EXPLOSIVE ATMOSPHERE ANALYSIS FOR SIMULATION OF ACETONE SOURCE OF RELEASE USING ALOHA SOFTWARE

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Abstract
The analysis of the explosive atmosphere for the simulation of acetone using ALOHA (Arial Location Hazardous Atmosphere) was evaluated against a previous evaporation measurement in the present study. With ALOHA, evaporation from large liquid surfaces can be studied on a global scale. Such fluid surfaces can be formed during high leakage from process units. In third world countries, there are still operating pools that, under normal operating conditions, contain large quantities of flammable and explosive substances that can be a source of highly explosive atmospheres. In the more developed countries of Europe, you are more likely to encounter puddles during overfilling and dumping. Unlike under normal operating conditions, failure may result in the formation of large liquid surface in storage salvage tray or transport tank leaks. The simulation considers several boundary conditions, such as the type and temperature of the solid or porous medium on which the fluid surface is located, as well as different weather factors. An additional advantage of the software is that it can be used to investigate the extent of hazardous areas geographically anywhere, depending on different concentrations.

Keywords: *acetone, flammable liquid, simulation, explosive atmosphere, ALOHA software*

1. Introduction

Safety is top of mind at all manufacturing plants. The increasing demand for various chemical products has led to an increased production situation. The spread of the chemical industry is progressively posing a threat, a risk and a vulnerability for the population and the environment. Releases of volatile chemicals under normal operating conditions or accidental releases can be life-threatening. Depending on the substance, it can pose a health hazard and cause destruction in the immediate vicinity as well as further away. The flammability and explosive properties of substances can be influenced (Davis et al., 2017; Yuan et al., 2021; Mikáczó & Szepesi, 2021) by a number of factors, such as concentration, temperature, pressure or even meteorological and terrain conditions.

ALOHA 5.4.7 versions allows (Agencia de Protección Ambiental U.S., 2007) the user to assess the potential for explosive atmospheres to be released into the air in a limited time, relative to unexpected events or normal operating conditions, using a suitable source algorithm(Islam & Ryan, 2016).

The time of emission at the source may vary between one minute and one hour, so that a flat and homogeneous ground must be assumed. During the investigation, whether a preliminary survey or an ex-post analysis is carried out, the time of leakage should be recorded at the moment of occurrence, whether day or night (Bhattacharya & Ganesh Kumar, 2015).

2. ALOHA modelling software

ALOHA allows the user to estimate the dispersion of the explosive cloud under the wind in the chemical/physical characteristics for different chemicals, based on atmospheric conditions and the specific conditions of the release. ALOHA is able to estimate the hazard zones associated (Da Silva Rodrigues et al., 2017) with several types of explosive material and present a visual representation of them.

The Mapping Application for Response, Planning and Local Operational Tasks (MARPLOT) is a strongly related mapping tool to the ALOHA software. It can be used to topographically investigate the dispersion of a simulated release anywhere. Without the addition of MARPLOT, the ALOHA software can only be used to determine fluid dynamics relationships (Agencia de Protección Ambiental U.S., 2007). The program has several global background base map options, both in street and satellite view. Users can add map information to their own objects, such as chemical facilities near where some community is located.

***Table 1.** Hazardous areas that can be modelled with ALOHA*

Source of release	Direct source	Tank	Puddle	Gas pipeline
Vapor cloud	Explosive/toxic vapor	Explosive/toxic vapor	Explosive/toxic vapor	Explosive/toxic vapor
Vapor cloud (explosion)	Flammable area	Flammable area	Flammable area	Flammable area
Pool fire	Not acceptable	Thermal radition	Thermal radition	Not acceptable
BLEVE (fireball)	Not acceptable	Thermal radition	Not acceptable	Not acceptable
Jet fire	Not acceptable	Thermal radition	Not acceptable	Thermal radition

Within the program, two types of dispersion models can be applied to the substance under investigation, Gaussian model (neutrally buoyant gases i.e., ethylene, ethane, carbon monoxide, ethanol, hydoregn) and heavy gases. The former is a model to predict how gases with similar buoyancy to air will disperse in the atmosphere. The density of these gases is about the same as air. According to this model, wind and atmospheric turbulence are the forces that move the molecules of gas emitted through the air. So as a released cloud is blown downward, it is dispersed upwind and crosswind by "turbulent mixing".

