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Consequence modeling and analysis of ethanol leakage from storage tank using the ALOHA program

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Abstract – Chemical spills pose a significant threat to the safety of people living nearby, as well as to air quality and occupational safety. Therefore, preventing chemical spills has become a key issue in environmental protection and process safety. This study aims to evaluate the effects of ethanol released from a tank at a chemical plant in Istanbul, Türkiye. The Areal Location of Hazardous Atmospheres model (ALOHA) version 5.4.7 estimates the storage tank's leakage radius and spread risk under three scenarios. ALOHA can assess the area affected by chemical hazards. The model shows that if the spill occurs 10 centimeters from the base of the tank, the toxic concentration of ethanol exceeds the Immediately Dangerous to Life or Health (IDLH) threshold (i.e., 3300 parts per million) at a distance of 31 meters from the place of release. In addition, when the ethanol concentration exceeds 60% of the Lower Explosive Limit (LEL) (i.e., 19800 parts per million), the flammable vapor cloud extends up to 31 meters from the place of release. For a Boiling Liquid Expanding Vapor Explosion (BLEVE), the mass of the fireball is assumed to be 100%, resulting in the worst possible scenario. During BLEVE, it is estimated that the fireball's diameter and time duration, determined by the amount of Ethanol present, would be 141 meters and 10 seconds, respectively. The results show that the thermal radiation effects caused by Ethanol BLEVE are extremely dangerous.

Keywords: *ALOHA, BLEVE, explosion, flammable, toxic*

1. Introduction

The chemical industry stores and uses flammable, explosive, and toxic chemicals. Therefore, fires, explosions, and releasing toxic substances are the most important risks in the chemical industry. In addition, fire and explosion are among the most important and unfortunate life-threatening events in factories producing and storing flammable and combustible solvents. The final assessment of the consequences of risks, such as releasing dangerous chemicals into the environment, is one of the most urgent measures to increase safety during the design stage or operation of industrial units. The evaluation of the behavior and release of fluids into the environment after release is essential to be aware of the maximum safe radius of fire, explosion, and release of toxic substances, consequences, and possible injuries, and can play a crucial role in handling accidents in crises [1]. Among flammable, explosive, and toxic chemicals, ethanol is a clear, colorless liquid with a pleasant odor and burning taste [2]. It is a flammable and volatile organic compound. Ethanol is found in alcoholic beverages, many cosmetics products, household cleaners and polishes, pharmaceuticals, disinfectants, pesticides, paints, and dyes. Ethanol is a good solvent used for many purposes, and it is stored in storage tanks for industrial plants. Ethanol in storage containers presents a serious danger, such as fire, explosion, and release of toxic substances. Therefore, it is vital to determine the risk consequence of ethanol from chemical plants [2]. Software is available to deal with the consequences of fire, explosion, and toxic

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release using various modeling tools such as Process Hazard Analysis Software Tool (PHAST) [3], Areal Locations of Hazardous Atmospheres (ALOHA) [4], and Flame Acceleration Software (FLACS) [5] modeling programs.

This study used the latest Areal Locations of Hazardous Atmospheres (ALOHA), updated in September 2016. The ALOHA dispersion model is supplied by the United States National Oceanic and Atmospheric Administration (USNOAA) and Environmental Protection Agency (USEPA), a tool recommended by the USEPA to assess toxic gas cloud hazard areas. The model is capable of simulating about 1000 chemical diffusion patterns and is used to simulate the accidental release of harmful substances and the spread of chemical vapors [6]. The purpose of this study is to simulate the threat zones in case of ethanol release following leakages and explosion from an above-ground storage tank for an unnamed chemical plant in the city of Istanbul, Türkiye, as a case study.

