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HAZARD MODELLING OF ACCIDENTAL RELEASE CHLORINE GAS USING MODERN TOOL-ALOHA SOFTWARE

Predrag Ilić¹, Svetlana Ilić¹, Ljiljana Stojanović Bjelić²

¹PSI Institute for protection and ecology of the Republic of Srpska, Banja Luka, Republic of Srpska, BiH, predrag.ilic@institutzei.net and svetlana.ilic@institutzei.net ²Pan-European University "APEIRON", Banja Luka, Republic of Srpska, BiH, ljiljana.v.stojanovicbjelic@apeiron-edu.eu

Abstract: This paper investigates the impact of accidental release of chlorine gas in surrounding areas consequences of chlorine gas leak studying the negative effects on both the environment and individuals. Chlorine and its consequences have a far more reaching effect in society that one may have imagined. The ALOHA software has been used in this paper to modelling of chlorine release. The modelling was performed for an accidental release of 3.373 tons chlorine gas from unsheltered single storied for one hour. For a typical average atmospheric condition in location, this accidental chlorine release would cause a red zone of 3.0 kilometres (AEGL-3=20 ppm), orange zone of 7.1 kilometres (AEGL-2=2 ppm) and yellow zone stretching to greater than 10.0 kilometres (AEGL-1=0.5 ppm) to downwind from the source.

Keywords: air pollution, ALOHA, chlorine, 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 be occurred inside or outside the establishment. Consequence assessment is very important to predict and prevent deleterious effects of these events [Setareshenas et al., 2014]. Oxidizing agents have the largest application in microbiological control of the water systems and include halogens, chlorine, bromine and iodine [Ruhipour et al., 2017]. Chlorine is a toxic material that is used in water treatment plants as disinfectants [Setareshenas et al., 2014]. Chlorine is a strong oxidizing agent that simply combines with Protoplasma and forms stable nitrogen-chlorine bonds in proteins. Therefore, it is toxic to all the living organisms. The toxicity of a chemical substance to a living organism is under influence of factors such as its concentration, pH, temperature, ionic strength and other chemicals and wastes in the system [Ruhipour et al., 2017]. A major objective of drinking water treatment is to provide water that is both microbiologically and chemically safe for human consumption. The combination of conventional drinking water treatment along with disinfection has proven to be one of the major public health advances in modern times. Chlorine is most often the disinfectant used to treat water for microbiological protection before it is discharged into a drinking water distribution system [Clark & Sivaganesan, 2002]. Chlorine is an essential material to protect human from outbreaks of waterborne disease. Population growth and developing the water treatment technology make extensive use of consequence analysis for prediction and prevent the harmful effects of chlorine release in chemical plants. There are various commercial codes including Gaussian model for consequence analysis of risk, such as SLAB, ALOHA, PHAST, etc. [Hosseini, 2016].

MATERIALS AND METHODS

LOCATION AND CHLORINE STATION

Subject of the research is impact of accidental release of chlorine gas in surrounding areas conse-

quences of chlorine gas in chlorine station (locality Grmić-water source) in the city of Bijeljina (Pictures 1). Bijeljina is a city in Republic of Srpska (Bosnia and Herzegovina). The city have around 100,000 inhabitants, and is situated on the plains of Semberija. It is located at 6 km (4 mi) from Serbia and 40 km (25 mi) from Croatia.

Bijeljina has temperate continental climate. It belongs to the Central European Time zone (GMT +1). The average annual temperature reaches 11 °C, the average January -1°C, whereas the average temperature in July reaches 22°C. Relative air humidity is 70-80%.

