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Original scientific paper

ACCIDENTAL RELEASES OF TOXIC GAS ACETYLENE-SIMULATION WITH ALOHA SOFTWARE

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ABSTRACT: Uncontrolled acetylene release during production processes, transportation, or storage can lead to explosions and detonations endangering safety of people and material assets. This paper investigates the impact of accidental release of acetylene gas in surrounding areas. The ALOHA software has been used in this paper to modelling of acetylene release. The modelling was performed for an accidental release of 2,000 kg acetylene from direct source for one minute. F or a typical average atmospheric condition in location, this accidental acetylene release would cause a red zone of 197 m (15,000 ppm) and yellow zone of 483 m (2,500 ppm) to downwind from the source. Inadequate storage can lead to accidental situations and negative impact on people and the environment.

Keywords: air pollution, ALOHA, acetylene, modelling.

INTRODUCTION

In the recent years, world has seen a wide range of major accidents with a number of fatalities, economic losses, and damage to the environment. These accidents can lead to serious danger to human health and the environment, which can occur inside or outside the establishment (Ilić et al., 2018). The chemical industry is one of the major potential environmental polluters. The release of any chemical may lead to toxic effects, fire, and explosion, and it makes the activity critical for safety systems to be made efficient and adequate to mitigate the haphazard in case of emergency. (Yadav et al., 2022). A great variety of its negative impacts affect both living organisms and material assets. Particularly dangerous are industrial sites, where emergencies are possible with the sudden formation of intense, diverse impact factors (shock waves, heat waves, emission of toxic substances). In this case, it is extremely important to predict the risk of damage to personnel in the workplace during emergencies (Biliaiev et al., 2020a).

According to European Union Directive–Seveso II, a chemical accident is defined as a result of unplanned and unpredicted events in the course of industrial activity being manifested through the emission of toxic substances in the environment or through fire or explosion. The accidents comprising one or more hazardous chemicals jeopardize humans and the environment both immediately or with delay, inside or outside the installation (Komatina et al., 2018). In addition to the proven impact on humans, the impact on plant life has also been confirmed (Ilić and Maksimović, 2011). Improper handling and accidental release of hazardous chemicals pose serious public health hazards. The intensity of such accidents depends on the nature of the release, toxicity of the material, population density, and meteorological factors (Ilić et al., 2019). The above can cause air pollution, which represents a significant risk to the health of the population (Ilić, 2015; Ilić et al., 2018, 2019, 2020; Radović et al., 2022; Ćirišan et al., 2023). In case of emergencies, it is very important to assess the risk of damage to people (Biliaiev et al., 2020b).

Acetylene (C_2H_2) is the simplest hydrocarbon (Pässler et al., 2000). It is the unsaturated hydrocarbon belonging to the alkyne group. Its molecule is linear and built up from two carbon atoms bonded together in a triple bond. One hydrogen atom is bonded to every carbon atom (Komatina et al., 2018). Before oil became the main feedstock of the chemical industry, acetylene was the predominant building block of industrial organic chemistry (Pässler et al., 2000). Pure acetylene is colorless, odorless, and tasteless at normal temperature and pressure. At higher temperatures and under higher pressures, acetylene decomposes spontaneously, releasing a large quantity of energy and causing chain reactions that result in explosion. Uncontrolled acetylene release during production processes, transportation, or storage can lead to explosions and detonations, endangering the safety of people and material assets (Komatina et al., 2018). Pässler et al. (2000) provided information on some basic physical properties of acetylene. Acetylene has a molecular mass of 26.0379. Its critical temperature is reported as 308.32 K (35.17 ˚C), and its critical pressure is 6.139 MPa. The critical volume of acetylene is 0.113 m^3/kmol. The triple point of acetylene occurs at 192.4 K (80.75 ˚C), and its corresponding pressure is 128.3 kPa. The normal sublimation point of acetylene is 189.15 K (4.0 ˚C). Acetylene also has a crystal transition point at 133.0 K (140.15 ˚C), and its enthalpy of transition is 2.54 kJ/mol.

