Evaluating the Consequences of Chemical Accidents in Fertilizer Plants using ALOHA Program

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Abstract - *The fertilizer industry is an essential component of modern agriculture, providing critical nutrients for crops to grow and produce yields. However, the production, storage, and transportation of fertilizers can also pose significant risks to workers and communities due to the potential for accidents and incidents. Fertilizer industry accidents can result in severe injuries, loss of life, environmental damage, and economic impacts. In this paper, simulations of chemical accidents are presented. The accident was caused by an uncontrolled release of ammonia from a storage tank in the fertilizer plant. The simulation was conducted using the ALOHA software, which anticipates the development of the accident and determines the areas of risk and safety. The experiment is based on the physical and chemical properties of the substance involved in the accident, and the paper discusses the various scenarios that could occur under the most unfavorable atmospheric conditions.*

Key Words: **Fertilizer, ALOHA, Simulation, Risk, Uncontrolled.**

1. Introduction

Safety should be a top priority in the fertilizer industry, especially in high-risk areas like ammonia-urea plants that operate under intense pressure and temperature. So, what's the first step in ensuring industrial safety? It's identifying potential hazards, which means looking for any undesired events that could lead to a hazardous situation and the mechanisms that could cause them. Once we've identified these hazards, we need to assess the potential damage they could cause to the surrounding area and come up with ways to lower the risk as much as practically possible. In order to effectively address potential safety hazards associated with the storage and handling of ammonia, the advanced software ALOHA will be employed to conduct sophisticated simulations. Upon careful evaluation and analysis of the simulation results, appropriate preventive measures can be taken by the relevant authorities to ensure the safety of personnel and the environment.

2. Theoretical part

According to the World Health Organization, a chemical accident in a fertilizer industry is an alarming occurrence that poses a significant threat to public health and the environment. It refers to the uncontrolled release of a toxic substance, which has the potential to cause harm, either immediately or over an extended period. Chemical incidents can occur due to natural causes, such as volcanic eruptions, earthquakes, or hurricanes. Conversely, they can also arise as a result of human error, system failure, or deliberate acts of sabotage, terrorism, or warfare. The severity of a chemical incident can vary, depending on the nature, quantity, and concentration of the substance released, the environmental conditions at the time of release, and the proximity of humans and animals to the source of contamination. The incident can be sudden and acute, leading to rapid onset of symptoms and potentially fatal consequences. Alternatively, it can have a delayed onset, with the harmful effects not becoming apparent until days, weeks, or even years after exposure. This type of incident is commonly known as a "silent" release of a chemical and can pose long-term health risks to those exposed. The range of chemical incidents can also vary from small-scale releases, which can typically be handled by local emergency services, to full-scale major emergencies, which require a coordinated response from multiple agencies at local, national, and even international levels. The latter can involve large-scale evacuations, decontamination efforts, and medical treatment for affected individuals, all of which require careful planning, resource mobilization, and communication. The increasing production and use of chemicals worldwide have raised concerns about the potential health and environmental impacts of these substances. Consequently, the health sector has had to expand its traditional roles and responsibilities to address the public health and medical issues associated with chemical usage and its health effects. This includes providing expertise and guidance on chemical safety, monitoring and assessing the health impacts of chemical exposures, developing emergency response plans, and supporting research on the health effects of chemicals. In this regard, the health sector plays a critical role in ensuring the protection of public health and the environment in the face of chemical incidents.

2.1 Ammonia

Table -1: Physical-chemical characteristics of ammonia

Chemical formula	NH3
Name	Ammonia, Azane (IUPAC)
Molar mass	17.031 g/mol
Apperance	Colorless gas
Odor	Pungent odor
Density	0.76 g/L at STP
Melting point	-77.37 ^{0}C
Vapour pressure	1003 kPa (at 25^{0}C)
Auto-ignition Temperature	651^{0}C
Explosive Limits	14.8 - 33.5 %

