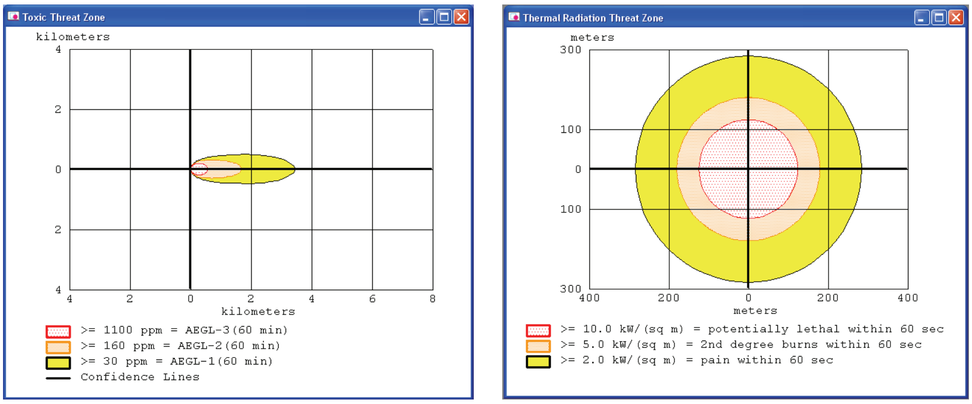


Fig. 1. Visualisation results in the post-processing phase

With respect to source intensity representation during the accident, the software provides a gradual curve with a discretized quantum of the quantity of interest in accordance with the risk assessment criteria.

The software package is a good base for further upgrades in the direction of implemented model development by including a number of phenomena that follow an accident scenario, and which are not already included in it because their influence is considered to be small (e.g. photochemical effect, presence of other contaminants in the atmosphere, potential chemical reactions, etc.), as well as detonation pressure change with the given distance from the accident source.

3. Mathematical Model of Gas and Fumes Explosion

Authors Koretkova (et al.) discuss the dependence of the detonation pressure on distance during accidents [4, 5].

The creation of a mathematical model for the calculation of the effects of the explosion of gas mixtures and fumes is the following:

Considering the high speed of detonation (1000 m/s), it has to be taken into account when calculating that the wave front is unchanged until the outer boundaries of the mixture cloud, limited by a hemisphere with a radius r_o.

Pressure on the detonation wave front in gas mixtures can reach values from 2 MPa to 10 MPa. The parameters of the detonation wave in the process of spreading within the cloud mixture do not change substantially. At the exterior layer of the mixture cloud, the detonation products expand and initiate the air shock wave. If the entire quantity of liquid does not turn into a cloud during leakage, according to the calculated values for this product mass, the coefficient υ takes a value lower than one.

Figure 1 graphically represents the change of maximum pressure at a distance from the centre of the mixture explosion, translated to the equivalent of the explosion of regular explosives.

The radius r_o (m) of the mixture cloud hemisphere depending on volume V_o (m^3) is determined by the equation:

$$r_o = \sqrt[3]{3V_o/(2\pi)} \quad (1)$$

According to Avogadro's law, a kilomole of ideal gas occupies a volume of $V_a=22,4\ m^3$.

The volume of a gas cloud with stoichiometric composition with aconcentration C_{sth} and molecular mass M_g of the flammable component of a mass m is determined by the equation:

$$V_o=V_a \cdot \upsilon \cdot m \,/\, M_g \cdot C_{sth} \quad (2)$$

The value of coefficient υ is determined depending on the storage manner of flammable matter:

υ=1 - for gas under atmospheric pressure;
υ=0,5 - for gas under pressure;
υ=0,1 - for cooled gas under pressure;
υ=0,02-0,07 - during leakage of highly flammable liquids.

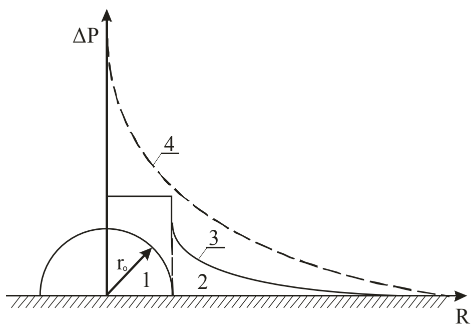


Fig. 2. Maximum ΔP pressure variation in relation to the distance from the explosion centre R:
1 - area of gas and liquid vapour mixture cloud with a radius r_o;
2 - spread zone of detonation and shock wave products;
3 - pressure variation during gas mixture and fumes explosion;
4 - pressure variation during a TNT explosion.