As its name implies, the heavy gases model is when a heavier than air gas is released, it initially behaves very differently from gases with a lower relative density. The heavy gas first "falls" or sinks because it is heavier than the surrounding air. As the gas cloud descends, it spreads out due to gravity. For example, this can cause some of the vapour to move away from its release point.

ALOHA automatically lets you choose whether you want to predict the dispersion of a substance as a Gaussian or as a heavy gas release. This choice is based primarily on the molecular weight, the size of the emission and the gas cloud temperature. In particular, if a substance with a molecular weight more than the air which has been stored at low temperatures or high pressures, it may behave as a heavy gas (example of hydrogen sulfide, LPG,).

But sometimes it may be worth specifying the model to use rather than choosing ALOHA. For global studies, ALOHA can be a good solution, but licensed software such as Phase 3D Explosion, CFD-FLACS. For local, more flow-focused scientific studies, ANSYS CFD, Autodesk CFD are recommended.

The source model is used to calculate the emission rate (kg/s) and the dispersion model (Vishnu et al., 2016) is used to estimate the air concentration rate (ppm or mg/m^3). Finally, the fire and explosion model is used to calculate the heat flux. The rate of liquid release from the storage tank (He et al., 2020) can be calculated using flow equations.

The outflow of liquids through a sharp-edged orifice/nozzle is given by the following equation

$$G_L = C_D \cdot A \cdot \rho_l \cdot \left(\frac{2 \cdot (p - p_a)}{\rho_l} + 2 \cdot g \cdot H \right)^{1/2}, \tag{1}$$

where the characters stand for:

- G_L is liquid mass emission rate $\left(\frac{\mathrm{kg}}{\mathrm{s}} \right)$,
- C_D is discharge coefficient $(-)$ (Bohl, 1983),
  - Sharp-edge = 0.59 -62
  - Thick-plate square edge ≅ 82
  - Rounded = 0,97-0,99
- A is discharge hole (m^2),
- ρ_l is liquid density $\left(\frac{\mathrm{kg}}{\mathrm{m}^3} \right)$,
- p is liquid storage pressure (Pa),
- p_a is ambient pressure (Pa),
- g is acceleration of gravity $\left(9.81 \frac{\mathrm{m}}{\mathrm{s}^2} \right)$,
- H is height of liquid above hole (m).

The flash fraction of the superheated liquid can be calculated using the following equations. The flash fraction means the fraction part will boil off immediately (the flash part) if the pressure is suddenly reduced whereas some evaporate slower.

$$F_V = C_p \cdot \frac{\Delta T}{H_{vap}}, \tag{2}$$

$$\Delta T = (T - T_b), \tag{3}$$

where the characters stand for:

- F_V is flash fraction $(-)$,
- C_p is specific heat at ambient pressure $\left(\frac{\mathrm{kJ}}{\mathrm{kg}\cdot\mathrm{K}}\right)$,
- H_{vap} is heat of vaporation at ambient pressure $\left(\frac{\mathrm{J}}{\mathrm{kg}}\right)$,
- T is temperature of the medium (K),
- T_b is normal boiling point of the medium at ambient pressure (K).

Concentration of a chemical in air due to dispersion from a continuous source of release using the Gaussian dispersion model (Schnelle, 2003):

$$C(x,y,z)=\frac{G}{2\cdot\sigma_y\cdot\sigma_z\cdot u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\cdot\left[\exp\left(-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right)+\exp\left(-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right)\right]. \quad (4)$$

where the characters stand for:

- C is concentration at location x,y,z $\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$,
- x,y,z are distance from source (Figure 1) (m),
  - x is downwind,
  - y is crosswind,
  - z is vertical,
- G is vapour emission rate $\left(\frac{\mathrm{kg}}{\mathrm{s}}\right)$,
- H is height of source above ground level plus plume rise (m),
- σ_x,σ_y is dispersion coefficient what function of distance downwind (m),
- u is wind velocity $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$.