This paper investigates the impact of the accidental release of acetylene gas in surrounding areas. The aim of this paper is to point out the inadequate storage and handling of acetylene, i.e. the consequences for human health and the environment.

MATERIALS AND METHOD

Location and acetylene station

The subject of the research is the impact of the accidental release of acetylene gas in the business zone "Ramići-Banja Luka", Banja Luka (Figure 1). Banja Luka is a city in the Republic of Srpska, Bosnia and Herzegovina (B&H). Banja Luka is located in Vrbas valley and is surrounded by hills 200-600 meters above sea level high. Banja Luka is the second biggest city in B&H, with a population of 200,000. Situated in a basin 164 m above sea level, where the Dinaric Alps from the south descend into the Pannonian Basin in the north.

Acetylene station is about 200 m away from the first residential building, north (Figure 1).

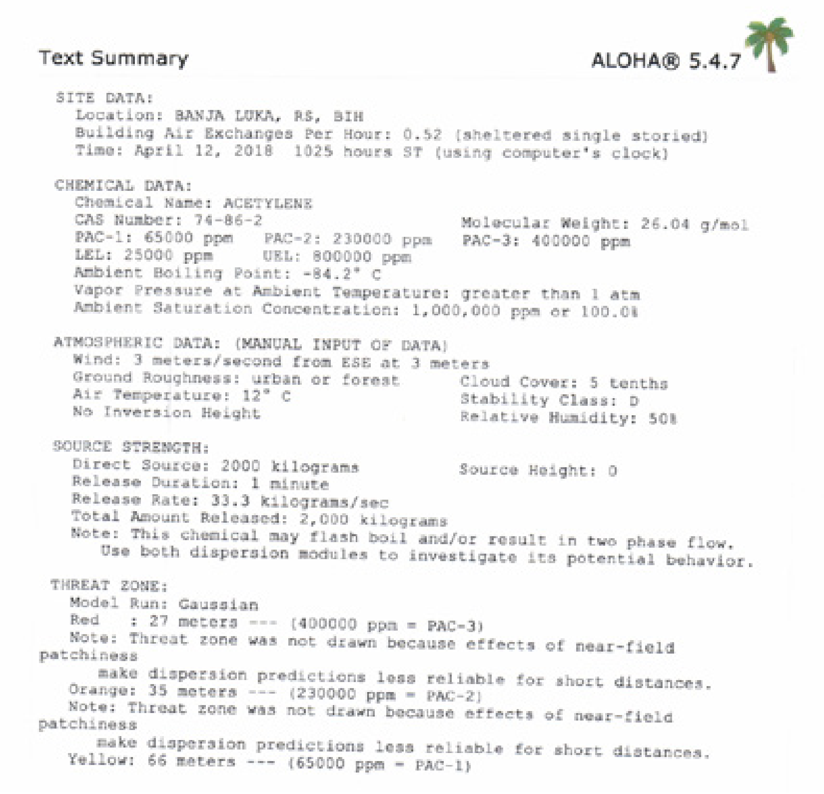
Figure 1. Position and distance of station from the first residential object (Google Earth)

Banja Luka has a temperate continental climate with prevailing influences from the Pannonian plain. It belongs to the Central European Time zone (GMT +1). The average annual temperature reaches 10.7°C, the average temperature in January reaches 0.8ºC, whereas the average temperature in July reaches 21.3ºC.

