SIMULATION AND CONSEQUENCE ANALYSIS OF TOXIC GAS RELEASE

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ABSTRACT

Chemical leaks threaten public health, air quality, and worker safety. The prevention and simulation of chemical leaks are essential topics in environmental protection and process safety today. This research selected chlorine and ammonia, two common yet poisonous industrial gases, to simulate accidental release scenarios and analyse the ensuing hazards and repercussions. Areal Locations of Hazardous Atmospheres (ALOHA) Software has been used in this paper to model chlorine and ammonia release. The simulation was run for a one-hour release of 3.5 tonnes of chlorine and ammonia from an unsheltered, single-story building. ALOHA software was used to model each event using relevant parameters, and the accident threat zones were obtained. The surrounding regions that harm humans at various levels of concern (LOC) were identified based on the toxic gas concentration. This research also investigates seasonal climatic parameters that influence chemical release rate and duration. The simulation helps avoid and control chlorine and ammonia storage tank leak incidents and gives a scientific guideline for regular safety management.

Keywords: *ALOHA, LOCs, accidental release, Hazardous*

1. INTRODUCTION

Due to the rapid growth of industry in Bangladesh, many chemicals are required to be used in our industry sector. The utilisation of hazardous chemical compounds requires appropriate management. Accidents can release hazardous substances into the atmosphere without proper handling or safety measures, causing significant contamination of the surrounding ecosystem. Considering the population density of Bangladesh, the general public faces more danger from such situations. So, it is essential to conduct investigations into the impacts of these situations in order to anticipate and prevent unfavourable consequences. Bangladesh uses a range of toxic chemical substances in its industrial sector for various purposes. Among them, chlorine and ammonia are the industry's most usable toxic chemical elements. Chlorine is widely used in water treatment, as a disinfectant, in the manufacture of PVC, in the manufacture of paper and paper products, in the manufacture of pharmaceuticals, and so on. Ammonia is used as a refrigerant gas, fertiliser, water purifier, explosives, textiles, insecticides, polymers, dyes, etc. In recent years, the demand for chlorine and ammonia has increased sharply. Inadequate management or negligence in handling and storing dangerous chemicals during production, use, or storage can lead to catastrophic consequences. In 2011, an accidental chlorine release occurred at Global Heavy Chemical Company Limited in Dhaka, Bangladesh, due to a pipe burst. Approximately 100 individuals were affected by a toxic gas leak from a factory in Keraniganj (Toxic Gas Runs Havoc, 2011). In 2016, an incident occurred at the DAP Fertiliser Company Limited in Chittagong, Bangladesh, which unintentionally released 250 metric tonnes of ammonia into the atmosphere (Gas disaster averted in Ctg, 2016). A fire occurred at a container depot on June 5, 2022, followed by a significant chemical explosion. The explosion was attributed to hydrogen peroxide stored in containers at the depot. The explosion resulted in the projection of fireballs into the atmosphere. The blast's impact was perceptible at a considerable distance. A total of 49 fatalities occurred, with numerous injuries sustained by firefighters, volunteers, and journalists (Bangladesh fire: Nearly 50 killed, hundreds injured in depot blast, 2022).