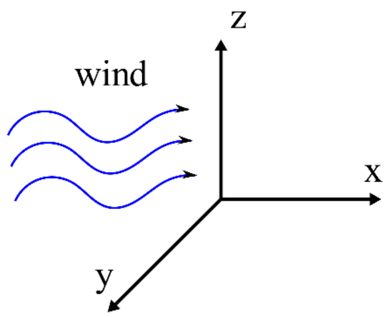

Figure 1. *Wind directions*

3. Experimental and simulation results

The phenomenon of acetone explosive liquid evaporation (Heymes et al., 2020; Akterian, 2020; Pénelon et al., 2020) under different airflows (u) was investigated in a previous study, where the measured results were compared with the results of different models. Based on the results published in this study, the best approach is the context of the Risk Management Program Guidance for Offsite Consequence Analysis, United States Environmental Protection Agency, 1994. The aim of the study is to compare the results of the aforementioned evaporation model with the reliability of the program and its adequacy. The measurement results obtained and the calculations according to this evaporation model are summarised in Table 2.

***Table 2.** Results of measurements and Evaporation model*

	u=0.2 m/s	u=2 m/s	u=4 m/s	u=6 m/s
Measurements	0.904 mg/s	6.171 mg/s	9.311 mg/s	12.8 mg/s
Evaporation model	0.904 mg/s	5.449 mg/s	9.356 mg/s	12.837 mg/s

The test fluid surface area was 0.00096 m^2, which is considered to be a very small area. In the ALOHA program, the evaporation rate was examined, which is shown in Figure 2. The simulation did not run with the surface area of the crucible under test. The results were compared to a factor of 10. The value obtained by the program is 3.59 grams/min, which corresponds to 59.833 mg/s. This result falls between the measured and modelled values, so it can be assumed that the correlations used by the program are consistent with the real values. The mathematical relationships used to model the propagation in the simulation studies are correct.

SITE DATA:
Location: SAJÓBÁBONY, HUNGARY
Building Air Exchanges Per Hour: 0.30 (unsheltered double storied)
Time: July 12, 2022 0930 hours ST (user specified)

CHEMICAL DATA:
Chemical Name: ACETONE
CAS Number: 67-64-1 Molecular Weight: 58.08 g/mol
AEGL-1 (60 min): 200 ppm AEGL-2 (60 min): 3200 ppm AEGL-3 (60 min): 5700 ppm
LEL: 26000 ppm UEL: 130000 ppm
Ambient Boiling Point: 55.6° C
Vapor Pressure at Ambient Temperature: 0.32 atm
Ambient Saturation Concentration: 322,056 ppm or 32.2%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
Wind: 2 meters/second from E at 3 meters
Ground Roughness: open country Cloud Cover: 0 tenths
Air Temperature: 26° C
Stability Class: D (user override)
No Inversion Height Relative Humidity: 50%

SOURCE STRENGTH:
Evaporating Puddle (Note: chemical is flammable)
Puddle Area: 0.0096 square meters Puddle Volume: 0.1 liters
Ground Type: Default soil Ground Temperature: 24° C
Initial Puddle Temperature: 21° C
Release Duration: 32 minutes
Max Average Sustained Release Rate: 3.59 grams/min

***Figure 2.** Result of the 2 m/s airflow simulation tested in the measurement*

The simulation required a much larger effective surface area for a proportional visual comparison of the results.

For the simulation, the Sajóbábony Chemical Park in Hungary was chosen as the geographical location of the emission source, as many companies and enterprises in this industrial park use flammable and explosive materials, both at the product and storage level.

The available weather data for the area was collected, determined by the prevailing climatological conditions and selected the best scenario to model the case study. In this paper, I chose a summer date of June 12th, 2022 at 9:30 AM as the time of the event. Figure 3 shows the metrological and additional boundary conditions entered in the ALOHA software, which were necessary to create the model. The average airflow in territory of Sajóbábony is 2-8 m/s. The lowest, most frequently occurring value was used as the basis for the simulation. At the given boundary conditions, the first things the program does is drawing the danger zones and placing them on the map in MARPLOT.