PHYSICAL-CHEMICAL CHARACTERISTICS AND IMPACT OF CHLORINE GAS

Chlorine (Cl₂) is considered a pollutant gas for dispersion modelling since it is one of the most commonly produced and used industrial chemicals in the world [Paul et al., 2014]. The chlorine gas is heavier than air (3.2 g/l at 0 °C) which tends to form a cloud near to ground. Its odour is suffocating and pungent at a concentration of less than 1 ppm. The Cl, effects on the human health are linked to its irritant potential. At a low atmospheric concentration less than 15 ppm, the chlorine irritates the eyes quickly, the skin and the respiratory system cells (nose, throat, respiratory tract). In the case of a longer exposure and with a higher concentration (around 1,000 ppm for 1 minute of exposure), a pulmonary oedema can occur in few minutes and causes the death of the contaminated persons [Garbolino et al., 2009]. Chlorine is produced by the electrolysis of brine in mercury or diaphragm cells, with the co-products sodium hydroxide and hydrogen. It is used mainly for the manufacture of a wide range of organic and inorganic chlorine compounds and for the chlorination of water and for bleaching. A large chlorine release is potentially one of the most severe hazards from a common bulk chemical presented by the chemical industry. As an oxidant chlorine is in many ways comparable with oxygen. Organic compounds may have flammability limits in chlorine rather similar to those, which they have in oxygen. Reactions between organic compounds and chlorine are generally highly exothermic and tend to go to complete chlorination, often with some violence. The major accidents which can occur in industrial installations or during the transportation of hazardous materials are usually related to a loss of containment. The loss of containment can be caused by an impact, by the failure of a piece of equipment (a pipe or tank) due to the effects of corrosion, by human error during a loading or unloading operation, or by various other factors. The loss of containment can also be a consequence of the accident itself, for example in the case of the explosion of a pressurized tank [Ruhipour et al., 2017].

SOFTWARE ANALYSIS

Numerical models may be considered from two angles: first, as operational models applied by decision makers in which results should be clear and instantly available, and second, as models in which 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 toxicity of chemical materials. Losses and damages caused by the release and spread of toxic chemicals depend on the concentration of toxic chemical and its contact time. In order to conduct incident modelling, ALOHA software (Arial Location Hazardous Atmosphere) Version 5.4.7 was used. ALOHA allows the user a choice of several accident scenarios, 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 purposes of solar radiation and day/ night decisions, time is fixed at the moment the leak begins [Ruhipour et al., 2017]. ALOHA is the hazard-modelling program for the CAMEO software suite, which is used widely to plan for and respond to chemical emergencies. ALOHA allows to enter details about a real or potential chemical release, and then it will

generate threat zone estimates for various types of hazards. ALOHA can model toxic gas clouds, flammable gas clouds, BLEVEs (Boiling Liquid Expanding Vapour Explosions), jet fires, pool fires, and vapour cloud explosions. The threat zone estimates are shown on a grid in ALOHA and they 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 [https://www.epa.gov/cameo/aloha-software].

RESULTS AND DISCUSSION

Chlorine station is located at an altitude of 92 m. The chlorine station is about 360 m away from the first residential building, north (Pictures 1). It is noticeable that chlorine is mainly used for disinfection of drinking water in this station. Since chlorine is a toxic material, thus, its dispersion can be dangerous for human health [Setareshenas et al., 2014, Hosseini, 2016].



Picture 1. Position and distance of chlorine station from the first residential object [Google Earth]

To model hazards with ALOHA, we have entered the required scenario information. Required In-

puts:

- Enter basic scenario information (such as date, time, and location).
- Choose a chemical from ALOHA's chemical library.
- Enter atmospheric information (such as wind speed and direction, air temperature, and cloud cover) by hand or automatically using a portable station for atmospheric measurements (SAM).
- Choose a source: direct, puddle, gas pipeline, or tank.
- Enter source information (such as release amount, tank dimensions, and whether the chemical is burning).
- Specify the Levels of Concern (LOCs) you want ALOHA to use when estimating the threat zones or use the default LOCs ALOHA offers.
- Choose the type of hazard (such as toxicity or thermal radiation) you want ALOHA to use when estimating the threat zones.

The entered data in software is shown in the Picture 2.