2. Materials and Methods

2.1. ALOHA Software

This study aims to model and assess the environmental impacts caused by a chemical ethanol spill from a storage tank. The ALOHA v.5.4.7 estimates the threat radius of an ethanol leak and spread from the container. The latest version of ALOHA model 5.4.7 (updated September 2016) was selected for this study. ALOHA is a free computer-based hazard modeling program that models toxic gas clouds, flammable gas clouds, shower fires, pool fires, Boiling Liquid Expanding Vapor Explosion (BLEVE) fires, and vapor cloud explosions. ALOHA can simulate the accidental release of about 1000 hazardous chemicals and generates hazard zone estimates for various types of hazards following actual or accidental potential chemical releases. These estimated three threat zones, red, orange, and yellow, are displayed on the ALOHA grid. The red zone indicates the worst level of danger, followed by the orange and yellow danger zones, which represent areas of decreasing danger. The three danger zones can also be drawn on maps in MARPLOT, a mapping program developed jointly by USNOAA and the Environmental Protection Agency (EPA) [7]. ALOHA is limited to airborne chemicals and includes models to estimate the rate at which chemicals are released and volatilized from the environment. These "source strength" models can be critical components of the threat assessment process. ALOHA combines source strength models with a dispersion model to predict the spatial extent of explosive vapor clouds, toxic clouds, and flammable vapors. On the other hand, ALOHA cannot model all combinations of source intensity, scenario, and hazard class into fire scenarios. Table 1 shows the combination of hazard category models and scenarios allowed in ALOHA.

Table 1. Hazard categories modeled in ALOHA [8]

Scenario\Source	Direct source	Tank	Puddle	Gas Pipeline
Vapor cloud	Toxic vapors	Toxic vapors	Toxic vapors	Toxic vapors
Vapor cloud (flash fire)	Flammable area	Flammable area	Flammable area	Flammable area
Vapor cloud (explosion)	Overpressure	Overpressure	Overpressure	Overpressure
Pool fire	NA	Thermal radiation	Thermal radiation	NA
BLEVE (fireball)	NA	Thermal radiation	NA	NA
Jet fire	NA	Thermal radiation	NA	Thermal radiation

On the other hand, ALOHA has some disadvantages. It does not include the effects of chemical mixtures, chemical reactions, particles, etc. In addition, it is not used in closed places, in certain weather conditions such as snow or rain, and with an emission duration of less than one hour. This assumes that the wind speed and direction are constant during the simulation during chemical release downwind [9].

2.2. Definition of the Thereat Zones

ALOHA software uses Level of Concern (LOC) guidelines such as Emergency Response Planning Guidelines (ERPG) and Lower Explosive Limit (LEL) to identify the hazard area of toxic and flammable vapor clouds as follows: Toxic Vapor Cloud Level by ERPG values; three danger distances were defined as the danger zone [10]. Here, ERPG-1 refers to the maximum concentration in air. Almost everyone can be exposed for up to 1 hour without experiencing minor, transient adverse health effects or detecting a well-defined unpleasant odor below this value. ERPG-2 refers to the maximum concentration in air. Almost all people can be exposed for up to 1 hour without experiencing irreversible or other serious health effects that may interfere with a person's ability to take preventive measures below this value, and ERPG-3 refers to the maximum concentration in air. Almost all people can be exposed for up to 1 hour without having or experiencing life-threatening health effects below this value.

The minimum concentration of flammable gas or vapor necessary to burn in air is called LEL. The mixture is too "weak" to burn below that level. On the other hand, the maximum concentration of flammable gas or vapor in air is called the Upper Explosive Limit (UEL). The mixture is too "rich" to burn above this level. The ignition range of this gas or vapor is defined between LEL and UEL [11-12].

However, the concentration levels estimated by ALOHA are time-averaged, and the instantaneous concentration at a given time determines whether the cloud ignites in certain areas of an actual burning vapor cloud. Therefore, any ALOHA-enabled LOC is, by default, part of the LEL, not the LEL itself. ALOHA uses 60% LEL as the default LOC for the red danger zone and 10% LEL for the yellow danger zone, which is the default LOC for ALOHA. The red and yellow danger zones indicate areas where fuel and air concentrations are expected to exceed that LOC sometime after the release begins; however, the red area is the most dangerous area where pockets of flame can occur [13]. Therefore, in this study, based on this criterion, the LOC level for the two ethanol concentrations is defined as follows:

Level 1: 19800 parts per million (ppm) Ethanol concentration corresponds to the value LEL=60%. In this instance, extreme explosion safety considerations should be taken into account.