The simulation shows an initial evaporation rate of 77.2 kilograms/min from a surface area of 290 m^2, which decreases continuously in proportion to the combustible surface. The hazard areas due to evaporation are shown in Figures 4 and 5. This is the amount of liquid that could form in the event of a surface water hazard in the area for example level control failure of a stationary cylindrical steel tank.

SITE DATA:
Location: SAJÓBÁBONY, HUNGARY
Building Air Exchanges Per Hour: 0.33 (unsheltered double storied)
Time: July 12, 2022 0930 hours ST (using computer's clock)

CHEMICAL DATA:
Chemical Name: ACETONE
CAS Number: 67-64-1 Molecular Weight: 58.08 g/mol
AEGL-1 (60 min): 200 ppm AEGL-2 (60 min): 3200 ppm AEGL-3 (60 min): 5700 ppm
LEL: 26000 ppm UEL: 130000 ppm
Ambient Boiling Point: 55.6° C
Vapor Pressure at Ambient Temperature: 0.37 atm
Ambient Saturation Concentration: 380,855 ppm or 38.1%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
Wind: 2 meters/second from E at 3 meters
Ground Roughness: open country Cloud Cover: 0 tenths
Air Temperature: 30° C Stability Class: B
No Inversion Height Relative Humidity: 50%

SOURCE STRENGTH:
Evaporating Puddle (Note: chemical is flammable)
Puddle Area: 290 square meters Puddle Volume: 1450 liters
Ground Type: Default soil Ground Temperature: 35° C
Initial Puddle Temperature: 20° C
Release Duration: 17 minutes
Max Average Sustained Release Rate: 77.2 kilograms/min
(averaged over a minute or more)

Figure 3. *ALOHA acetone evaporation modelling text summary*

From the evaporation value calculated by the program under the given boundary conditions, the vapour propagation is determined based on the heavy gas model. Figure 4 shows the distribution of LEL20% concentration (ppm) as a function of horizontal and vertical distance. The other concentration distributions cannot be visualised on the diagram, as they would require a larger surface area. It cannot interpret the dispersion of the nearer fields as homogeneous, and thus cannot be considered reliable.

When placing the emission source on the map, data from the nearer zones can be extracted. A conservative approach towards safety is correct for these extents, as smaller distances are less reliable from a safety point of view.

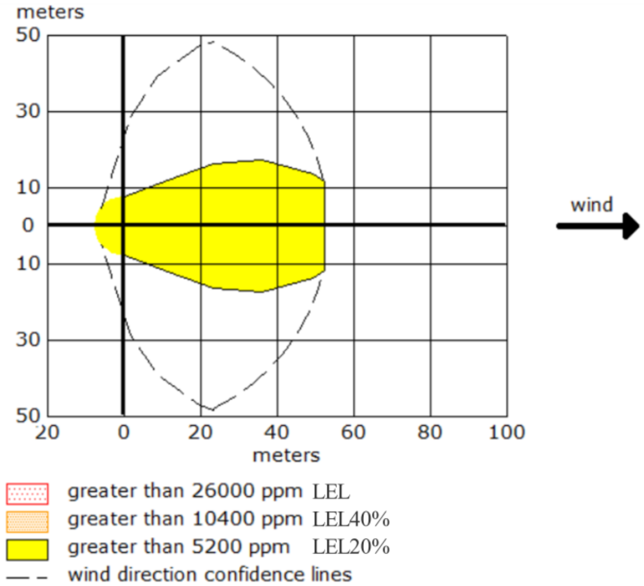

Figure 4. *Expansion of explosion boundary zones*

Figure 5 illustrates the lower explosion limit, with the extents at 20% and 40% of its value expressed in ppm. The program is still partially limited with the present parameters, only plotting the LEL20% value, but it is possible to extract the distances for the other zones. LEL extension is 20 metres, LEL40% extension is 34 metres.