The spread speed of the detonation wave D (m/s) is determined by the equation:

$$D = \sqrt{2(\gamma^2 - 1)Q_m} \tag{3}$$

Where Q_m is the released heat upon explosion (J/kg).

The duration of a complete cloud detonation t_v (s) is determined by the equation:

$$t_v = r_o/D \tag{4}$$

The maximal overpressure at the detonation wave front is determined by the equation:

$$\Delta P_1 = 4(\gamma - 1)Q_m\rho_{sth} - P_o \tag{5}$$

During a very small time interval t, the detonation wave pressure is reduced twice.

$$\Delta P_2 = 2(\gamma - 1)Q_m\rho_{sth} - P_o = \rho_{sth}D_2/(\gamma + 1) - P_o \tag{6}$$

Time t has a scale of ten microseconds - the duration of the transfer into the chemical reaction zone, i.e., transition from the adiabatic process of initial matter to the adiabatic process of detonation products.

Variation of overpressure during detonation at a distance of $R \leq r_o$ (m) from the explosion centre is approximated by a triangle with an effective action time θ (s), Figure 2 line 2.

$$\Delta P(t) = \Delta P_2(1 - t/\theta)\ (0 < t \leq \theta) \tag{7}$$

In the case of a flat vertical barrier, pressure ΔP_{orp}, at $R<r_o$, is determined by the expression:

$$\Delta P_{orp} = 2{,}5\Delta P_2 \tag{8}$$

Spreading properties of the mixture are given in Table 1, where:

ΔP_2 - detonation wave overpressure (effective pressure);

γ_{sth} - adiabatic index of detonation products;

ρ_{sth} - density;

$Q_{m,sth}$ and $Q_{V,sth}$ - explosion heat per mass unit or mixture volume unit, where the index *sth* indicates stoichiometric composition.

Table 1. Properties of gas-air and fume-air mixtures

Flammable substances	D m/s	ρ kg/m^3	$Q_{m,sth}$ MJ/kg	$Q_{v,sth}$ MJ/kg	γ_{sth}	M_g g/mol	C_{sth} zap.%	ΔP_2 MPa
GASS MIXTURE								
ammonia	1630	1,180	2,370	2,791	1,248	17	19,72	1,29
acetylene	1990	1,278	3,387	4,329	1,259	26	7,75	2,14
butane	1840	1,328	2,776	3,684	1,270	58	3,13	1,88
butane	1840	1,329	2,892	3,843	1,260	56	3,38	1,89
vinyl chloride	1710	1,400	2,483	3,980	1,260	63	7,75	1,71
hydrogen	1770	0,933	3,425	3,195	1,248	2	29,59	1,20
divinyl	1870	1,330	2,962	3,967	1,260	54	3,68	1,96
methane	1750	1,232	2,763	3,404	1,256	16	9,45	1,57
arbonmonoxide	1840	1,280	2,930	3,750	1,256	28	29,59	1,82
propane	1850	1,315	2,801	3,676	1,257	44	4,03	1,89
propylene	1840	1,314	2,922	3,839	1,259	42	4,46	1,87
ethane	1800	1,250	2,797	3,496	1,257	30	5,66	1,69
ethylene	1880	1,285	3,010	3,869	1,259	28	6,54	1,91
FUME MIXTURE								
acetone	1910	1,210	3,112	3,766	1,259	42	4,99	1,85
kerosene	-	1,350	2,973	3,770	-	94	2,10	-
benzene	1860	1,350	2,937	3,966	1,261	78	2,84	1,96
hexane	1820	1,340	2,797	3,748	1,261	86	2,16	1,86
dichloroethane	1610	1,400	2,164	3,224	1,265	99	6,54	1,60
diethyl ether	1830	1,360	2,840	3,862	1,261	74	3,38	1,91
xylene	1820	1,355	2,830	3,834	1,259	106	1,96	1,89
methanol	1800	1,300	2,843	3,696	1,253	32	12,30	1,77
pentane	1810	1,340	2,797	3,748	1,258	72	2,56	1,84
toluene	1830	1,350	2,843	3,838	1,260	92	2,23	1,90
cyclohexane	1770	1,340	2,797	3,748	1,248	84	2,28	1,77
ethanol	1770	1,340	2,804	3,757	1,256	46	6,54	1,76

