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Simulation and Risk Analysis of the Accidental Release of Toxic Gas from an Industrial Complex

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ABSTRACT
Toxic gas is capable of causing serious damage to human health and surrounding living things if it is ingested, inhaled, or absorbed. The amounts required to cause the damaging effects vary with the nature of the substance and duration of exposure. In this study, two common but toxic industrial gases, Chlorine and Ammonia were selected for modeling the accidental release cases and analyze the subsequent risks and impacts. For each case, a hypothetical toxic release scenario was developed and simulated with the help of risk assessment software ALOHA (Areal Location of Hazardous Atmospheres). An industrial complex in Khulna was assumed to process the gases and selected as the geographical area for the analysis. The surrounding affected areas at different levels of concern (LOCs) were detected. The study also analyzed various parameters that affect the release rate and duration, such as wind speed, air temperature, relative humidity, etc. This study simulated probable scenarios of toxic industrial gas dispersion and its effect on surrounding areas, which can be used as a model to tackle actual incidents in the future.

Keywords: Toxic gas, modeling, accidental release, risk, levels of concern.

1. Introduction

Simulation and risk analysis is a key component of an effective emergency response plan for any chemical industry. To be able to mitigate damage from the accidental release of any toxic gas, it is important to carry out a predictive analysis of the nature of spreading and the concentration profile in the affected area in terms of duration of exposure for probable atmospheric, geographic, and release conditions.

Ammonia and Chlorine are two toxic gases having extensive industrial applications. Ammonia is predominately used as a refrigerant, in water treatment, to produce Urea fertilizer, textiles, pesticides, dyes, and many other chemicals. Chlorine finds application in water treatment and the manufacture of many products ranging from paper to pesticides. Hence, these gases are stored in large amounts in different industrial complexes worldwide, including Bangladesh.

Since these two gases are widely used, and that too in amounts large enough to create hazards, instances of the hazardous release of Ammonia or Chlorine are persistent in countries around the world, Bangladesh not being any exception. In 2016, 250 tons of Ammonia was accidentally released, resulting from the rapture of a tank at the plant of DAP Fertilizer Company Limited, Chittagong, Bangladesh [1]. Accidental release of Chlorine occurred in 2011 when a pipe leaked at the Global Heavy Chemical Company Limited on the outskirts of Dhaka, Bangladesh [2]. With many industrial complexes in the country involving the use and storage of these two gases, there are always risks of accidental release. Hence, it is worthwhile to perform consequence assessments of the release of these gases focusing on the local atmospheric and geographic conditions.

Bosanquet and Pearson (1936), in their seminal work on dispersion modeling, derived equations for plume dispersion of gas [3]. It was Sutton (1947) who first included the assumption of Gaussian distribution and considered the effect of ground reflection to derive the plume dispersion equations for pollutants, to be later modified and developed by many researchers [4]. With the advancement in computer science, this model has been used to build computer programs to estimate the dispersions of the pollutants.

The nature of the gas dispersion is primarily affected by its density – whether it is heavier or lighter than air. When the gas is heavier, the emitted plume is called heavy gas clouds. Heavy gas clouds might involve either a gas having a higher molecular weight than that of air (e.g., Chlorine), or might result from conditions including low-temperature release, reactions of emitted gas with atmospheric water vapor, or high storage pressure and aerosol formation (as is the case with Ammonia).

Since the 1970s, there have been many works on heavy gas dispersion modeling. Markiewicz (2012) presents an overview of these works, which have been classified into different categories: empirical models, box models, steady-state plume models, generalized steady-state plume models, one-dimensional integral models, Lagrangian particle trajectory and Lagrangian puff dispersion models, and sophisticated/CFD models [5].

The software ALOHA (Areal Locations of Hazardous Atmospheres) encapsulates the DEGADIS (DEns Gas DISpersion) model, which falls in the category of generalized steady-state plume models. The DEGADIS model was developed from the HAGADAS (HeAvy GAs Dispersion from Area Sources) model, based on the original work of Riele (1977).