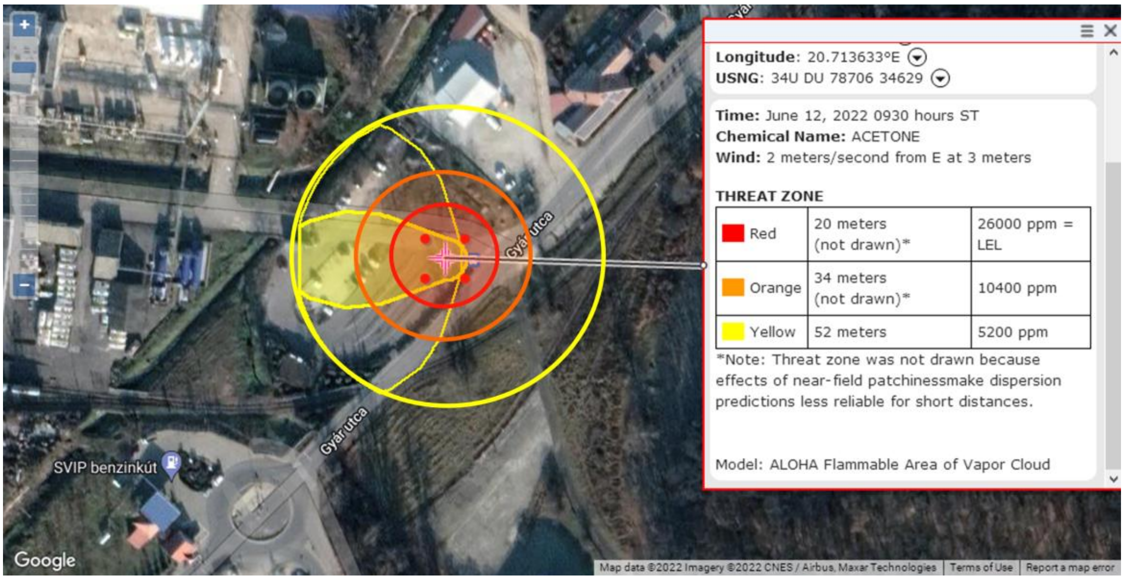

Figure 5. *Representation of explosion threat zone of 2 m/s air flow from east*

Figure 5 shows the extent to which explosive gas clouds can form. In principle, the program assumes a one-way airflow at a time. Conservatism is kept in mind due to the different wind direction, the yellow (LEL20%) zone representation has been extended to a circle. With further individual graphical correction, the LEL40% and LEL boundaries were also considered.

Within the zone of the lower explosive limit if an effective ignition source of some form is present. There is a high probability that an explosion will occur. In these studies, ignition source analysis can be used to rule out the possibility of in-area hazards. By installing an appropriate gas detector in the LEL20% area, an acoustic and light warning signal can be used to inform those in the area of the initial potential hazard. For LEL40%, further reinforcement of the warning signal and the de-energising of electrical fabrications can ensure the exclusion of effective ignition sources.

4. Summary

The study discusses a case study of acetone chemical emissions during a hypothetical, fictitious case. To demonstrate the simulated model of the case study, ALOHA software with scatter modelling was developed. The 100% utilization of all units of the program only works on a global scale, it is more suitable for control calculations locally.

The program and similar software have long been used in the field of industrial safety to determine the dispersion of hazardous materials in connection with serious accidents. The experiment and the simulation confirm the assumption that the program is actually suitable for investigating dangerous situations. It is not suitable for the exact identification of explosive atmosphere, as it can be used properly on a global scale. On the other hand, in the case of chemical plants where, in the case of potential emission sources and equipment, the lack of maintenance is highly neglected, and in the case of omission of further measures, an increased leakage is assumed, the operator can be encouraged to make immediate repairs by using the program.

The application of these software is important from the point of view of risk values, as it helps to avoid undesirable events due to safety, loss of life and property. It is free to use, regardless of time or circumstances. Its applicability is subject to these conditions.

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