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ALOHA-Based Dispersion and Risk Assessment of Toxic and Flammable Chemical Releases from ISO Tankers in a Coastal Port Environment

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Abstract: The transportation and storage of hazardous chemicals in ISO tankers pose significant safety risks, particularly in coastal port environments where accidental releases can affect both industrial facilities and nearby populations. This paper includes, consequence and dispersion analysis of the effects of accidents such as leaks of Styrene Monomer and n-Hexane in the area through the ALOHA (Areal Locations of Hazardous Atmospheres) computer modeling software. On a representative meteorological coastal environment, the Terminals located at the Kamarajar Port at India was simulated. The Acute Exposure Guideline Levels (AEGLs) was used to assess toxic threat areas, whereas lower explosive limit (LEL) levels and vapor cloud explosion overpressure levels were used to determine flammability and explosion dangers. It is observed that Styrene Monomer is unsafe mainly due to localized yet serious toxic risks because it is low in volatility and heavy, but n-Hexane exhibits widespread flammable and explosion risks because it is of high volatility and evaporates quickly. The comparative analysis indicates the effects of chemical properties and the environment on the dispersion behavior. This paper reveals the efficiency of ALOHA in supporting emergency preparations, risk prevention, and safety control within the scope of the chemical transportation and port operations.

Keywords: ALOHA; Chemical Dispersion Modeling; ISO Tanker; Styrene Monomer; n-Hexane; Risk Assessment; AEGL; Flammable Vapor Cloud; Port Safety.

I. INTRODUCTION

This growth in chemical production and world logistics has seen an increase in the transportation and storage of hazardous chemical substances especially in terminals and industrial cores by the use of ISO container tanks. Though ISO tankers provide safe and uniform ways of containment, any releases that happen in handling, storage, or transportation may cause serious effects which include toxic exposures, fire outbreak, explosion, and environmental pollution [1], [2]. The environment of coastal ports is particularly susceptible because of the large population, complicated logistical processes, and unstable weather conditions.

It has been found repeatedly that due to a series of industrial incidents, minute leakage of dangerous chemicals can lead to disastrous outcomes when coupled with a bad weather pattern or ignition sources [3]. Fire and explosion incidents with burning materials and toxic releases of vapours have caused high human costs and destruction of infrastructure that need to be systematized with the need to evaluate risks and consequences [4]. Therefore, making forewarned comparisons of the dispersion pattern and the path of impact of hazardous chemical releases is the key factor in making emergency preparedness and safety management possible.

There is widespread distribution of atmospheric dispersion modeling to assess the possible effect of the events of chemical release. One of the most widely used platform towards the simulation of the effects of toxic gases dispersion, flammable vapor clouds, and explosion overpressure is the use of the ALOHA (Areal Locations of Hazardous Atmospheres) platform [2], [5]. ALOHA uses a combination of chemical properties, release properties, and site-specific meteorological parameters as a way of estimating threat zones including Acute Exposure Guideline Levels (AEGLs) and lower explosive limit (LEL) contours. It has been applied in numerous industrial processes such as the storage tanks, pipeline, power plants and transportation accidents [6]–[8].

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The effectiveness of ALOHA has been proved by a number of researchers in consequence and risk assessment studies. ALOHA was applied by Bhattacharya et al. [2] to model the hazardous chemical dispersion under various atmospheric stability conditions and its ability to aid emergency plans. Tseng et al. [9] tested the toxic chemical releases by using ALOHA, and it was found to be accurate in predicting the down wind hazard areas. Recent research has also incorporated ALOHA into the quantitative risk assessment and spatial analysis integrated in the ensuing decision enhancing the industrial safety [10], [11].

The physicochemical properties of chemicals that are released (vapor pressure, molecular weight, toxicity, and flammability limits) are a sensitive indicator of the dispersion of chemicals released as well as their hazard potential. According to volatile substances such as n-Hexane collapse quickly and generate large clouds of vapors which lay favorable chances of ignition or explosion of vapors clouds [12], [13]. On the other hand, less volatile chemicals like Styrene Monomer are prone to clouding into heavy vapor and may extend themselves over long distances as clouds nearer to the ground thus the risk of severe toxic exposure is severely localized especially in low lie or poorly ventilated places [14], [15]. At least the behavior of heavy gas dispersion has been highly researched and known to cause more exposure, near the source [16].