Both domestically and internationally, researchers have extensively studied hazardous chemical substances leaking diffusion models, including theoretical, experimental, and practical applications. Numerous models of expected accident outcomes, such as the Gaussian model, BM model, Sutton model, FEM3 model, and P-G model, have been developed. Several simulation tools, such as PHAST, SAFETI, ALOHA, etc., have been created in conjunction with various models of leakage effects to predict the release of hazardous substances. These models help predict the occurrence of accidents, which will help mitigate the effects of these accidents. In 1936, the first mathematical model for air pollutant plum dispersion was developed, but this model did not assume a Gaussian distribution for air pollution dispersion (Bosanquet & Pearson, 1936). Afterwards, a mathematical model for the dispersion of air pollutants in the vertical and crosswind directions was introduced. This model was based on the foundational assumption of a Gaussian distribution (Sutton, 1947). A heavy gas dispersion model for released gases was developed. It was observed from the model that the initial behaviour of a heavy gas will be different from that of a neutrally buoyant gas. A heavy gas will initially sink since it is heavier than the surrounding air. As the gas cloud moves downwind, it becomes diluted, its density reduces, and it behaves like a neutrally buoyant gas (Eidsvik, 1980). A computational fluid dynamics (CFD) simulation was conducted using Fluent 6.3 software. The main objective of this simulation was to model the dispersion of discharged ammonia from a pressurised storage tank. Additionally, the researchers compared the simulation outcomes and the data obtained from the Fladis field experiment conducted in 1997. Fladis field studies for liquid ammonia leaks were conducted by the Riso National Laboratory (Labovský & Jelemenský, 2010). Using standard dispersion modelling techniques, the effects of an accidental release of chlorine gas into the surrounding area are investigated, taking into account a variety of locations with varying surface conditions (rural or urban), seasons, and meteorological conditions. The Areal Locations of Hazardous Atmospheres (ALOHA) software was used to identify the affected areas that pose a risk to human exposure at various levels (Paul et al., 2014). A numerical simulation based on CFD theory was conducted to study ammonia's dispersion law in a food factory. The dispersion of ammonia is affected by the concentration, pressure, and wind direction (Tan et al., 2020). The threat zone for ammonia vapour cloud dispersion, flammable ammonia vapour cloud area, blast force from ammonia vapour cloud explosion overpressure, jet fire, and fireball from BLEVE were all predicted by ALOHA. The threat zone was estimated based on the LOC, which included hazards that were harmful to people's health and safety and property damage. The yellow zone represented the least hazardous area, and the red zone represented the most hazardous one (Mustapa, 2018).

However, accurately predicting the environmental consequences of a dangerous chemical accident remains challenging. The primary goal of this paper is to model the effects of harmful gas dispersion and estimate its radius in three different seasons.

2. METHODOLOGY

In this research, a chemical plant located in Narayangong, Bangladesh, was chosen. Chlorine and ammonia have been used on this plant. The ALOHA software has been used to create hypothetical situations for the accidental release of those chemicals to estimate the radius of hazardous gas dispersion.

3. Study Area Selection

For this research, a chemical industry in Narayangong, Bangladesh, has been considered. This chemical plant uses both chlorine and ammonia. Two chemical storage tanks of identical dimensions and operating at atmospheric pressure are in the factory. The tanks are located at 23°47'20" north, 90° 31'59.5" east, and 23°47'19" north, 90°32'3" east, respectively. Narayanganj is one of the most populous cities in Bangladesh. This city is also a central commercial and industrial hub. Around 2 million people are living there ("Narayanganj," 2023). The storage tanks are situated in an inhabited location. If ammonia and chlorine were to escape, the dangerous vapour clouds might potentially migrate to the adjacent densely populated portion of the city.

Figure 1: Location of chlorine and ammonia storage tanks

4. ALOHA Software

The ALOHA dispersion model, which is based on the continuous Gaussian model and heavy gas dispersion mode, is used in this study. A heavy gas model is used when the density of a dangerous substance exceeds that of air (Purnama et al., 2020). The ALOHA model's latest version is 5.4.7, which was released in September 2016 (US EPA, 2013). ALOHA can simulate hazardous and explosive gas clouds, BLEVEs, jet flames, pool fires, and vapour cloud explosions. The estimated threat zone from ALOHA is split into three parts: red, orange, and yellow. MARPLOT, Google Earth, and ArcMap can be used to plot these estimated zones on the map.

5. Atmospheric Parameter

To model the dispersion of ammonia and chlorine accidentally discharged from a storage tank using ALOHA, the atmospheric variables required are temperature, wind speed, stability, and atmospheric humidity. The average values of these variables for the months of the rainy season (July), winter (January), and summer (April) are shown in Table 1 (Nārāyanganj Winter Weather, Average Temperature (Bangladesh) - Weather Spark.Pdf, n.d.)

Table 1: Atmospheric variables for simulation

Scenarios	Seasons	Temperature	Humidity	Wind speed	Cloud cover	Atmospheric stability
I.	Winter	65° F	51%	5.4 mph	17%	B
II.	Summer	84° F	60%	8.5 mph	23%	D
III.	Rainy Season	84° F	81%	9.9 mph	89%	E

6. Chemical Data

In order to assess the potential danger area resulting from an unintentional discharge of a dangerous chemical, ALOHA requires the physical and chemical characteristics of the chemical substance. The physical and chemical properties of chlorine and ammonia are given in Table 2.