Software analysis

Numerical models may be considered from two perspectives: first, as operational models applied by decision-makers where results should be clear and instantly available, and second, as models where simulation time is less important, and more importance is given to the accuracy of results and the most thorough consideration of the complexity of phenomena. There are various parameters and criteria for assessing the impacts of the toxicity of chemical materials. Losses and damages caused by the release and spread of toxic chemicals depend on the concentration of the toxic chemical and its contact time. In order to conduct incident modelling, ALOHA software (Areal Location of Hazardous Atmosphere) Version 5.4.7 was used (Ruhipour et al., 2017). ALOHA is the hazard-modelling program for the CAMEO (Computer-Aided Management of Emergency Operations) software suite, which is widely used to plan for and respond to chemical emergencies. ALOHA allows the user to choose from several accident scenarios and then uses an appropriate source algorithm to inject material into the air over a limited time. The source emission time may vary between limits of one minute to one hour. A flat, homogeneous Earth is assumed. For the purposes of solar radiation and day/night decisions, time is fixed at the moment the leak begins. ALOHA can model toxic gas clouds, flammable gas clouds, Boiling Liquid Expanding Vapor Explosions (BLEVEs), jet fires, pool fires, and vapor cloud explosions. The threat zone estimates are shown on a grid in ALOHA and can also be plotted on maps in MARPLOT, Esri's ArcMap, Google Earth, and Google Maps. The red threat zone represents the worst hazard level, and the orange and yellow threat zones represent areas of decreasing hazard (www.epa.gov/cameo/aloha-software; Ilić et al., 2018; Joseph & Williams, 2022).

To model hazards using ALOHA, several required inputs are entered into the software. These inputs include basic scenario information such as the date, time, and location of the event. A chemical is chosen from ALOHA's chemical library, and atmospheric information, including wind speed and direction, air temperature, and cloud cover, is entered either manually or automatically using a portable station for atmospheric measurements (SAM). Additionally, a source is chosen from options such as direct, puddle, gas pipeline, or tank, and corresponding source information, including release amount, tank dimensions, and whether the chemical is burning, is entered. The Levels of Concern (LOCs) to be used for estimating the threat zones are specified, or default LOCs offered by ALOHA are used. Furthermore, the type of hazard, such as toxicity or thermal radiation, to be used when estimating the threat zones is also chosen. The entered data for acetylene in ALOHA is presented in Figure 2.



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Text Summary                                              ALOHA® 5.4.7

 SITE DATA:
   Location: BANJA LUKA, RS, BIH
   Building Air Exchanges Per Hour: 0.52 (sheltered single storied)
   Time: April 12, 2018  1025 hours ST (using computer's clock)

 CHEMICAL DATA:
   Chemical Name: ACETYLENE
   CAS Number: 74-86-2                      Molecular Weight: 26.04 g/mol
   PAC-1: 65000 ppm   PAC-2: 230000 ppm     PAC-3: 400000 ppm
   LEL: 25000 ppm     UEL: 800000 ppm
   Ambient Boiling Point: -84.2° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 3 meters/second from ESE at 3 meters
   Ground Roughness: urban or forest        Cloud Cover: 5 tenths
   Air Temperature: 12° C                   Stability Class: D
   No Inversion Height                      Relative Humidity: 50%

 SOURCE STRENGTH:
   Direct Source: 2000 kilograms            Source Height: 0
   Release Duration: 1 minute
   Release Rate: 33.3 kilograms/sec
   Total Amount Released: 2,000 kilograms
   Note: This chemical may flash boil and/or result in two phase flow.
      Use both dispersion modules to investigate its potential behavior.

 THREAT ZONE:
   Model Run: Gaussian
   Red   : 27 meters --- (400000 ppm = PAC-3)
   Note: Threat zone was not drawn because effects of near-field
patchiness
      make dispersion predictions less reliable for short distances.
   Orange: 35 meters --- (230000 ppm = PAC-2)
   Note: Threat zone was not drawn because effects of near-field
patchiness
      make dispersion predictions less reliable for short distances.
   Yellow: 66 meters --- (65000 ppm = PAC-1)
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Figure 2. Entered data in software for acetylene

The rate at which a chemical becomes airborne is critical for determining the size and duration of a toxic or flammable cloud. ALOHA utilizes a range of models known as source strength models to estimate the rate at which a chemical is released from containment and enters the atmosphere (Jones et al., 2013). For this study, a direct source model was employed, involving the instantaneous or continuous release of chemical vapors into the air from a single point. This option is the only one that permits an elevated release.