The parameters of shock waves at a distances $R \geq r_o$ (m) are determined with the equation by the approximation of the solution of the propane-air mixture detonation model. The solution is obtained by integrating the system of non-stationary equations of gas dynamics into spherical coordinates with the Lagrange variables. Real equations of the state of the initial mixture of detonation products and speed ratio of mixture reaction in the reaction zone were applied [1].

The universal dependence of the maximum effective overpressure P_m (Pa) and specific impulse I (Pa·s) was obtained in the shock wave at a distance R from the centre of the explosion, which is in concordance with the experimental data for the combustible mixture of hydrocarbons with air or oxygen [1].

$$\Delta P_m = P_o P' \tag{9}$$

$$\log P' = 0{,}65 - 2{,}18 \cdot \log R' + 0{,}52(\log R')^2 \tag{10}$$

$$R' = R / \sqrt[3]{m_t} \tag{11}$$

$$\log I' = 2{,}11 - 0{,}97 \log R + 0{,}04(\log R)^2 \tag{12}$$

$$I = I' \sqrt[3]{m_t} \tag{13}$$

Where:
m_t – the TNT explosion equivalent of the hemisphere mixture cloud (kg):

$$m_t = 2mQ_{m,sth}/Q_t \tag{14}$$

m – mass of flammable mixture (kg)

$$m = r_{sth} V_o \tag{15}$$

Q_t – heat released during the TNT explosion ($4{,}184 \cdot 10^6$ J/kg),
P_o – atmospheric pressure (Pa).

In order to determine the parameters of the cloud border, values $r_{o,}$ are replaced with the values of R_o obtained from the conditions of continuity of the functions $\Delta P_m(R)$ in the point $R=R_o$.

$$R_o = 10^{\alpha} \sqrt[3]{m_t} \tag{16}$$

$$\alpha = K_1 - \sqrt{K_1^{\,2} - A} \tag{17}$$

$$K_1 = 1{,}09/0{,}52 \tag{18}$$

$$A = 1{,}25 - \log(\Delta P_2/P_o)/0{,}52 \tag{19}$$

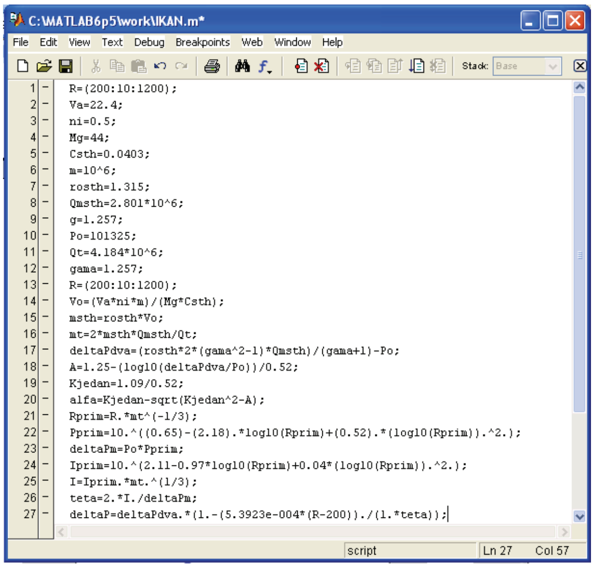
The impulse magnitude *at* $R \leq R_o$ is taken to be equal to the magnitude $I(R_o)$ from equation (13).