Level 2: 3300 parts per million (ppm) Ethanol concentration corresponds to the value LEL=10%. In this instance, explosion safety considerations should be taken into account.

2.3. Explanation of Scenarios

The location under consideration is Organized Industrial Zone (OSB)/Istanbul, Türkiye. Atmospheric data for Istanbul was obtained from the Turkish National Meteorological Service, with an average air temperature of 19.6 degrees Celsius (°C) in 2022, an average wind speed of approximately 4.5 meters per second (m/s), and a northeast (NE) wind direction [14]. In the diffusion modeling, a relative humidity of 50% and stability class D were considered neutral conditions based on the recommendation of ALOHA.

In this study, the total tank volume is considered 20 000 liters, containing 18 000 liters of liquid ethanol, which occupies 90% of the tank. Due to the pipeline rupture, the leak is 100 mm from the bottom. The mass percentage of the fireball is assumed to be 100%, and the ALOHA software automatically selects the discharge model as Gaussian.

This study is conducted under three different scenarios expressed as follows:

Scenario 1: A liquid chemical leaks from a storage tank and spreads into the environment.

Section 1-1: Modeling of Ethanol Toxic Vapor Cloud Formation.

Section 1-2: Modeling of Ethanol Vapor Cloud Flammability.

Section 1-3: Modeling of Ethanol Vapor Cloud Explosion.

Scenario 2: A liquid chemical leaks from a storage tank and burns into the environment in a pool fire.

Scenario 3: A storage tank explodes, and the liquid chemical burns like a fireball.

Table 2 shows the Parameters ALOHA software requires to model a chemical spill of ethanol from an above-ground storage tank, including chemical, spatial, and atmospheric parameters.

Table 2. Input parameters of ALOHA

Parameters	**ALOHA Data**
Local Information	Türkiye, Istanbul
Material	Ethanol (ethyl alcohol)
CAS Number	64-17-5
Molecular Weight	46.07 grams per mole (g/mol)
ERPG-1:	1800 ppm
ERPG-2	3300 ppm
IDHL	3300 ppm
Ambient Boiling Point	78.3 ° C
Building type	Single storied building
Type of terrain for dispersion	Sheltered surroundings
Tank type	Horizontal Cylindrical Tank
Tank diameter	2.50 m
Tank length	4.07 m
Tank Volume	20 m^3 (18 m^3, 90% full)
Mass of compound	14232 kg (90% full)
Wind speed, direction /Stability Class	4.5 m/s, North to East / D
Measurement height	10 m above ground
Ambient Temperature	19.6 ° C
Relative Humidity	50%
Air Temperature	19.6 ° C
Leak type, dimension	Circular opening, 100 mm

3. Results and Discussion

ALOHA was selected as a software tool to make a consequence assessment of toxic chemical release scenarios [6]. This study was conducted on three unnamed factories in Twain with three toxic substances: chlorine, phosgene and epichlorohydrin. Two scenarios have been considered by changing parameters: wind speed and total duration time for direct leakage of these hazardous chemicals from storage tanks. The results are then shown in accordance with the ERPG and Dangerous to Life or Health (IDLH) values for the summer and winter seasons. As a result, the dispersion simulation results of all three factories indicate that the biggest hazard areas for each scenario were the phosgene leak in factory C, followed by the chlorine leak in factory A and the epichlorohydrin leak in factory B, respectively.

Patel and Sohani [15] conducted a risk assessment using ALOHA on a storage tank that stores hazardous chemicals at an oil refinery in India. In this study, naphtha, kerosene, butane, and propane, which are stored hazardous materials, leak locations from the bottom of the tank such as 6, 2, 15, and 3 meters, vertical/horizontal cylindrical and sphere, pressurized and unpressurized scenarios were changed according to the types of the storage tank. After the ALOHA simulation, the pressurized butane leakage scenario stored in a sphere tank under jet fire had the worst results, with the longest threat zones red-2.3 km, orange-2.8 km, and yellow-5.5 km. On the other hand, the unpressurized kerosene leaking from a vertical cylindrical tank under a pool fire had the smallest threat areas as red 106-meter, orange-117 meters, and yellow-142 meters compared to different scenarios. This shows that the type of hazardous chemical, whether the chemical leakage from the tank is accomplished by pressure, and the type of fire or explosion were critical parameters affecting the outcomes of accidents.