Shuxia *et al*. (2012) used the software ALOHA to investigate the consequence of liquefied ammonia leakage [6]. Using the same software, Paul *et al*. (2014) performed the consequence assessment of the accidental release of Chlorine gas in surrounding areas for typical

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tropical atmospheric conditions in Bangladesh [7]. In another work on the impact of toxic release, Syeda *et al.* (2017) analyzed the case study of the aforementioned Ammonia release in Chittagong through a simulation in ALOHA [8].

This study performs a consequence assessment of hypothetical scenarios of Ammonia and Chlorine release from an industrial complex in the Khulna region of Bangladesh. In particular, this study identifies the probable threat zones arising from toxic chemical release, which in turn aids in identifying potentially hazardous situations and devise an emergency plan. Several critical parameters that influence the gas dispersion are also comparatively analyzed for further understanding.

2. Methodology

At first, an area in Khulna district was selected for a hypothetical industrial complex. The industrial complex was assumed to be a chemical processing plant. Two common industrial gases, namely Chlorine and Ammonia, were selected for their wide usage. Using ALOHA software, two hypothetical scenarios were created for the accidental release of the above two chemicals. The variation of relevant atmospheric and geographic factors from base cases were carried out for assessing the relationship with toxic gas dispersion. The findings were then analyzed.

2.1 Selection of Study Area

Khulna, situated on the bank of the Rupsha river, is the third-largest city of Bangladesh [9]. The metropolitan area comprising an area of around 50 square kilometers, has more than two million residents, making it one of the densely populated cities of the country. Khulna has the potential to be a major industrial hub because of its proximity to Mongla port, ideal geographic location, and good connectivity with the capital. For this study, an area close to the Rupsha river was earmarked as a hypothetical industrial complex processing the selected gases.

2.2 Software Selection

For the simulation of toxic gas dispersion and analyzing the effects, a number of software are available, both commercial and free. ALOHA, being a free software, is widely used to model various hazardous scenarios arising from accidental chemical releases such as toxicity, fire, and explosions. Though it has a number of limitations, Emergency responders often use this tool to quickly estimate the severity of hazardous situations and take necessary actions accordingly. ALOHA is adequate for modeling a toxic release scenario of pure chemicals, and hence, it has been used in this study.

2.3 Level of Concern Selection

Level of Concern (LOC) is a threshold value for a specific type of hazard arising from toxicity, fire, or explosion. For example, a toxic LOC indicates the limiting concentration of a toxic chemical that is injurious to people exposed to it for a certain duration. Any value above the corresponding LOC may pose a severe threat to the surrounding people or properties. Based on the various release scenarios, ALOHA predicts the threat zones which exceed the specified LOCs after some point of time from the initial release. For toxicity-related LOCs, several public exposure guidelines are available among which, Acute Exposure Guideline Levels (AEGLs) are the most distinguished. AEGLs are subdivided into three tiers based on severity, namely AEGL-1, AEGL-2, and AEGL-3, the last one being the most damaging. The three tiers are further developed for five exposure periods. For this study, 60 minutes exposure duration was used for LOC determination. The AEGLs for Chlorine and Ammonia exposure are given in Table 1 [10,11].

Table 1 AEGLs for Chlorine and Ammonia exposure (in ppm).

Duration of Exposure	Level of Toxicity					
	AEGL-3		AEGL-2		AEGL-1	
	Chlorine	Ammonia	Chlorine	Ammonia	Chlorine	Ammonia
10 minutes	50	2,700	2.8	220	0.5	30
30 minutes	28	1,600	2.8	220	0.5	30
60 minutes	20	1,100	2.0	160	0.5	30
4 hours	10	550	1.0	110	0.5	30
8 hours	7.1	390	0.71	110	0.5	30

2.4 Chemical Release Scenario

Two separate base scenarios were considered-one for toxic Chlorine release, another for Ammonia release from the industrial complex site mentioned in section 2.1. On a partly cloudy day with a temperature of 30 ^{o}C, toxic chemical was released from a cylindrical vertical storage tank through a circular hole of a 1.5-inch diameter located 2 feet from the bottom of the tank. On both cases, 2.5 tons of toxic chemical was stored in the tank and got released from the hole into the atmosphere. Based on the properties, a varied amount of chemicals got released, which were modeled using ALOHA for identifying the respective LOCs. For comparative analysis, most of the parameters of the base cases were assumed identical, as shown in Table 2. The geographical location was taken into consideration for environmental parameters [12]. Later, some of the critical input parameters were varied for identifying the impacts on the outcomes.