With the direct source option in ALOHA, the user can specify the amount of chemical vapors introduced into the air from a specific point in space. The user can select between an instantaneous or steady-state release of finite duration. This option is appropriate for gases that are denser than air and are affected by gravity or gases that behave as neutrally buoyant. ALOHA allows for a release above ground level for gases that behave as neutrally buoyant (Jones et al., 2013). The source emission time may vary between limits of one minute to one hour (Bhattacharya & Ganesh Kumar, 2015). For this study, the direct source option was used for one minute.

ALOHA employs a graphical interface to display the results and for data entry. Threat zones, which depict the area within which there is a potential for exposure to toxic vapors, a flammable atmosphere, overpressure from a vapor cloud explosion, or thermal radiation from a fire, are represented graphically. These threat zones indicate the area where ground-level exposure exceeds the user-specified level of concern at some time after the release. All points within the threat zone experience a transient exposure exceeding the level of concern at some point following the release, serving as a record of the anticipated peak exposure over time. In certain scenarios, the user may also view the time dependence of the exposure at specific points (Jones et al., 2013).

For the accidental release of 2,000 kg of acetylene, modeling was performed. The accident simulation was positioned in accordance with the entered coordinates (44°84'19.80"N 17°17'85.34"E) and can be rotated to face the direction of the wind that blows at a certain point.

RESULTS AND DISCUSSION

Modelling the effects of acetylene release and spread - toxic effect

For a typical average atmospheric condition at this location, iso-concentration lines of toxic zones based on the gas model have been calculated, and the following zones have been obtained: the red zone (27 m, 400,000 ppm = PAC-3) and the orange zone (35 m, 230,000 ppm = PAC-2) are not plotted because the prediction dispersion is less reliable for short distances, and the yellow zone (66 m, 65,000 ppm = PAC-1).

As the gas moves towards the limits of the vulnerable zones, it creates a toxic effect that can be life-threatening. Workers who are in the yellow zone (Figure 3) may experience serious health effects or symptoms that can weaken their ability to take protective measures.

Protective Action Criteria (PACs) are essential components for planning and responding to uncontrolled releases of hazardous chemicals. These criteria, in combination with exposure estimates, provide the necessary information to evaluate chemical release events and take appropriate protective actions. During an emergency response, PACs may be used to evaluate the severity of the event, identify potential outcomes, and decide what protective actions to take (Protective, 2012).

The PACs dataset is a hierarchy-based system of the three most common public exposure guideline systems: Acute Exposure Guideline Levels (AEGLs), Emergency Response Planning Guidelines (ERPGs), and Temporary Emergency Exposure Limits (TEELs). AEGLs are established by the U.S. Environmental Protection Agency (EPA) and represent threshold concentrations of a substance in the air that can cause adverse health effects, such as respiratory or neurological impairment, to individuals exposed to it for a short period of time (up to 8 hours). ERPGs are developed by the American Industrial Hygiene Association (AIHA) and represent airborne concentrations of a substance above which an emergency response plan should be implemented to protect workers and the public. TEELs are established by the U.S. Department of Energy (DOE) and represent threshold concentrations of a substance in the air that can cause immediate and irreversible health effects, such as severe respiratory distress or death, to individuals exposed to it for a short period of time (up to 30 minutes) (Acute Exposure Guideline, 2018).

The PACs dataset uses a hierarchy-based system when choosing which values to use for the PACs of a hazardous substance. The preferred values are the Final, 60-minute AEGL values, followed by the Interim, 60-minute AEGL values. If those values are not available, the dataset uses the ERPG values, and if those are not available either, it uses the TEEL values.

The PACs dataset provides a set of values (PAC-1, PAC-2, and PAC-3) for each chemical, but the source of those values may vary. For instance, the PAC-3 value for one chemical may be an ERPG-3, while for a different chemical, it may be the TEEL-3. A hierarchical system is useful for selecting levels of concern for chemicals that are defined under two or more public exposure guidelines. In Aloha, PAC-1, PAC-2, and PAC-3 values can be selected to estimate threat zones. The yellow, orange, and red zones indicate areas where these values are predicted to be exceeded after the release of the chemical. For acetylene, ALOHA provides the PAC values as the default toxic LOCs until AEGL or ERPG values are established.