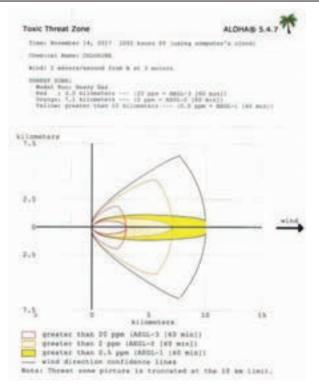
```
at ALOHA 5.4.7 - Text Summary!
The Est SteCuts SetUp Deplay During Help
 SITE DATA:
   Location: BIJELJINA, ES, BIH, ES, BIH
   Building Air Exchanges Per Hour: 0.52 (unsheltered single storied)
   Time: November 14, 2017 1055 hours ST (using computer's clock)
 CHENICAL DATA:
   Chemical Mame: CHLORINE
   CAS Humber: 7782-50-5
                                         Molecular Weight: 70,91 g/mol
   AKGL-1 (60 min): 0.5 ppm AEGL-2 (60 min): 2 ppm AEGL-3 (60 min): 20 ppm
   IDLM: 10 ppm
   Ambient Bolling Points -34.1* C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.04
 ATHOSPHERIC DATA: (HANUAL INFUT OF DATA)
   Winds 2 meters/second from N at 3 meters
   Ground Roughness: open country Cloud Cover: 5 tenths
   Air Temperature: 11" C
                                          Stability Class: C
   Ho Inversion Seight
                                          Relative Humidity: 70%
 SCHOCK STRENGTH:
   Direct Source: 3375 Wilcorame
                                        Source Height: 1 meters
   Release Duration; 1 minute
   Release Rate: 14.7 kilograms/sec
   Total Amount Released: 3,373 kilograms
   Note: This chemical may flash hoil and/or result in two phase flow.
 THREAT JONE:
   Model Run: Heavy Gas
   Red | 3.0 kilometers --- (20 ppm = AEGL-3 (40 min))
   Grange: 7.1 Milometers ---- (2 ppm = AEOL-2 [40 min])
   Yellow: greater than 10 kilometers ---- (0.5 ppm = AEOL-1 [40 min])
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Picture 2. Entered data in software

The rate at which a chemical becomes airborne is critical to the size and duration of a toxic or flammable cloud. ALOHA employs a variety of models to estimate the rate at which a chemical is released from confinement and enters the atmosphere; these are referred to as source strength models [Jones et al., 2013]. In this study is used direct source. An instantaneous or continuous release of chemical vapours into the air from a single point. This is the only option that allows for an elevated release.

A direct source option allows the user to directly specify the amount of chemical vapours introduced into the air from a point in space. The user can specify an instantaneous release, or a steady-state release of finite duration. This option can be used with 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]. The study was used for 1 minute.

Picture 3 shows the threat zone in case of accidental release of chlorine.



Picture 3. Toxic threat zone

ALOHA uses a graphical interface for data entry and display of results. The area where there is a possibility of exposure to toxic vapours, a flammable atmosphere, overpressure from a vapour cloud explosion, or thermal radiation from a fire are represented graphically as threat zones. Threat zones represent the area within which the ground-level exposure exceeds the user-specified level of concern at some time after the beginning of a release. All points within the threat zone experience a transient exposure exceeding the level of concern at some time following the release; it is a record of the predicted peak exposure over time. In some scenarios, the user can also view the time dependence of the exposure at specified points [Jones et al., 2013].

ALOHA software used 60 minutes Acute Exposure Guideline Levels (AEGLs), as Toxic Levels of Concern (LOCs). LOCs are used to assess the toxicity threat of a chemical release. LOCs are used to assess the toxicity threat of a chemical release. A toxic LOC indicates threshold concentration of exposure to a chemical that could hurt people if they breathe it in for a defined length of time. Generally, the lower the toxic LOC value for a substance, the more toxic the substance is by inhalation. The most common public exposure guidelines are Acute Exposure Guideline Levels (AEGLs), Emergency Response Planning Guidelines (ERPGs) and Temporary Emergency Exposure Limits (TEELs). available to date and all three tiers (AEGL-1, AEGL-2, and AEGL-3) are developed for five exposure periods: 10 minutes, 30 minutes, 60 minutes, 4 hours and 8 hours [Paul et al., 2014] (Table 1).

Exposure Time –	Toxic level		
	AEGL-3	AEGL-2	AEGL-1
10 minutes	50	2.8	0.5
30 minutes	28	2.8	0.5
60 minutes	20	2.0	0.5
4 hours	10	1.0	0.5
8 hours	7.1	0.71	0.5

Table 1. AEGLs for Chlorine exposure in ppm [Paul et al., 2014]

AEGL-3 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population could experience life-threatening health effects or death. AEGL-2 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population could experience irreversible or other serious, long-lasting adverse health effects. AEGL-1 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population could experience notable or other serious, long-lasting adverse health effects. AEGL-1 is the airborne concentration (expressed as ppm or mg/m³) of a substance above which it is predicted that the general population could experience notable discomfort and irritation. However, the effects are not disabling and are transient and reversible upon cessation of exposure [Paul et al., 2014].