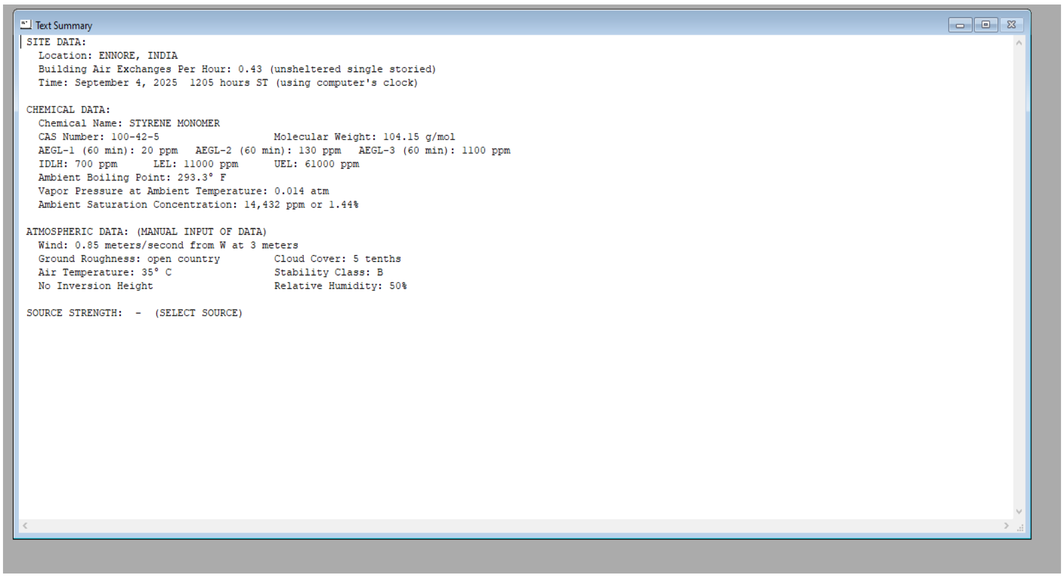
This paper will provide a consequence assessment of the possible consequences of an accidental leaking into the Styrene Monomer and n-Hexane stored in the ISO tankers in the Terminals inside Kamarajar Port, Tamil Nadu, India. Toxic dispersion, flammability zones, and effects of overpressure of the explosion are simulated using ALOHA software under typical coastal meteorological conditions. The aim is to make a comparison between the nature of hazards of the two chemicals and to illustrate the utility of ALOHA as a decision-support instrument on emergency preparedness and risk reduction on port-based chemical transportation systems [17]–[20].

II. METHODOLOGY AND SIMULATION SETUP

This paper uses the ALOHA (Areal Locations of Hazardous Atmospheres) program to simulate the circumstances associated with a polluted accidental release of chemicals by ISO tankers containing hazardous chemicals in a port environment. The ALOHA is a generally accepted conjunction modeling software that is applied to forecasting the effects of toxic dispersions, flammable vapor cloud, and explosion overpressure released following accidental spills of hazardous materials [2], [3], [10]. The approach that is being applied in this work brings about a level of consistency in the terms of a particular environment and release parameters in order to carry out a comparative risk analysis of Styrene Monomer and n- hexane.

A. Study Area Description

The simulation study was conducted for the Terminals located inside Kamarajar Port, Tamil Nadu, India. The reasons why this site was chosen include its strategic location as a significant chemical processing and transportation centre and closeness to the industrial sites and living areas. The unintended emissions of such coastal port settings can be disastrous because of open grounds and unpredictable weather conditions.


Text Summary

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SITE DATA:
  Location: ENNORE, INDIA
  Building Air Exchanges Per Hour: 0.43 (unsheltered single storied)
  Time: September 4, 2025  1205 hours ST (using computer's clock)

CHEMICAL DATA:
  Chemical Name: STYRENE MONOMER
  CAS Number: 100-42-5                   Molecular Weight: 104.15 g/mol
  AEGL-1 (60 min): 20 ppm   AEGL-2 (60 min): 130 ppm   AEGL-3 (60 min): 1100 ppm
  IDLH: 700 ppm      LEL: 11000 ppm      UEL: 61000 ppm
  Ambient Boiling Point: 293.3° F
  Vapor Pressure at Ambient Temperature: 0.014 atm
  Ambient Saturation Concentration: 14,432 ppm or 1.44%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
  Wind: 0.85 meters/second from W at 3 meters
  Ground Roughness: open country         Cloud Cover: 5 tenths
  Air Temperature: 35° C                 Stability Class: B
  No Inversion Height                    Relative Humidity: 50%

SOURCE STRENGTH:  -  (SELECT SOURCE)
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Fig. 1. ALOHA simulation layout showing release source and dispersion direction

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Fig. 1 shows the ALOHA simulation layout, which has the release point, wind direction, and downwind hazard regions. To capture the behavior of the vapor clouds, the open-country terrain was chosen because it describes the almost unobstructed port environment that greatly affects the control and behavior of cloud dispersion.