There are three levels of PAC value, with each level indicating a higher level of exposure and an increasingly severe effect. The levels are PAC-1, PAC-2, and PAC-3, with PAC-1 associated with mild, transient health effects, PAC-2 associated with irreversible or other serious health effects that could impair the ability to take protective action, and PAC-3 associated with life-threatening health effects (Protective, 2012).

Table 1. PACs (Protective Action Criteria) (https://cameochemicals.noaa.gov/chemical/18)

Chemical	PAC-1	PAC-2	PAC-3	
Acetylene (74-86-2)	65,000 ppm 🔥🔥🔥	230,000 ppm 🔥🔥🔥	400,000 ppm 🔥🔥🔥	LEL = 25,000 ppm

🔥🔥🔥 indicates value is 100% or more of LEL.

Figure 3 shows the threat zone in case of accidental release of acetylene.

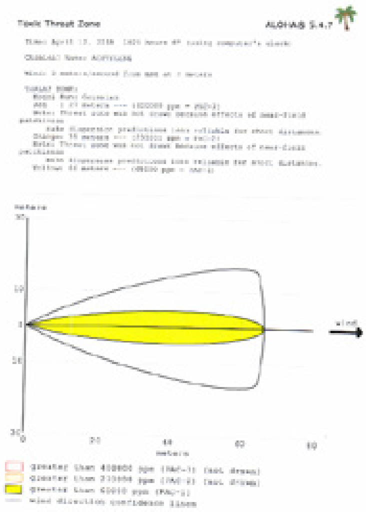

Figure 3. Toxic threat zone of release and spread of toxic effect-acetylene

Table 2. PACs values for Acetylene in ppm (https://sp.eota.energy.gov/pac/docs/Revision_29_Table2.pdf)

PACs based on AEGLs, ERPGs, or TEELs		
PAC-1	PAC-2	PAC-3
65,000*	230,000*	400,000*

* indicates PAC ≥ LEL

MODELING THE EFFECT OF THE POSSIBILITY OF IGNITING A VAPOR CLOUD OF A DANGEROUS SUBSTANCE - ACETYLENE

According to the results obtained from the calculation of the vulnerable zone using the heavy gas model, the flammable zones for acetylene are represented by two iso-concentration lines. The first line is the red zone, which covers an area of 197 m and is characterized by a concentration of 15,000 ppm (parts per million) of acetylene, equivalent to 60% of the lower explosive limit (LEL). The second line is the yellow zone, which covers an area of 483 m and is characterized by a concentration of 2,500 ppm of acetylene, equivalent to 10% of LEL. It is important to note that the LEL is defined as the lowest concentration (percentage) of a gas or vapor in air that is capable of producing a flash of fire in the presence of an ignition source. Safety professionals often consider it to be the same as the lower flammable limit (LFL). If concentrations of a flammable gas or steam are greater than 10%, evacuation of the area should be carried out as a precautionary measure.

The red zone includes a portion of the business zone, while the yellow zone covers both the population and a portion of the business zone (as shown in Figure 4).