Table 2: Properties of ammonia & chlorine

Properties	Ammonia	Chlorine
Molecular weight	17.03 g/mol	70.90 g/mol
Ambient boiling Point	-28.20° F	-29.2° F
Vapor pressure at ambient temperature	more than one atm	more than one atm
Freezing point	-107.9° F	-150.16° F

More than 900 chemical substances are included in ALOHA's chemical library with their toxic LOC (Level of Concern). The term "toxic LOC" refers to the threshold level of a hazardous material that, with prolonged exposure, causes illness in individuals. ALOHA uses public exposure guidelines for toxic substances to predict danger zones that exceed LOCs. This research considers AEGLs for toxic LOC. The toxic LOCs of ammonia and chlorine are shown in Table 3 (US EPA, 2014a) and Table 4 (US EPA, 2014b).

Table 3: AEGLs for ammonia

Toxic Level of Concern (ppm)			
Duration of Exposure	AEGL-1	AEGL-2	AEGL-3
10 minutes	30	220	2700
30 minutes	30	220	1600
60 minutes	30	160	1100
4 hours	30	110	550
8 hours	30	110	390

Table 4: AEGLs for chlorine

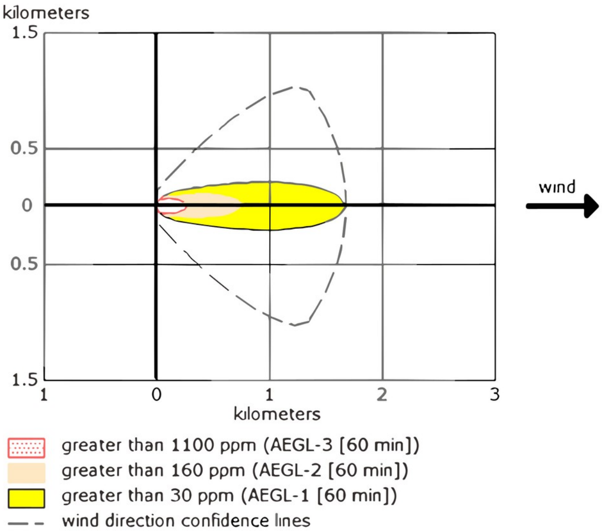
Toxic Level of Concern (ppm)			
Duration of Exposure	AEGL-1	AEGL-2	AEGL-3
10 minutes	0.50	2.8	50
30 minutes	0.50	2.8	28
60 minutes	0.50	2.0	20
4 hours	0.50	1.0	10
8 hours	0.50	0.71	7.1

7. Source Strength

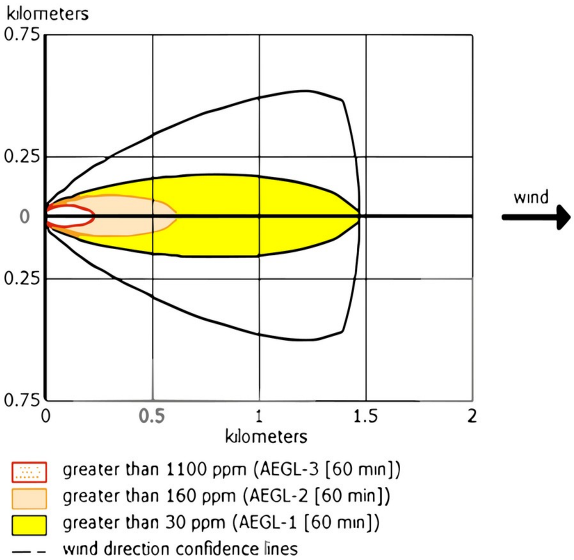
ALOHA utilises source strength information to predict the chemical release rate. This study considers two separate hypothetical cases of ammonia and chlorine release from a chemical complex in a storage tank at the factory at atmospheric pressure. Let us assume a cylindrical chemical storage tank which is 15 feet long and 10 feet in diameter. Due to leakage in the storage tank, about 3.5 tonnes of chemicals are directly released into the atmosphere through a 2.5-inch-diameter circular-shaped hole. The speed at which chemicals are dispersed into the atmosphere substantially impacts a hazardous cloud's magnitude and longevity.