Table 2: Input parameters for base case simulation.

Parameters	Values/Description
Ambient Temperature (^{o}C)	30
Wind Speed (mph)	7
Wind Direction	South-West
Measurement Height (m)	3
Ground roughness (cm)	3
Relative Humidity (%)	50
Stability Class	E
Source Type	Tank
Storage Tank Dimension (ft)	Length=10, Diameter=7
Hole Dimension(in)	1.5

3. Results and Discussion

3.1 LOCs for base cases

The modeling was set up and run using the input parameters from Table 2, and corresponding LOCs were estimated using ALOHA. The threat zone outputs were then superimposed on Google Earth for better visualization. Fig.1 and Fig. 2 show the threat zone plots for the accidental release of Chlorine and Ammonia, respectively.

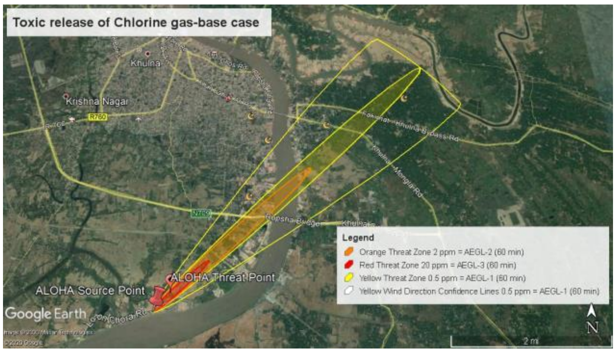

Fig.1 Various threat zones for Chlorine release.

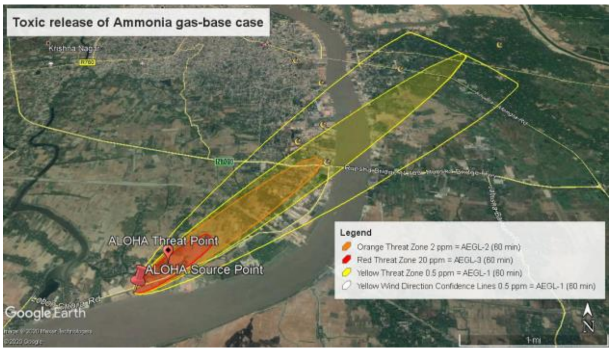

Fig.2 Various threat zones for Ammonia release.

From the outputs, it was found that, over a 12-minute period, the material released from Chlorine and Ammonia tanks was 500 kg and 1,567 kg, respectively. The LOCs varied for two cases, consequently, as shown in Table 3.

Table 3: Threat zone distances for base case simulation.

Threat Zones	AEGL (60 min)	Distance from source (km)	
		Chlorine	Ammonia
Zone-1 (Red)	AEGL-3	1.5	1.1
Zone-2 (Orange)	AEGL-2	4.6	3.1
Zone-3 (Yellow)	AEGL-1	8.4	6.8

The area and perimeter coverage under each LOC is shown in Fig 3 and Fig.4 for Chlorine and Ammonia, respectively. The figures were obtained using MARPLOT. As can be seen from the figures, for Chlorine, the areas ranged from 0.068 sq. miles for AEGL-3 to 1.32 sq. miles for AEGL-1, and perimeters ranged from 1.92 miles to 10.6 miles respectively. For Ammonia, the range for areas and perimeters was 0.103 to 1.47 sq. miles and 1.55 to 8.60 miles, respectively. So, it is clear that, even though the amount released for Chlorine was much less than that of Ammonia, it reached the farthest downwind. This is due to the molecular structure of Chlorine, which being heavier than air, gets diluted slowly compared to Ammonia, and hence, it spreads less sideways but reaches longer distance downwind.