Fatemi et al. [16] studied the effects of a chemical accident on chlorine storage facilities near residential areas in Iran using the ALOHA model simulated hazard zones in a Geographic Information System (GIS) representation. The scenarios for chlorine leakage from the storage tank were based on climatic conditions varying in different seasons, including atmospheric stability class, temperature, wind speed, and relative population. The result showed that the release of chemicals under the selected scenario affected two cities and seven villages. The highest loss result of 25 400 people and 6.5 km of danger area occurred in autumn, the lowest 24 100 people and 8.8 km of danger area.

Anjana et al. [17] studied the Ammonia leakage scenario using the ALOHA Model simulated threat zones in a GIS presentation. In this study, scenarios of ammonia leakage from the storage tank were based on changed atmospheric parameters in summer and winter. After analyzing four scenarios in four different weather conditions, it was found that the greatest distance of influence of the toxic threat of ammonia was in scenario 1, with 4 km from the source in winter as the worst scenario. Instead, scenario 4 showed a minimum zone of 1.6 km in summer. GIS analysis capabilities also provide insight into how much of the population needs to be evacuated from an area in crisis. The study demonstrates the validity of these data and analysis methods to effectively understand the consequences of an accident. The study provides guidelines for decision-makers on how to act immediately in an emergency.

Anandhan et al. [18] carried out the risk assessment of liquefied petroleum gas (LPG) tanks by using ALOHA with different fire scenarios (i.e., Vapor Cloud Explosion (VCE), BLEVE, and Jet) that can occur in LPG storage area. ALOHA software utilized dispersion models to predict dispersion concentrations, thermal radiation, toxic effects, flammability effects, and explosion effects when LPG is released from its container.

Siddiki and Ahmed [19] studied two toxic industrial gases - Ammonia and Chlorine - chosen to model accidental releases from their tanks in Khulna, Bangladesh. They analyzed the subsequent risks and impacts by simulating atmospheric conditions on ALOHA. Both toxicity levels were identified through analysis using Acute Exposure Guideline Levels (AEGLs). Three levels of AEGLs are present in each one, with a level that is more harmful than the others: AEGL-1, AEGL-2, and AEGL-3. Risk areas were identified and evaluated based on a model of the first two conjectural baseline scenarios. Environmental and geographical factors examined the distribution of gas.

Özay et al. [20] investigated the potential explosion and fire-effect area of 10 000 m^3 liquefied natural gas (LNG) tankers passing through the Istanbul Strait. This study analyzed a BLEEVE scenario in the LNG tank using the open-access software ALOHA. The explosion was found to have destroyed buildings, caused serious injuries, and broken windows in a 4.4 km threat area. In addition, it has been determined that 10.0 kW/m^2 of thermal radiation occurs within a 2.0 km danger zone and is potentially fatal within a minute.

Barjoee et al. [21] conducted a study using ALOHA to estimate the threat zone of benzene released from a tank in a coke and tar processing industry in Kerman, Iran. These leak scenarios were based on varying four seasonal conditions by simulating the dispersion of toxic clouds and pool fire formation. According to the result, the hazard area for the benzene toxic vapor cloud is divided into three levels: yellow, orange, and red. AEGL-3, located at a distance of 53, 62, 99, and 61 meters from the reservoir in spring, summer, autumn, or winter, is depicted in the red zone. The maximum danger area was obtained in autumn. This showed that different seasons affected accident outcomes.

Therefore, after the related studies on risk assessment of hazardous chemical spill scenarios using ALOHA, modelling the consequences of ethanol in different scenarios was calculated in this study using ALOHA.