Simulation of the accident positioned according to the entered coordinates (44°45'01.17"N 19°14'06.03"E), rotated in the direction of the wind (south, north, east, west) (Picture 4).



Pictures 4a, 4b, 4c and 4d. Simulation of the accident (south, north, east, west)

The affected areas which are harmful to human exposures at different levels are detected. The affected areas are divided into three level of concerns namely red zone, orange zone, yellow zone. Red zone is the affected area in which there is severe concentration of toxic gas and exposure to which may cause life threatening health effects or even death. Exposure to Orange Zone may cause long lasting adverse health effects and in Yellow zone average individual may feel notable discomfort, irritation but reversible upon cessation of exposure.

The modelling was performed for an accidental release of 3.373 tons chlorine gas from steel pressure bottles for one hour. For a typical average atmospheric condition in location, this accidental chlorine release would cause a red zone of 3.0 kilometres (AEGL-3=20 ppm), orange zone of 7.1 kilometres (AEGL-2=2 ppm) and yellow zone stretching to greater than 10.0 kilometres (AEGL-1=0.5 ppm) to downwind from the source (Picture 4). It is expected that the red zone will expand at least 3 km along the wind.

The Oregon OSHA exposure limit for Cl_2 is very low due to the extreme irritation hazard and is noted as a ceiling value. The exposure limit of 1 part per million (ppm) should never be exceeded and is an

instantaneous limit. Therefore, it is not averaged over an eight-hour period (Table 2).

The American Conference of Governmental Industrial Hygienists recommends an eight hour Time Weighted Average (TWA) of 0.5 ppm and 15 minute Short Term Exposure Limit (STEL) of 1 ppm to minimize the potential for eye, mucous membrane and respiratory irritation [Chlorine, 2015].

Concentration (ppm)	Agency	Limit	Comments	
0.02-0.2	-		Odour threshold (varies with individuals).	
< 0.5	-		No known acute or chronic effect.	
0.5	ACGIH	BHR TWA		
	OSHA	Ceiling Limit	Odour threshold for all individuals.	
1 -	ACGIH	STEL		
	AIHA	ERPG-1		
1-10	-		Irritation of the eyes and mucous membranes of the upper res- piratory tract. Severity of the symptoms dependent on the concentration and	
			length of the exposure.	
3	AIHA	ERPG-2	Slight imitation of the nose and throat.	
5	-		Irritation of the respiratory tract and eyes.	
10	NIOSH	IDLH		
20	AIHA	ERPG-3	Immediate severe irritation of the respiratory tract intense coughing and choking.	
30	-		Shortness of breath, chest pain; possibly nausea and vomiting.	
40-60	-		Development of chemical bronchitis and fluid in the lungs, which may occur after several hours; chemical pneumonia may occur several days later.	
500	NIOSH	5 min.	Lowest concentration reported to have caused death in humans and animals.	
840	NIOSH	30 min.	Lethal to 50% of human population.	
1000	-		Immediately life threatening.	

Table 2. Chlorine gas Exposure Limits [Chlorine, 2008]

The National Institute for Occupational Safety and Health (NIOSH) has set a Recommended Exposure Limit (REL) of 0.5 ppm as a ceiling limit not to be exceeded as a 15-minute average. The immediately dangerous to life and health (IDLH) value is 10 ppm for Cl_2 . IDLH is defined as exposure to airborne contaminants that is likely to cause death or immediate or delayed permanent adverse health effects or prevent escape from such an environment [Chlorine, 2015] (Table 2).

High levels of chlorine concentration in the air can affect in plants. Injury caused by chlorine (Cl_2) is somewhat similar to that caused by sulfur dioxide and fluorides, in that it is marginal and interveinal. On broad-leaved plants, necrotic, bleached, or tan to brown areas tend to be near the leaf margins, tips, and between the principal veins. Conifers may show tip burn on the current season's needles. Very susceptible plants show symptoms when exposed for 2 hours or more at concentrations of chlorine ranging from 0.1 to 4.67 ppm. Chlorides do not accumulate in plant tissues after exposure to chlorine [Sikora & Chappelka, 2004].

CONCLUSION

Chlorine is a toxic material, thus and its dispersion can be dangerous for human health. Dispersion modelling was performed for an accidental release of 3.373 tons chlorine gas from unsheltered single storied for one hour using ALOHA software. For a typical average atmospheric condition of Bijeljina, this accidental chlorine release would cause a red zone of 3.0 kilometres (AEGL-3=20 ppm), orange zone of 7.1 kilometres (AEGL-2=2 ppm) and yellow zone stretching to greater than 10.0 kilometres (AEGL-1=0.5 ppm) to downwind from the source.

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