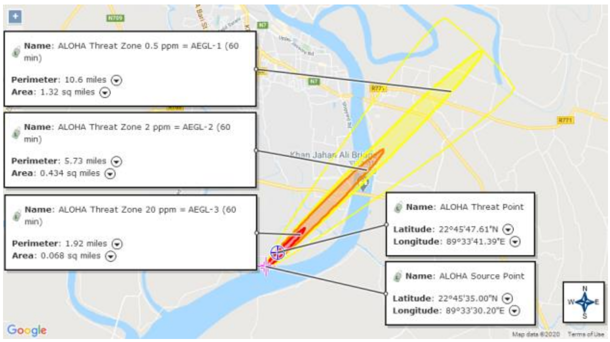

Fig.3 Area and perimeter coverage for Chlorine release.

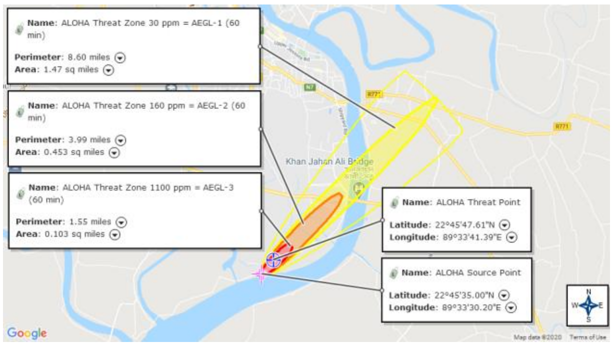

Fig.4 Area and perimeter coverage for Ammonia release.

Further, threat at point was considered for a particular point located downwind 500 meters and crosswind 50 meters from the source. The maximum concentration for outdoor exposure was estimated as 65.2 ppm for Chlorine falling under the most severe Zone-1 (Red) and the indoor concentration of 2.21 ppm fell under the less severe Zone-2 (Orange) as shown in Fig. 5.

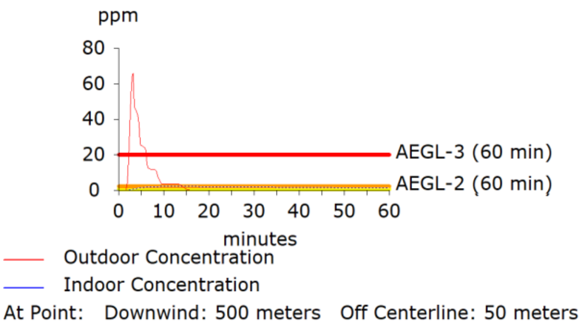

Fig.5 Threat at point for Chlorine release.

For Ammonia release at the same point, outdoor (4350 ppm) and indoor (49.8 ppm) concentrations were found to fall under Zone-1 (Red) and Zone-2 (Orange), respectively as shown in Fig. 6.

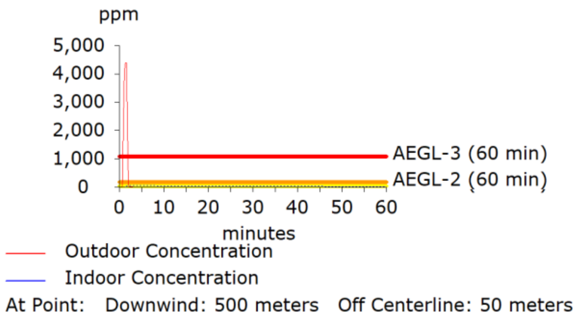

Fig.6 Threat at point for Ammonia release.

3.2 Variation of key parameters and their effects

The base case scenarios discussed above are dependent on several key parameters. Environmental factors contribute significantly to changing the release scenarios of the hazardous chemicals. The surrounding landscape also impacts release scenarios. Consequently, several such variations from the base case are analyzed for assessing their effects.