3.1. Scenario 1: A Liquid Chemical Leak from a Storage Tank and Spreads into the Environment

Section 1-1: Modeling of Ethanol Toxic Vapor Cloud Formation

The ALOHA simulation gives the toxic vapor cloud hazard area: If the ethanol concentration is above 1800 ppm and below the IDLH level of 3300 ppm, the orange zone extends 31 to 32 meters from the spillage source. People may experience eye and nasal irritations when they get in touch with the orange area. The red zone is visible up to 31 meters from the spillage source if the ethanol concentration exceeds the IDLH level of 3300 ppm. Exposure to the red zone can result in health effects that are life-threatening or fatal for people.

Section 1-2: Modeling of Ethanol Vapor Cloud Flammability

The ALOHA simulation shows a fire hazard area caused by ethanol vapor. Two different color ranges were detected in this scenario. These areas were marked with red and yellow, which indicates the concentration of ethanol in the air. When ethanol comes into contact with any combustion source, it will burn.

In the red area, the amount of ethanol was more than 19 800 ppm, corresponding to the lower explosive limit (i.e., 60% of ethanol). In the yellow area, ethanol was higher at 3300 ppm, corresponding to the lower explosive limit (i.e., LEL =10% of ethanol). In the red hazard area, the concentration of chemical vapors at a distance of 31 meters is >19,800 ppm, and in the yellow hazard area, at a distance between 31 to 33 meters, it is >3,300 ppm.

The hazard areas were 31 meters for the red zone and 33 meters for the yellow zone. In case of emergency, all work should be suspended in this area to avoid sources of heat/spark/flame. A red danger zone represents a fire hazard; anything closer than 31 meters from the source is a high fire hazard.

Section 1-3: Modeling of Ethanol Vapor Cloud Explosion

Rapid combustion in the air generates an explosive force when a vapor cloud is produced. ALOHA simulation displays the explosion zone of the vapor cloud. According to the ALOHA simulation, no explosion exists because no part of the cloud is above the LEL.

3.2. Scenario 2: A Liquid Chemical Leaks from a Storage Tank and Burns into the Environment in a Pool Fire

The thermal radiation hazard area of a pool fire caused by ethanol can be identified using ALOHA software, as shown in Figure 1. The yellow area is 30 to 43 meters away from the spillage source, where the thermal radiation from an ethanol pool fire exceeds 2 kilowatt/square meter (kW/m²) but remains below 5 kW/m². Individuals affected by thermal radiation in this yellow area may experience pain within a minute. The orange area extends 23 to 30 meters from the spillage source, where the thermal radiation from the ethanol pool fire exceeds 5 kW/m² but remains below 10 kW/m². Exposure to heat radiation in this orange area can cause second-degree burns within a minute. The red area includes an area located at a maximum distance of 24 meters from the spillage source, where the thermal radiation from an ethanol pool fire exceeds 10 kW/m². Individuals affected by heat radiation in this red area can die within a minute.