Effective time θ (s) of the compression achieved by shock wave is approximated by triangle $\Delta P(t) = \Delta P_m(1 - t/\theta)$ and determined according to the equation:

$$\theta = 2I/\Delta P_m \tag{20}$$

4. Results of the Gas and Fumes Explosion Process Simulation

Simulation of the above mentioned mathematical model was implemented in the software package MATLAB designed for computing in science and technology. With its numerous toolboxes, its use is even more diverse. The mathematical model of the explosive process is presented as a series of programming functions of number fields whose execution provides numerical values of the variables of interest, which characterize an explosive process, Figure 3.




```
R=(200:10:1200);
Va=22.4;
ni=0.5;
Mg=44;
Csth=0.0403;
m=10^6;
rosth=1.315;
Qmsth=2.801*10^6;
g=1.257;
Po=101325;
Qt=4.184*10^6;
gama=1.257;
R=(200:10:1200);
Vo=(Va*ni*m)/(Mg*Csth);
msth=rosth*Vo;
mt=2*msth*Qmsth/Qt;
deltaPdva=(rosth*2*(gama^2-1)*Qmsth)/(gama+1)-Po;
A=1.25-(log10(deltaPdva/Po))/0.52;
Kjedan=1.09/0.52;
alfa=Kjedan-sqrt(Kjedan^2-A);
Rprim=R.*mt^(-1/3);
Pprim=10.^((0.65)-(2.18).*log10(Rprim)+(0.52).*(log10(Rprim)).^2.);
deltaPm=Po*Pprim;
Iprim=10.^(2.11-0.97*log10(Rprim)+0.04*(log10(Rprim)).^2.);
I=Iprim.*mt.^(1/3);
teta=2.*I./deltaPm;
deltaP=deltaPdva.*(1.-(5.3923e-004*(R-200))./(1.*teta));
```

Fig. 3. Program file for the simulation of the explosive process mathematical model

By revocation of the commands from the toolbar menu, in the post-processing phase, a graphic representation is obtained of the dependency on the variables of the explosive processes in the function of time and/or distance.

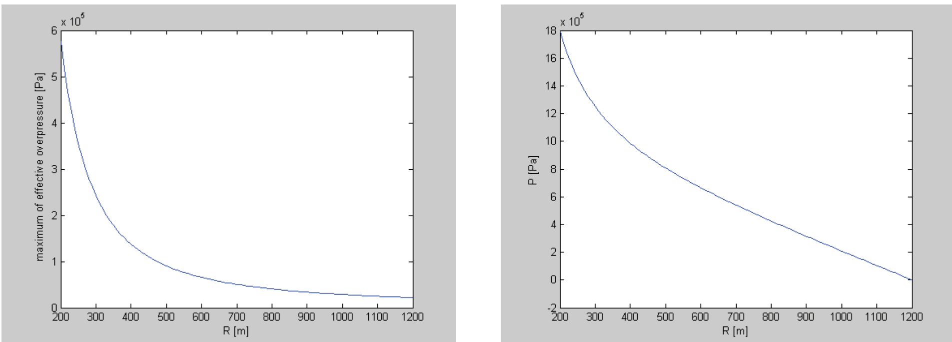


Fig. 4. Results of the explosive process simulation

The chart on the left shows the change in the maximum effective overpressure in the explosive process in the function of distance. It is evident that the overpressure decreases with distance.

The chart on the right shows the detonation wave pressure in the function of distance, which also decreases with distance.

From the aspect of the assessment of the safe zone, these diagrams can be used by reading the distance at which a pre-determined maximum quantitative indicator of the explosive process is reached. The safe zone is defined as a set of points in space with a distance from the centre of the explosion greater than the previously described distance.

Since there are two independent variables in the mathematical model, it is possible to generate a 3D view of variable dependency which describes an accident in the function of distance from the accident centre and time elapsed from the moment of its initialization.

Figure 5 shows a 3D view of the detonation pressure dependency on the distance from the centre of the explosion and the time elapsed from the moment of its initialization. The diagram on the left clearly shows isobars which follow a 3D grid chart with a purpose of an efficient representation of the state of variables (pressure) in space and time. The chart on the right was obtained by the rotation of the left chart providing a clearer view of the safe zone in the function of time and distance.