Ammonia is an inorganic compound, comprised of a single nitrogen atom that is covalently bonded to three hydrogen atoms. It is a potent inhibitor of amidase and neurotoxin, and is both synthetically manufactured and naturally produced through bacterial processes and the decomposition of organic matter. Its uses span across a wide range of industries, including its applications as a refrigerant and fertilizer. Ammonia is identified by its characteristic pungent odor and is commonly found in a colorless gas or compressed liquid form, with exposure typically occurring through inhalation, ingestion, or contact. Both long-term inhalation of low concentrations and short-term inhalation of high concentrations of ammonia vapors can result in adverse health effects. Despite this, ammonia continues to be used as a fertilizer, refrigerant, and in the manufacture of other chemicals. Its rate of onset is immediate and it persists for minutes, with an odor threshold of 17 parts per million. It is worth noting that ammonia is also utilized in explosives manufacture, pesticides, and the detergents industry, and poses a range of other hazards as well. The label depicted in Figure 1 serves as a comprehensive reference to identify and highlight all of the common hazards associated with the storage and handling of ammonia.

In its anhydrous form, ammonia is a clear and colorless gas that can be shipped as a liquid under its own vapor pressure. Its liquid form is known to be highly dense, weighing in at approximately 6 pounds per gallon. Contact with the unconfined liquid can cause severe frostbite. While the gas is typically regarded as lightly flammable, it has been known to ignite within certain vapor concentration limits and with strong ignition sources. The presence of oil or other combustible materials can significantly increase the risk of fire. It is important to note that, despite being lighter than air, the vapors from a leak initially cling to the ground. Prolonged exposure to fire or heat can cause violent rupturing and rocketing.

One of the key features of ammonia is its combustion characteristics. Ammonia does not burn readily or sustain combustion under most conditions. This is due to several factors, including its low heat of combustion, high auto-ignition temperature, and narrow flammability range. In other words, ammonia requires a specific mixture of fuel and air to burn, which limits its potential as a fuel source. However, when ammonia does burn, it produces a distinct flame that is pale yellowish-green in color. This flame is a result of the chemical reaction between ammonia and oxygen, which forms nitrogen and water. This reaction is exothermic, meaning it releases energy in the form of heat. The standard enthalpy change of combustion for ammonia is -382.81 kJ/mol, which indicates the amount of energy released per mole of ammonia combusted. Interestingly, the combustion of ammonia can also produce nitrogen oxides, which are important industrial chemicals. When ammonia reacts with oxygen in the presence of a catalyst, it can produce nitric oxide (NO) and water. This reaction is important in the production of nitric acid, which is a key ingredient in fertilizers, explosives, and other products.

4 NH3 + 3 O2 → 2 N2 + 6 H2O(gΔH°r = −1267.20 kJ),

Nitrogen oxides can also react with other compounds in the atmosphere to form smog and acid rain, which can have negative effects on human health and the environment.

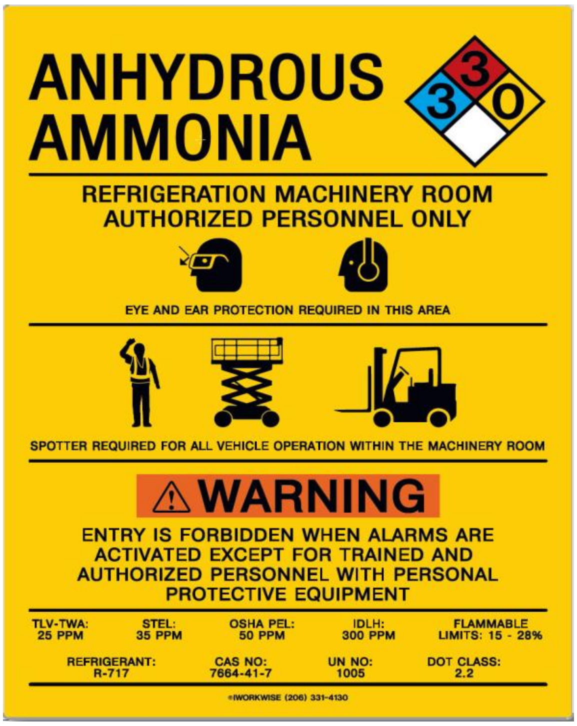


Fig -1: Label of Anhydrous Ammonia

2.2 Causes of Ammonia Leakage

To Identify the causes of leakage of ammonia, the root cause analysis method was used. A root cause analysis allows an employer to discover the underlying or systemic, rather than the generalized or immediate, causes of an incident. Correcting only an immediate cause may eliminate a symptom of a problem, but not the problem itself. It is important to consider all possible “what,” “why,” and “how” questions to discover the root cause(s) of an incident. This method was used to identify seven basic causes of ammonia leakage, which are listed below.