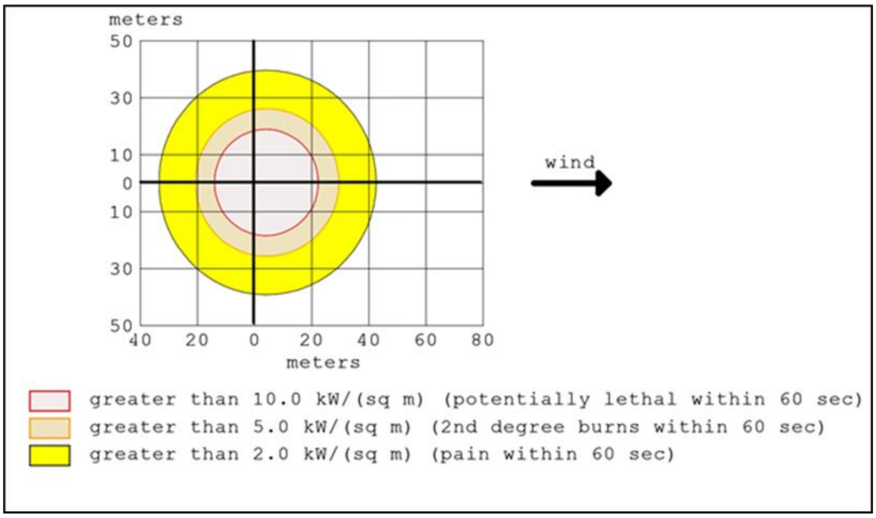

Figure 1. Threat zones of radiation during a thermal pool fire

3.3. Scenario 3: A Storage Tank Explodes, and the Liquid Chemical Burns Like a Fireball

BLEVE is an explosion that occurs when a container filled with pressurized liquid ruptures and exceeds its boiling point [22]. The tank pressure becomes abnormal when the ethanol temperature rises above the boiling point. This can be caused by a pool fire from the same tank, heat radiation from material in a neighboring tank, or BLEVEs from nearby tanks. The fireball's mass is assumed to be 100% in the most severe scenario. Using ALOHA software, it was determined that the ethanol fireball had a diameter of 141 meters and lasted 10 seconds. Figure 2 shows the hazard areas of thermal radiation.

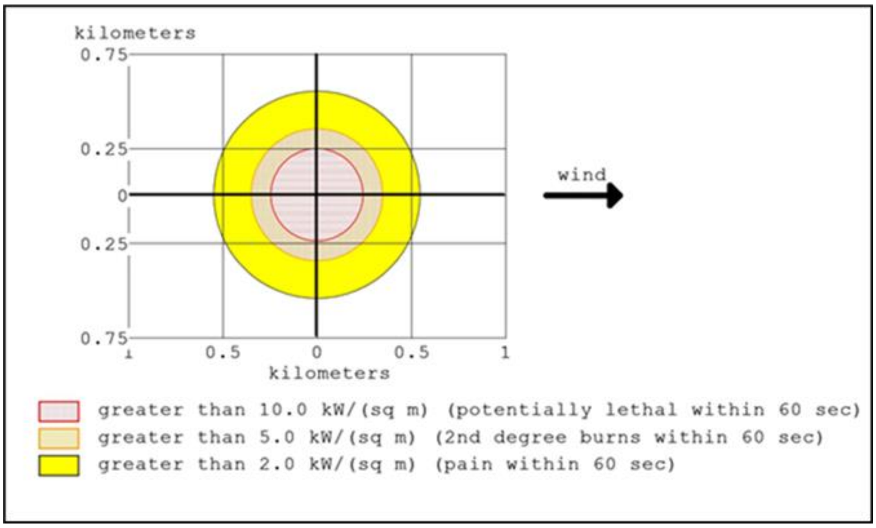

Figure 2. Threat zones of thermal radiation during BLEVE

The yellow area extends from 349 meters to 548 meters from the spillage source, where the ethanol BLEVE thermal radiation exceeds 2 kW/m^2 but remains below 5 kW/m^2. In this area, people can feel pain within a minute of exposure to heat radiation. The orange area extends 244 meters to 349 meters from the spillage source, where the ethanol BLEVE thermal radiation exceeds 5 kW/m^2 but remains below 10 kW/m^2. Exposure to heat radiation from a BLEVE in the orange area can result in second-degree burns within a minute. The red area is up to 244 meters from the spillage source, where the thermal radiation from a BLEVE of ethanol exceeds 10 kW/m^2. In the red area, individuals can succumb to death within a minute upon exposure to thermal radiation from a BLEVE.

Figure 3 shows the visual representation of the thermal radiation threat zone with a 100% percentage of mass in the fireball on Google Earth Map. The results from the graphs show three regions with yellow, orange, and red colors, represented on the map shown in Figure 3.