8. RESULTS AND DISCUSSION

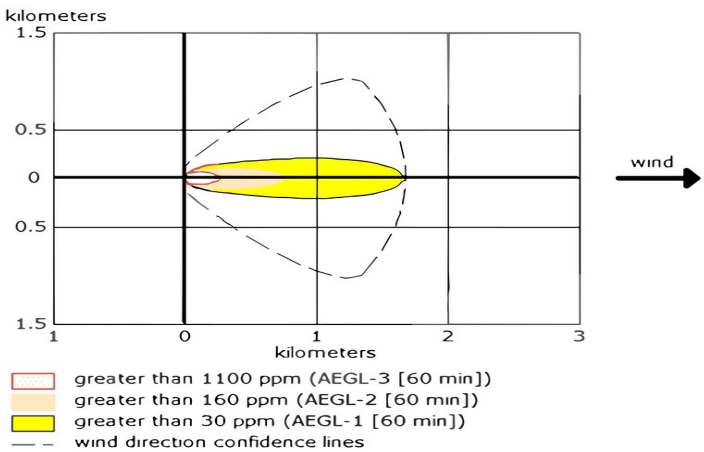
This paper simulated three distinct scenarios for three seasons using different atmospheric conditions and providing all other essential data as input. ALOHA predicted the effect of toxic clouds of ammonia and chlorine as red, orange, and yellow threat zones where the hazard would exceed the LOC during a release. Figure 2 and Figure 3 show the threat zones of ammonia and chlorine, respectively, for three seasons. According to both Figure 2 and Figure 3, dispersion threat zones are estimated in red, orange, and yellow, where the red zone (AEGL-3) represents the highest risk, while the orange (AEGL-2) and yellow (AEGL-1) zones show zones with decreasing risk. The collected danger zone outputs from ALOHA were projected onto Google Earth to estimate the potential extent of harm to persons caused by ammonia and chlorine in each scenario. Figure 4 and Figure 5 indicate ammonia and chlorine threat zones on Google Earth.



Scenario I(Winter)



Scenario II(Summer)



Scenario III(Rainy)