B. Atmospheric and Site Conditions

Meteorological parameters were manually entered into ALOHA based on realistic coastal afternoon conditions to represent a conservative but credible accident scenario. The same atmospheric inputs were applied to both the chemicals making the dispersion characteristics of the chemicals fairly comparable.

Table I: Site and Atmospheric Parameters Used in ALOHA Simulation

Parameter	Value
Study Location	Terminals, inside Kamarajar Port, Tamil Nadu, India
Terrain Type	Open country
Building Air Exchange Rate	0.43 h^{-1} (unsheltered, single-storey)
Date and Time	September 4, 2025, 12:05 IST
Wind Speed	0.85 m/s
Wind Direction	From West
Wind Measurement Height	3 m
Ambient Temperature	35 °C
Relative Humidity	50 %
Cloud Cover	5 tenths
Atmospheric Stability Class	B (slightly unstable)

The position and the environment of the simulations are presented in Table I. The atmospheric stability (B) and a wind speed (0.85m/s) were selected to show some unstable conditions resulting in greater horizontal dispersion of hazardous vapors. These conditions are often related to the increased risk in the occurrence of the accidental chemical releases [16], [17].

C. Chemical Properties and Tank Configuration

Two dangerous chemicals overall that are usually carried in ISO tankers Styrene Monomer and n-Hexane were chosen to be analysed as they belong to a number of contrasting physical and chemical properties. The Styrene Monomer belongs to a category of under-volatility and strong toxic hazards and n-Hexane belongs to a category of high volatility and severe flammability risks.

The two chemicals were presumed to be kept in the horizontal cylindrically shaped like the ISO tanks that are the common feature in port transportation activities. The tanks were filled partially (70–75%) and kept in an internal temperature of 35 °C. A leak case where there was a circular leak hole of 10 inches in diameter (around the lower part of the tank) was modeled to replicate a real life mechanical failure or accidental puncture, in line with practice of consequences assessment which has been reported in literature [43], [44].
The tank geometry, filling conditions, and leak characteristics used in the simulations are summarized in Table II.

Table II: ISO Tank and Leak Scenario Parameters for Styrene Monomer and n-Hexane

Parameter	Styrene Monomer	n-Hexane
Chemical State	Liquid	Liquid
Tank Type	Horizontal cylindrical ISO tank	Horizontal cylindrical ISO tank
Tank Diameter (m)	6.058	2.438
Tank Length (m)	2.591	6.058
Tank Volume (m^3)	74.7	28.3
Filling Level (%)	75 %	70 %
Chemical Mass in Tank (kg)	49,933	12,815
Internal Tank Temperature (°C)	35	35
Leak Type	Circular hole	Circular hole
Leak Diameter	10 inches	10 inches
Leak Position from Tank Bottom	1.09 m	1.0 m
Ground Type	Default soil	Default soil

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Ground Temperature	Ambient	Ambient
Release Duration	60 min	60 min
Max Sustained Release Rate	88.5 lb/min	407 lb/min
Release Behavior	Pool formation with evaporation	Pool formation with evaporation
Max Puddle Diameter	2 ft	49 yards
Dispersion Mode	Heavy gas	Heavy gas

D. ALOHA Modeling Approach

ALOHA uses source strength estimating, atmospheric dispersion, and chemical specific thermodynamic properties to compute dispersion. The Heavy Gas dispersion model has been used to conduct all simulations since both of the vapors of Styrene Monomer and n-Hexane are heavier than air, and they usually stay near the ground level once they have been released.

The software created threat areas on the basis of:

- Toxicity in terms of Acute Exposure Guideline Levels (AEGLs),
- Flammability based on fractions of Lower Explosive Limit (LEL), and
- Effects of explosion with using vapor cloud explosion overpressure criteria.

The model outputs had been evaluated considering the spatial extent of hazard zone which have been elaborated further later in Section III. The methodology embraced allows the assessment of the dominance of chemical specific hazards and the emergency preparedness and risk reduction planning in case of ISO tankers operations in port conditions [1], [11].

III. RESULTS AND DISCUSSION

This section gives the results of the ALOHA simulations in case of the accidental release of Styrene Monomer and n-Hexane at Terminals inside Kamarajar Port. The attacks involve the dispersion of toxic vapors, flammability and potential explosion, and a comparative analysis is made in a detailed manner.