Wind velocity variation affects toxic cloud dispersion in that, with the increase of wind speed, the gas can disperse quickly across a larger area, ultimately resulting in a smaller area of dense concentration, i.e., reduction of threat zone distance from the source. From Figure 7, it is observed that for Chlorine, the length of Zone-1 (Red), Zone-2 (Orange), and Zone-3 (Yellow) decreases gradually as the wind velocity increases. After the wind velocity increases more than 7 mph, the stability of the system is lowered, resulting in a sharp decrease of zone lengths. For Ammonia, the length of the three zones starts slightly increasing at first (indicating its lightness compared to air) and then decreases as the wind velocity increases beyond a certain value (indicating change of stability of the system).

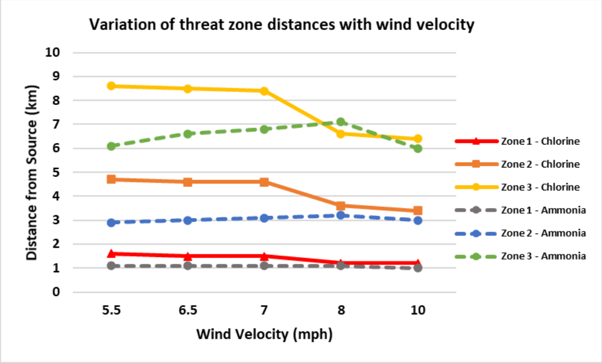

Fig.7 Effect of wind velocity on threat zones.

During a hot and dry day, more solar radiation reaches the earth's surface heating up the adjacent air, which causes larger turbulence and vertical motion of air. Therefore, any toxic release gets carried over to longer distances resulting in larger threat zones. From Figure 8, it is observed that for both of the cases of Chlorine and Ammonia, the length of the threat zones increases with increasing temperature. For Ammonia, the effect seems a bit less than Chlorine.

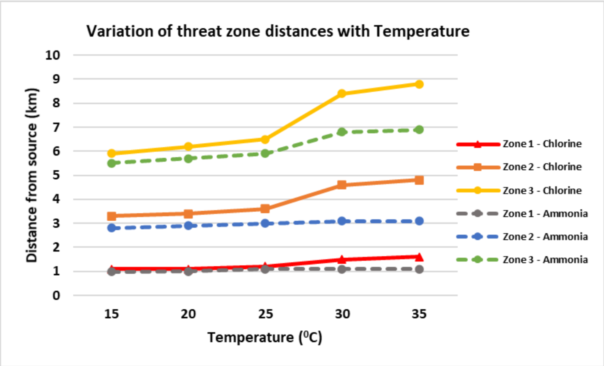

Fig.8 Effect of temperature on threat zones.

Surface roughness is an indicator of the amount and size of ground obstacles over which a pollutant mixture travels. An increase in surface roughness increases the mixing of air with the pollutant cloud, i.e., the pollutant gas gets more diluted. From Figure 9, it is observed that for both of the cases of Chlorine and Ammonia, the length of threat zones decreases slightly with increasing surface roughness. From surface roughness values of 10 cm onwards, ALOHA models the heavy gas systems identically. So, there is no change in threat zones once the surface roughness gets past 10 cm.

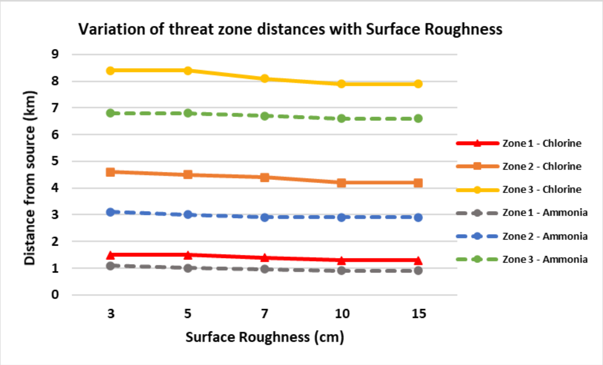

Fig.9 Effect of surface roughness on threat zones.