Figure 2: Toxic threat zone of ammonia under various atmospheric condition

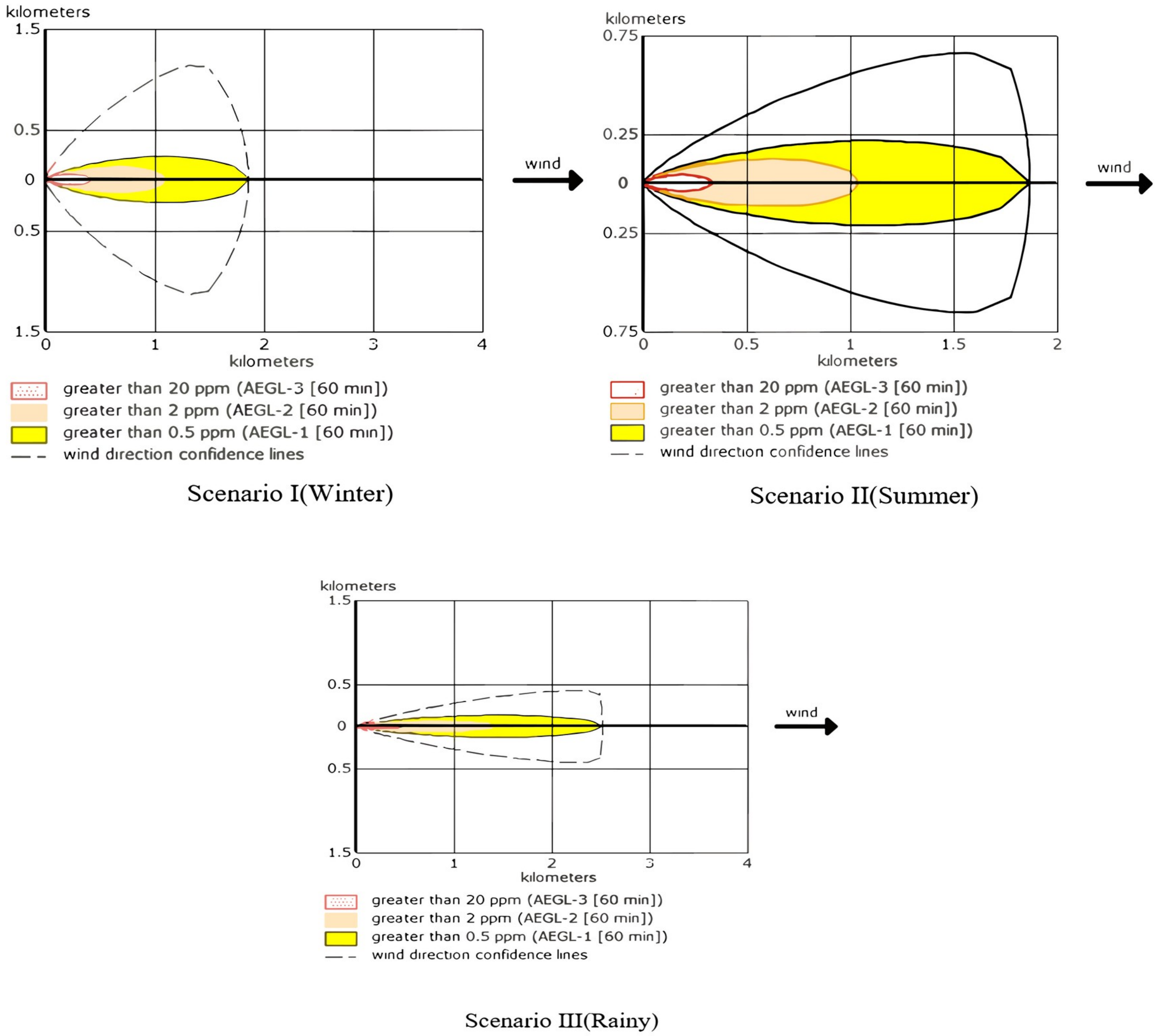


Figure 3: Toxic threat zone of chlorine under various atmospheric condition

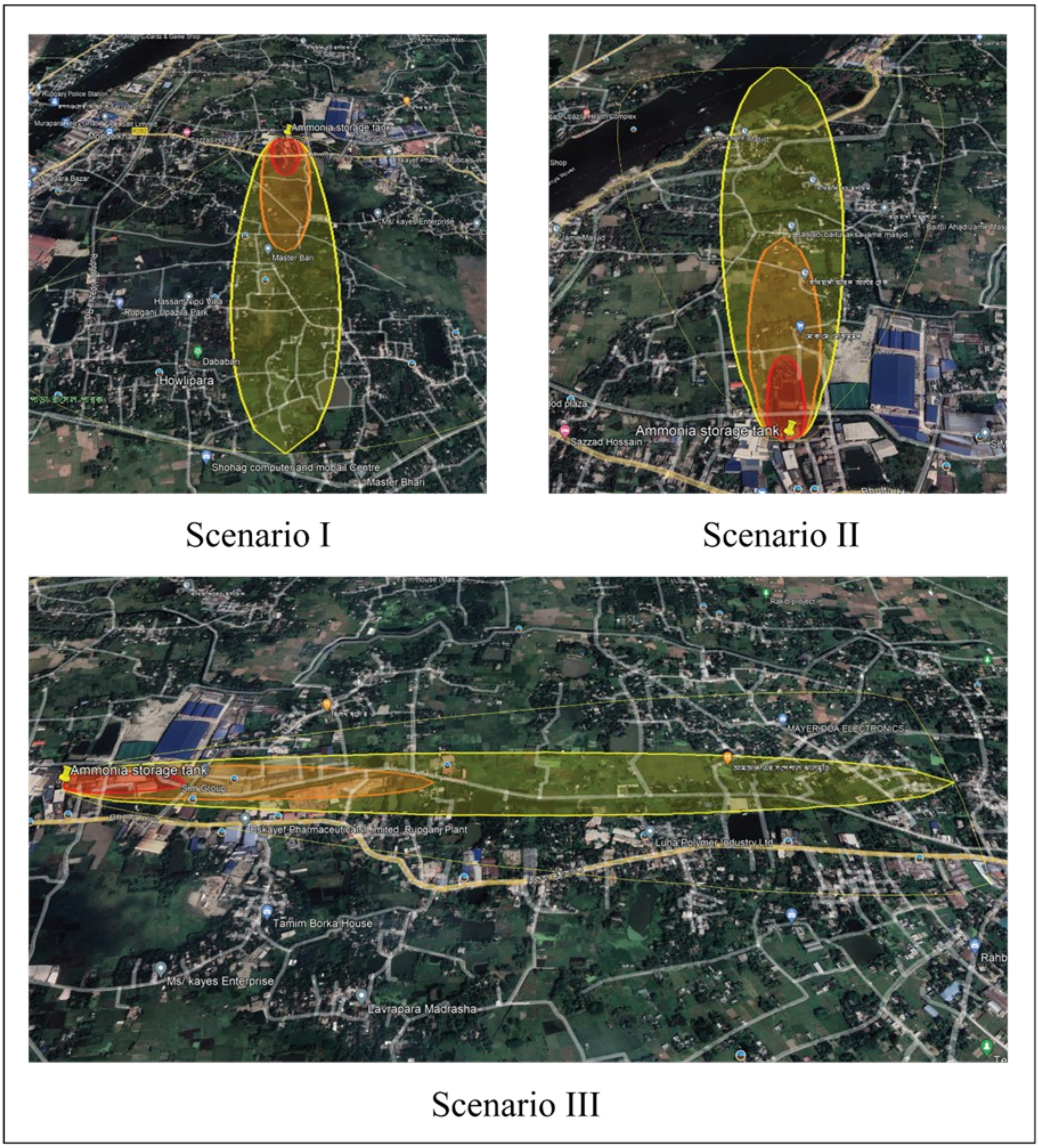


Figure 4: Threat zone of ammonia on google earth

The data shown in Figures 4 and 5 unambiguously demonstrate that the extent of ammonia and chlorine impact is subject to change depending on the atmospheric conditions specific to each scenario. The extent of the influence of ammonia and chlorine in each situation is shown in Table 5. According to the table, in scenario III, ammonia and chlorine had the greatest impact on the red zone at distances of 0.35 km and 0.60 km, respectively. Scenario II exhibits the lowest distance, measuring 0.25 km for ammonia and 0.35 km for chlorine, respectively. In scenario III, the orange danger zone has a maximum affected radius of 0.90 km for ammonia and 1.50 km for chlorine.

Conversely, scenario II exhibits the shortest distance, measuring 0.65 km for ammonia and 1.05 km for chlorine. In scenario III, the yellow danger zone extends to a maximum distance of 2.15 km for ammonia and 2.60 km for chlorine. In contrast, in scenario II, it reaches a minimum distance of 1.5 km for ammonia and 1.80 km for chlorine. In scenario I, the distance of the danger zone varies somewhat compared to the other two scenarios due to the influence of meteorological factors on the threat zone's fluctuation among different situations.