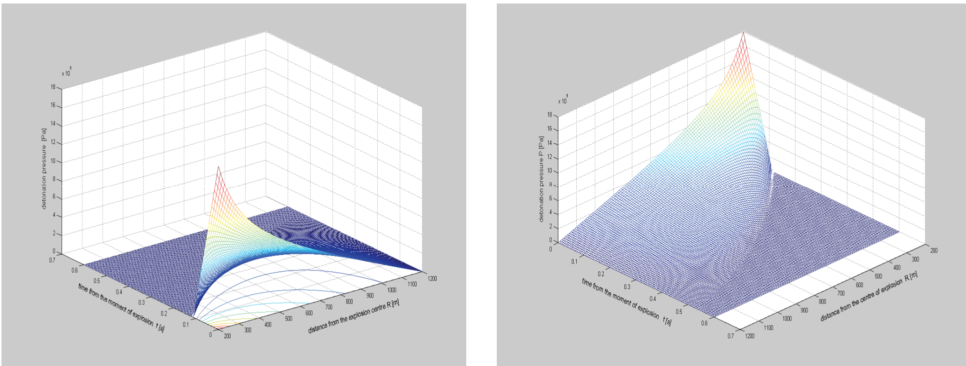


Fig. 5. 3D chart of the results of explosive process simulation

To gain a more precise view of the values of accident variables, the 3D graphic was projected to a plane of relevance, determined by an independent variable axis and a dependent variable axis which represents an accident property.

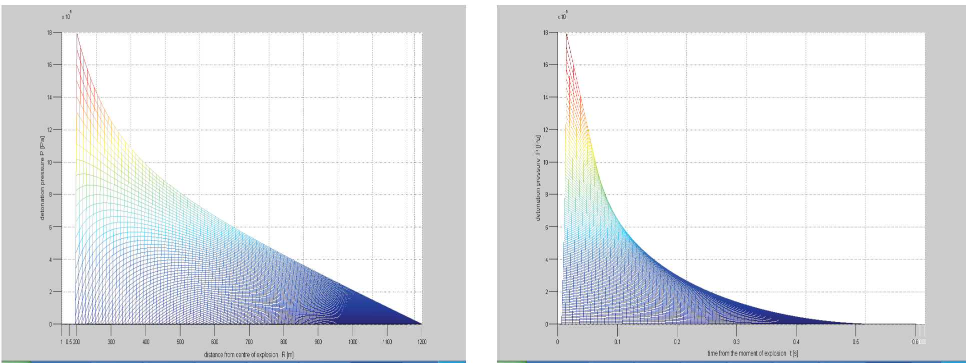


Fig. 6. 3D projection of the results of explosive process simulation to a relevant plane

The 3D view of the simulation results enables assessment of the effects on buildings and people, since the intensity and variable exposure time, which are accident properties, are clearly observable. The accident effect is proportional to the summary indicator of the intensity and exposure time.

5. CONCLUSION

This paper represents a review of the software packages which can be used for simulation of accidents. The ALOHA software package was used for the simulation of accidents and to provide an overview of the results. Based on a mathematical model of the explosive process, a simulation model implemented in the MATLAB software package was generated and a way of interpreting graphic representations of the simulation results was provided, in order to designate the safe zone and destructive effects of accidents.

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MODELIRANJE EFEKATA OBLAKA ZAPALJIVIH GASOVA I PARA

Predrag Stanković, Ivan Krstić, Emina Mihajlović

Pri odvijanju tehnoloških procesa može, u redovnom radu ili u slučaju udesa, doći do ispuštanja opasnih tečnih materija, izdvajanja zapaljivih i eksplozivnih gasova i para i stvaranja uslova za nastanak požara i eksplozija. Posebno je izražen i uticaj na ljude i životnu sredinu, kada dolazi do formiranja zapaljivog i toksičnog oblaka gasova i para. U tom smislu, predmet rada je modeliranje i simulacija efekata koji tom prilikom nastaju u cilju određivanja bezbedne zone. Na bazi mogućih scenarija udesnog događaja, korušćenjem matematičkog modela, procenjuju se ekološki rizik, pri čemu modeli u realnom vremenu daju sliku ugroženih zona.

Ključne reči: *zapaljivi gasovi i pare, matematički model, simulacija, bezbedna zona*