A. Styrene Monomer Release

In the Styrene Monomer release scenario, the liquid that was involved was 49,934 kg of Styrene and this is contained in a horizontal cylindrical ISO tank at a temperature of 35 °C. It has a low vapor pressure (0.014 atm) that restricted the amount of vaporized material though caused a heavy gas plume in the lower atmosphere.

1) Toxic Dispersion

AEGL-based toxic threat zones are summarized in Table III.

Table III: Styrene Monomer Toxic Threat Zones

AEGL Level	Concentration	Threat Zone Distance
AEGL-1	20 ppm	420 yards
AEGL-2	130 ppm	144 yards
AEGL-3	1100 ppm	25 yards

Observations:

- The main hazard is that of toxicity because it is characterized by persistent heavy vapor.
- The 25-yard area of the AEGL-3 zone is dangerous to life, in addition to the limited range of the release point.
- Moderate AEGL-2 and AEGL-1 zones are a clue that there should be evacuation and monitoring outside of the immediate storage facility.

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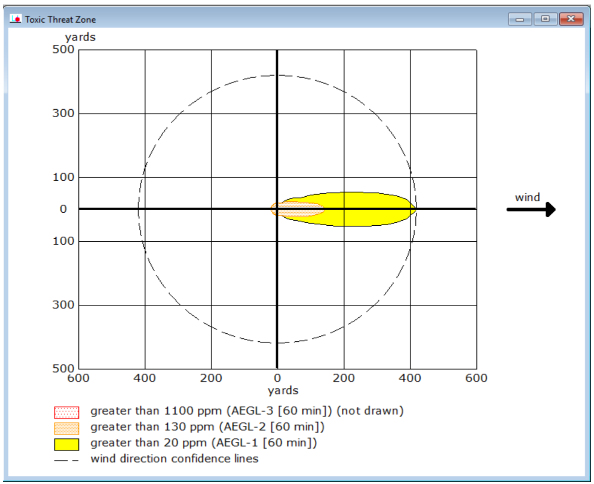

Fig. 4. AEGL-based toxic dispersion zones for Styrene Monomer

2) Flammability and Explosion Risk

- Styrene Monomer has a low volatility flammable zone.
- The 10% LEL zone was not projected to go much more than 25 yards and no serious vapor cloud explosion (VCE) was anticipated.
- Therefore, the risk of toxicity is prevailing, and the risk of fire and explosion is not great in the open air.

B. n-Hexane Release

The initial release of n-Hexane was associated with a 12,815 kg amount in a horizontal ISO tank at 35 °C pressure of a high vapor (0.30 atm), and generated a rapidly expanding vapor cloud.

1) Toxic Dispersion

Table IV: n-Hexane Toxic Threat Zones

AEGL Level	Concentration	Threat Zone Distance
AEGL-2	2900 ppm	153 yards
AEGL-3	8600 ppm	95 yards
AEGL Level	Concentration	Threat Zone Distance

Observations:

- Toxic hazard occurs locally around the release point.
- Inhalation can also result in central nervous system depression, dizziness, or nausea.

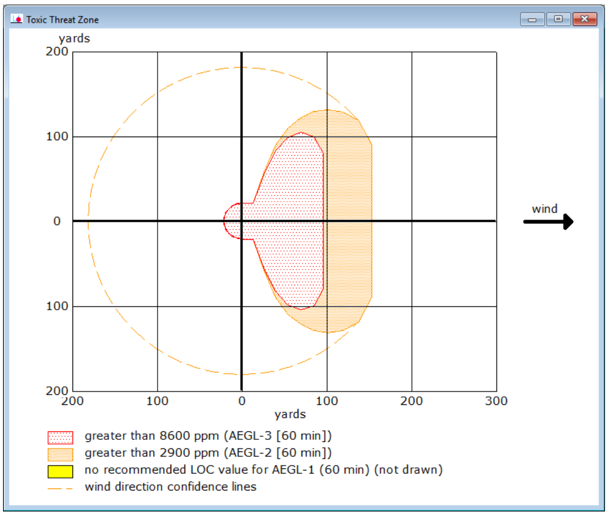

Fig. 5. AEGL-based toxic dispersion zones for n-Hexane

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2) Flammability and Explosion Risk

It has a great volatility; consequently, the flammable threat range of n-Hexane is much more substantial:

Table V: n-Hexane Flammable and Explosion Zones

LEL Threshold	Distance from Source	Overpressure
10% LEL	229 yards	–
60% LEL	101 yards	–
VCE (Explosive Mass)	43.2 lb	1–3.5 psi
Orange Zone	55 yards	1 psi
Red Zone	24 yards	3.5 psi

Observations:

- There is high likelihood of ignition in case of exposure to sparks or open flame.
- Explosion may result into structural damage (3.5 psi) and personnel injury (1 psi).
- n-Hexane is hazardous as both toxic and flammable.