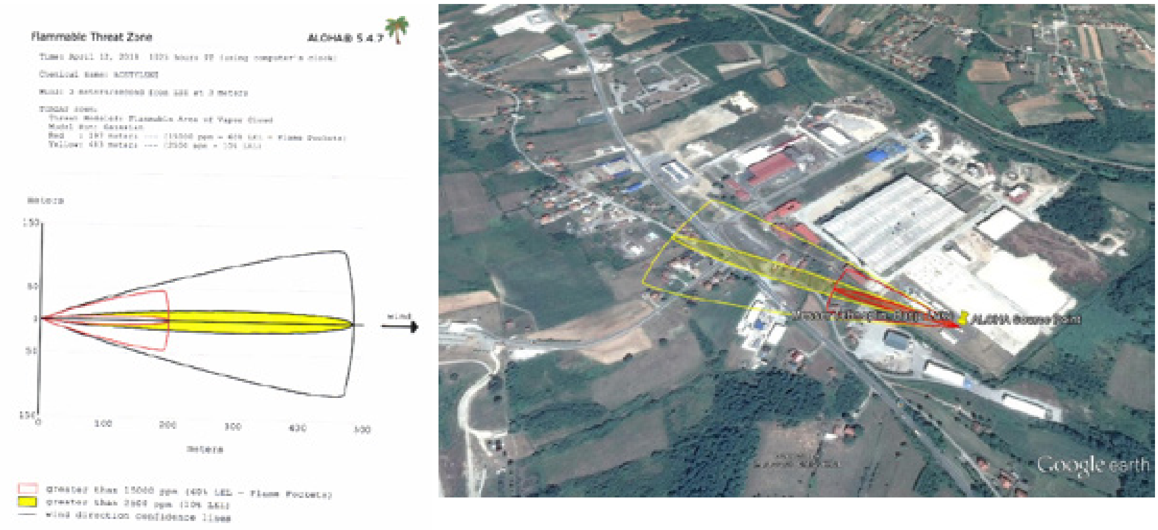

Figure 4. Iso-concentration lines of flammable zones and possible development of events - scenario of the possibility of ignition of a vapor cloud of dangerous substance - acetylene

MODELLING THE EFFECTS OF A VAPOR CLOUD EXPLOSION - ACETYLENE

ALOHA characterizes the damaging effect of the blast wave by using only the pressure peak. The blast wave can cause damage directly to pressure-sensitive organs, such as the ears and lungs, or indirectly, by accelerating debris or causing building collapse. ALOHA uses three levels of concern (LOCs) to quantify the direct and indirect effects. Glass windows can break at a pressure of 1 psi, at 3.5 psi there is a significant risk of ear and lung damage and injury from flying debris, and at 8 psi there is a significant risk of unreinforced building collapse, ear and lung damage.

The vulnerable zone is calculated based on the gas model and shock wave model, which considers the explosion of a gas cloud caused by a spark or flame. Isolines of overpressure from the center of the explosion are obtained, with the red zone representing areas where pressure is greater than 8 psi, causing damage to equipment and buildings. The orange zone (3.5 psi) represents a risk of serious injury, and the yellow zone (1.0 psi) is where glass windows could break, with a range of 174 m.

There are no accurate data on the number of employees per vulnerable zone. It is estimated that the total number of employees in the business zone is around 6,000. The population of Ramići is 2,105.

Figure 5 shows the overpressure due to an acetylene explosion and examples of steam cloud effects for acetylene.

Figure 5. Over-pressure due to Acetylene Explosion and Examples of scenario Steam Cloud effects for acetylene

CONCLUSION

The use of ALOHA software provides decision-makers with an effective tool for modeling the release of hazardous chemicals and estimating the potential impacts. The direct source model option in ALOHA allows for an elevated release and enables the user to specify the amount of chemical vapors introduced into the air from a particular point in space. The threat zones, which represent the area within which there is a possibility of exposure to toxic vapors or a flammable atmosphere, were represented graphically using ALOHA's graphical interface.

Acetylene is a highly flammable and explosive gas, and it poses significant dangers to the environment. Simulation of acetylene release scenarios indicates a high risk of fire and explosion, which could significantly endanger the working environment and the area around the "Ramići" business zone in Banja Luka. According to ALOHA software, damage may occur due to direct or indirect effects of the pressure shock wave. Direct effects may include damage to pressure-sensitive organs such as the ears and lungs. Indirect effects may result from glass fragments from broken windows, collapsing buildings, or debris accelerated by the blast wave. ALOHA includes three LOCs that quantify indirect and direct effects. Glass windows can break at a pressure of 1 psi; at 3.5 psi, there is a significant risk of eardrum injury and injury from flying debris; at 8 psi, there is a significant risk of ear and lung damage, as well as an indirect effect from the collapse of unreinforced buildings.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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