From Figure 10, it is observed that for both of the cases of Chlorine and Ammonia, the length of threat zones remains almost constant up to a relative humidity of 50% implying that, the effect of relative humidity is minimal up to 50%, and the stability class remains nearly unchanged After that, there is a noticeable decrease in threat zone distance with the increase of relative humidity, indicating a change of stability in the toxic and heavy gas dispersion. Ammonia, being lighter of the two, the effect of relative humidity seems a bit moderate.

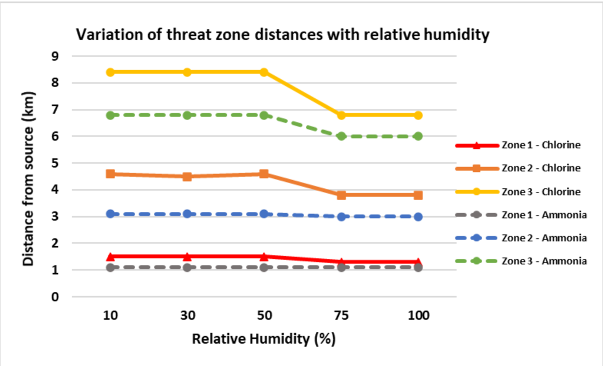

Fig.10 Effect of relative humidity on threat zones.

3.3 Additional threats from Ammonia leakage

Apart from being a toxic pollutant, Ammonia can also be a flammable species when exposed to an ignition source or cause explosion when exposed to high temperature and pressure. As such, any leakage from Ammonia may pose additional threats in the form of jet fire (as shown in Fig. 11), vapor cloud flash fire, or in the worst-case scenario, BLEVE (Boiling Liquid Expanding Vapor Explosion). Though this scenario is not common, the possibility remains for further damage, unlike Chlorine, which mainly acts as a toxic hazard. Such additional analysis is beyond the scope of the present study.

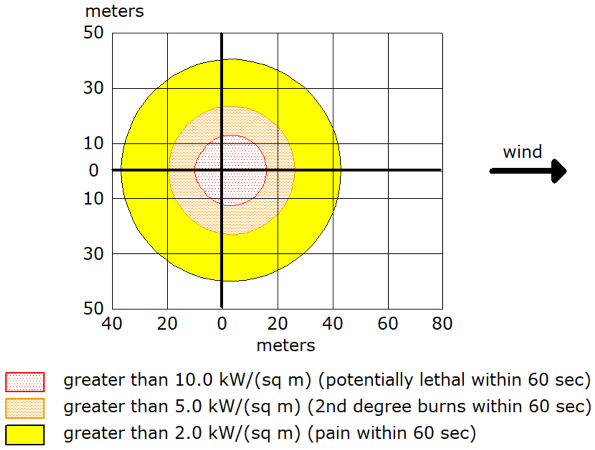

Fig.11 Jet fire caused by Ammonia leakage (output from ALOHA).

4. Conclusion

Bangladesh is a densely populated country with a minimal landscape. As such, the industries which process and handle hazardous chemicals are, in many places, adjacent to the locality. Any chemical can be hazardous based on its toxicity, flammability, or reactivity, among which, toxicity is given special attention as it has the potential to adversely affect and injure a large number of people and livings. In this study, accidental release and the associated effects of two common chemicals, Chlorine and Ammonia, has been investigated with the help of ALOHA software. Two hypothetical base case scenarios were first modeled, and the resulting threat zones were analyzed. Environmental and geographical factors that influence gas dispersion were then analyzed comparatively. Most of the results showed similar trends between the two chemicals under study. The variations were mostly due to their molecular structure, which was discussed in the relevant sections. Since accidents from the chemical release is a common phenomenon in our country, such type of analysis should be carried out on all possible sources beforehand to better prepare for any adverse situations and minimize damages to properties and livelihoods. The current work can be extended further by considering actual industry-specific data and accurate environmental inputs.

5. References

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NOMENCLATURE

KW : Kilo Watt, kJs^{-1}
sq m : Square meter, m^2
mph : miles per hour, $mileh^{-1}$
ppm : parts per million, mgL^{-1}
cm : centimeter
ft : foot