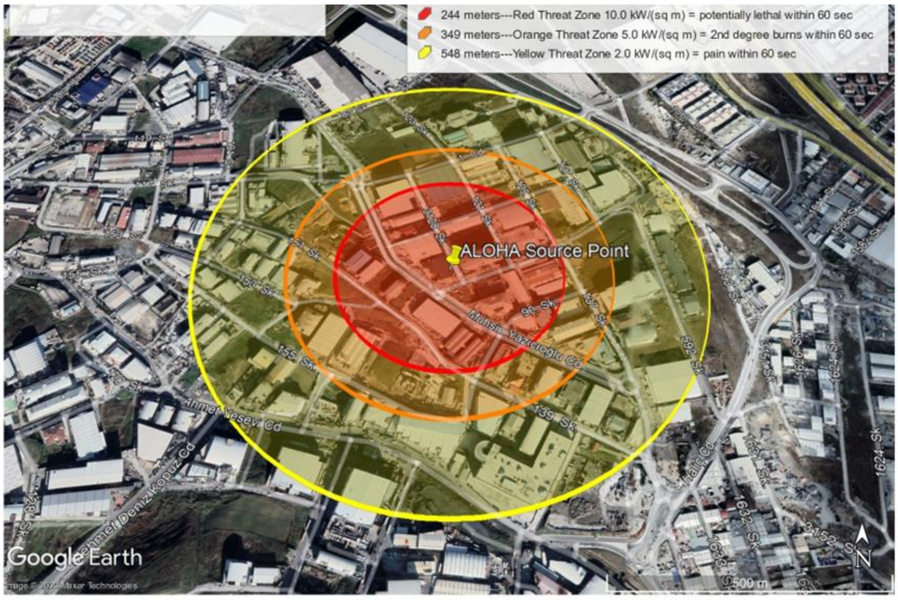

Figure 3. Visual representation of thermal radiation threat zone

As a result, Table 3 summarizes the scenario analysis results and its potential threat distance.

Table 3. Summary of the results of the consequence model of ethanol

Ethanol release scenarios	**Potential hazards and its effect**		**Threat zone distance in meters (m) for each scenario**
Leaking Tank: The Chemical is not burning and forms an evaporating puddle.	Toxic area of vapor cloud	> N/A=ERPG-3	N/A
		> 3300 ppm=ERPG-2 =(IDHL)	31 m (from the source)
		> 1800 ppm=ERPG-1	32 m (from the source)
	Flammable area of vapor cloud	>19800 ppm=%60 LEL	31 m (from the source)
		>3300 ppm=%10 LEL	33 m (from the source)
	The blast area of the vapor cloud explosion force	> 8.0 psi=destruction of buildings	no part of the cloud is above LEL at any time
		> 3.5 psi=serious injury likely	no part of the cloud is above LEL at any time
		>1.0 psi=shatters glass	no part of the cloud is above LEL at any time
Leaking Tank: Chemical is burning and forms a pool fire.	Thermal radiation	>10.0 kW/m²	23 m (from the source)
		>5.0 kW/m²	23-30 m
		>2.0 kW/m²	30-43 m
BLEVE, Tank explodes, and chemical burns in a fireball.	Thermal radiation	>10 kW/m²	244 m (from the source)
		>5.0 kW/m²	244-349 m
		>2.0 kW/m²	349-548 m

4. Conclusion

As a result, the consequences of ethanol in different scenarios were modeled in this study using ALOHA. Table 3 summarizes the scenario analysis results and its potential threat distance. The orange area covers between 31 to 32 meters from the spillage source and can cause eye and nasal irritations for people. In addition to that, the red area covers up to 31 meters and poses life-threatening health risks, including the possibility of death. In the event of a flammable vapor cloud, the red zone extends up to 31 meters from the container, and all emergency operations should be carried out outside this area. Finally, the red area encompasses up to 244 meters from the spillage source during thermal radiation from a BLEVE. Within this zone, humans will face lethal consequences within 60 seconds. The findings clearly show that the effects of thermal radiation from BLEVE involving ethanol are extremely dangerous.

The heat radiation effect caused by BLEVE is the most severe and hazardous risk of ethanol tank failure compared to other situations. In addition, the area affected by BLEVE is relatively wide and can destroy a wide area quickly. Secondary accidents can occur when a storage tank explodes, which then causes tertiary accidents in the surrounding tank and other related incidents. Therefore, considering the possibility of a chain reaction (domino effect) is crucial for risk management.

This study considers the area that would be affected by BLEVE from only one tank (20 m^3). The domino effect should be considered separately. The information gathered from this study will be valuable in strategizing the emergency readiness of the ethanol storage facilities.

Author Contributions

This paper is derived from the first author's doctoral dissertation supervised by the second author. They all read and approved the final version of the paper.

Conflicts of Interest

All the authors declare no conflict of interest.

Ethical Review and Approval

No approval from the Board of Ethics is required.

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