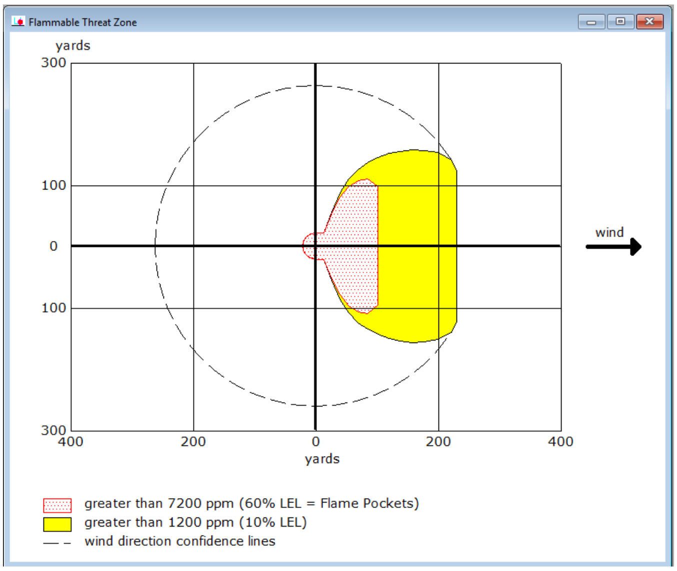

Fig. 6. Flammable vapor cloud and explosion threat zones for n-Hexane

C. Comparative Evaluation

The hazards of both Styrene Monomer and n-Hexane are presented in a comparative summary as shown in Table VI.

Table VI: Comparative Hazard Evaluation

Property	Styrene Monomer	n-Hexane
Vapor Pressure	Low (0.014 atm)	High (0.30 atm)
Primary Hazard	Toxic	Toxic + Flammable
AEGL-3 Zone	25 yards	95 yards
10% LEL Zone	25 yards	229 yards
Explosion Potential	None	High
Environmental Persistence	Moderate	Rapid Evaporation

- Styrene Monomer: Toxic hazard dominates; slow dispersion limits flammability.
- n-Hexane: Rapid evaporation increases flammability risk; toxicity is local.
- Environmental conditions such as wind speed, temperature, and atmospheric stability play a crucial role in hazard zone propagation.
- The results underscore the need for chemical-specific mitigation strategies at port storage and handling facilities.

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D. Safety and Risk Implications

- Styrene Monomer
  - Emphasize air quality monitoring and ventilation.
  - Train personnel for toxic exposure response and emergency evacuation.
- n-Hexane
  - Implement spark control, grounding, and ignition source isolation.
  - Maintain firefighting readiness due to high flammability.
- Recommendation
  - Regular safety audits, ISO tanker maintenance, and real-time monitoring improve hazard preparedness.
  - Emergency response planning must account for chemical-specific dispersion and threat zones.

IV. CONCLUSION

This study presented a comprehensive analysis of hazardous chemical releases from ISO tankers using ALOHA software, focusing on Styrene Monomer and n-Hexane at Terminals inside Kamarajar Port. Through its simulations it was found that Styrene Monomer as a substance has a toxicity threat is the most hazardous due to its low vapor pressure (0.014 atm) and the AEGL-3 limit is a low zone ranging to 25 yards with minimal flammability and explosive potential in the open environment setting. With a high volatile index n-Hexane, on the other hand, dispersed quickly (vapor pressure 0.30 atm) and was flammable, creating large flammable areas (10% LEL to 229 yards) with great explosion potential, but its toxic effects were confined locally. The relative analysis shows that chemical attributes, environmental factors, and tank layouts are the key elements in identifying the hazard levels and the extent of the risks. Results of the present paper show that hazard-specific safety precautions are vital, such as ventilation, leak detection, spark control, the isolation of ignition sources, and emergency preparedness. In general, the project proves ALOHA is a valuable predictive tool in the evaluation of chemical hazards as it allows to make informed decision-making during safe storage, transportation, and emergency response planning. Future studies can be expanded to other different environmental conditions and other chemical substances to boost predictive accuracy and safety measures in industries.

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