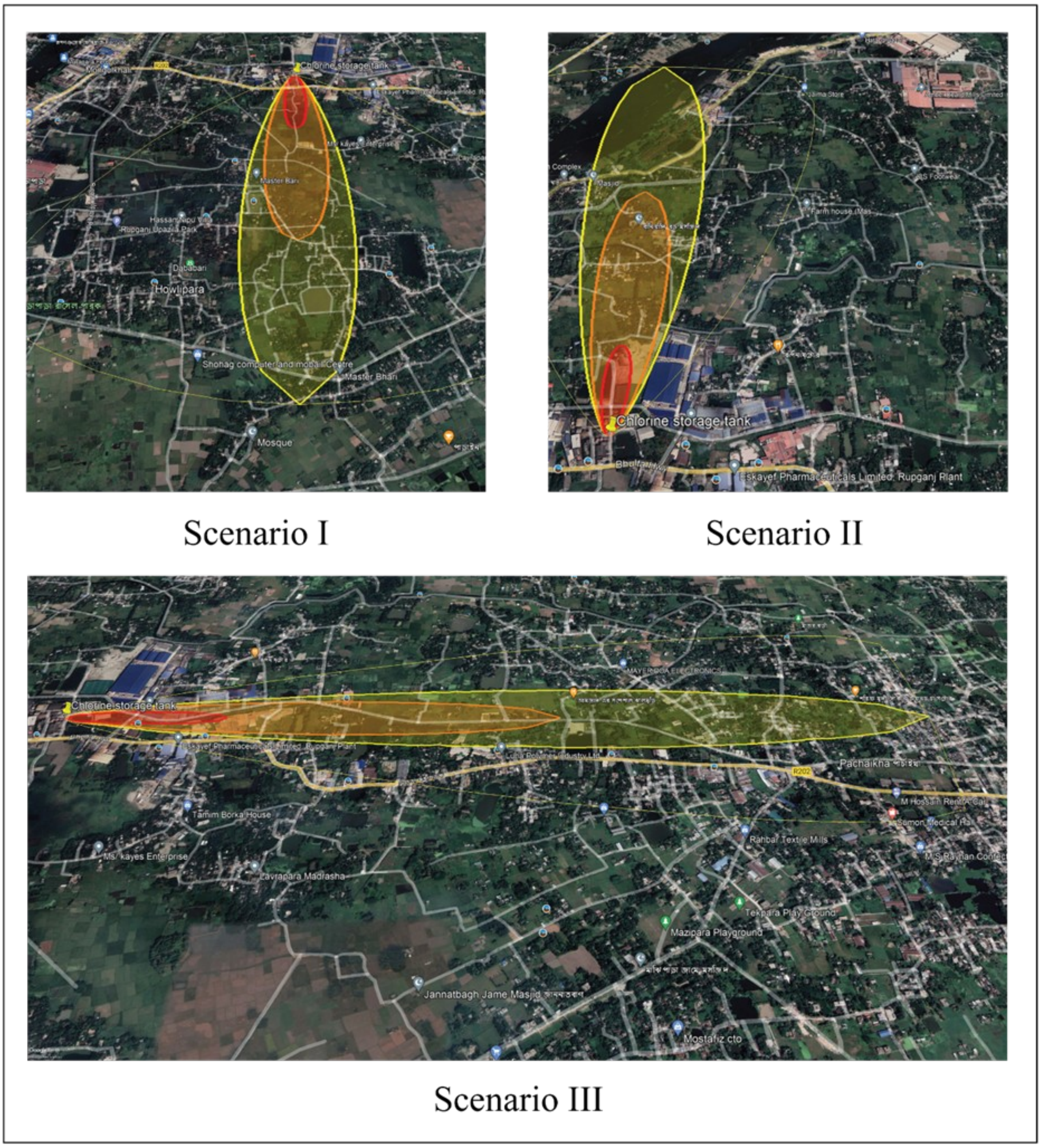


Figure 5: Threat zone of chlorine on google earth

The stability of the atmosphere plays a significant role in the area affected by noxious clouds including chlorine and ammonia. The atmospheric stability is primarily determined by factors such as temperature, cloud cover, and humidity. The increased stability of atmospheric conditions, along with elevated levels of temperature, cloudiness, and humidity, leads to an extended range of detrimental impacts. The atmospheric stability of scenario-III is more stable compared to the other scenarios. Hence, the distance of the threat zone affected is greater in comparison to other circumstances.

Table 5: Toxic threat zone distance from source for various scenarios

Scenario	**Threat zone distance for ammonia (km)**			**Threat zone distance for chlorine (km)**		
	Red zone (AEGL-3)	Orange zone (AEGL-2)	Yellow zone (AEGL-1)	Red zone (AEGL-3)	Orange zone (AEGL-2)	Yellow zone (AEGL-1)
I	0.30	0.80	1.70	0.50	1.15	1.90
II	0.25	0.65	1.50	0.35	1.05	1.80
III	0.35	0.90	2.15	0.60	1.50	2.60

A comprehensive set of scientific guidelines for regular safety management can be established based on the meticulous research conducted using ALOHA Software to simulate chlorine and ammonia leaks. First and foremost, creating evacuation plans with a well-defined zoning strategy is crucial. These plans should use the results of simulations to determine which areas should be evacuated first. The simulation provides a range of the affected areas caused by leaks of chlorine and ammonia, allowing us to determine the extent of influence from various accidents. Hence, during the evacuation procedure, utilizing the maximum accident impact range as the benchmark for conducting group evacuations is imperative. Based on the simulation results, it is recommended to enhance the daily supervision of safety management and establish emergency disposal cards in areas with varying levels of hazards. It is advantageous to affix many monitoring words in the storage tank area to minimize the likelihood of fire and static sparks.

9. CONCLUSIONS

This research has investigated the properties and behaviour of two widely encountered chemicals, namely ammonia and chlorine, utilising the ALOHA programme. The study provides evidence that the dispersion of a cloud containing ammonia and chlorine gases is subject to substantial influence from a range of meteorological variables. The simulation of this model incorporated the average atmospheric conditions of Bangladesh, although it is essential to note that the actual circumstances may exhibit variability. The dispersion of dangerous clouds in the atmosphere is significantly influenced by stability in the low-lying atmosphere. A highly stable atmospheric condition facilitates the dispersion of gas clouds over extensive areas, impacting a larger population. Furthermore, this study examines a range of meteorological variables impacting the ammonia and chlorine hazard zone. Given the frequency with which chemical accidents occur in our nation, they have become a common phenomenon. Based on the investigation findings, utilising the air dispersion model ALOHA holds promise as a valuable instrument for future research endeavours of a similar nature. Moreover, its application is anticipated to aid emergency management personnel in formulating an effective strategy for managing such situations.

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