1) Corrosion: Corrosion can occur through a variety of mechanisms, but one common cause is the combination of oxygen, ammonia, stress, and carbon steel. When carbon steel is exposed to an environment containing oxygen and ammonia, a reaction can occur that produces ammonium compounds. These compounds can react with the metal to form iron oxide, which is a type of rust. This reaction is accelerated by the presence of stress on the metal, which can weaken the metal and make it more susceptible to corrosion.

2) Over-pressure: The occurrence of over-pressure in an ammonia storage tank can have serious safety implications, including the risk of explosions or fires. The injection of warm ammonia into the tank or sudden mixing of ammonia solution and liquid ammonia due to the break up of an oil layer can lead to a rapid increase in pressure beyond the tank's design limits. Proper design, operation, and maintenance of the tank and associated equipment, along with appropriate safety measures such as relief valves and emergency shutdown systems, are essential in mitigating the risk of over-pressure and ensuring safe handling and storage of ammonia.

3) Overfilling: The accurate monitoring of the liquid level in tanks is critical to ensuring their safe operation. However, errors in level readings by operators, combined with the failure of the high-level alarm, can lead to overfilling of the tank. This can result in spills, leaks, or even rupture of the tank, which can pose serious safety hazards to personnel and the environment.

4) Fatigue: Fatigue is a common phenomenon that can occur in materials due to repeated stress cycles over a long period of time. In the case of ammonia storage tanks, fatigue can occur due to the tank's long lifetime, and the stresses that it experiences from the constant filling and emptying of the tank, as well as other factors such as temperature changes and corrosion.

5) Faulty design: Human error in the design phase of ammonia storage tanks can result in faulty tank design, which can compromise the safety and integrity of the tank.

6) Implosion: The collapse or implosion of an ammonia storage tank due to vacuum conditions can have serious safety consequences, including damage to the tank, release of ammonia, and injury or death to personnel. This can occur when pressure transmitters fail to accurately detect vacuum conditions in the tank, and the vacuum relief valve fails to open, resulting in the tank's roof partially collapsing due to the negative pressure.

7) Cooling system failure: Cooling water blockage in an ammonia storage tank can cause the cooling system to fail, leading to overheating and potentially catastrophic consequences.

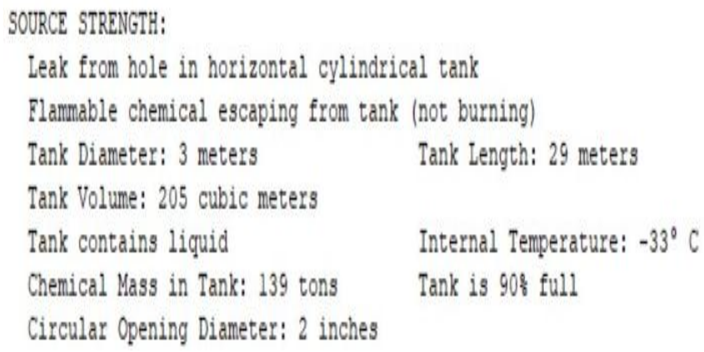
2.3 Modelling software

The Aerial Locations of Hazardous Atmospheres (ALOHA) model is a sophisticated computer tool jointly developed by the Environmental Protection Agency (EPA) and the National Oceanic and Atmospheric Administration (NOAA) of the United States. It is designed to estimate the movement and dispersion of gases, providing a quick and efficient way to predict the concentration of pollutants in the air downwind from a spill. The model takes into account a wide range of factors, including the physical and toxicological properties of the spilled material, site characteristics, atmospheric conditions, and release circumstances, using both the Gaussian and heavy gas models. With an extensive database containing information on thousands of chemicals, ALOHA can model the threat zone for any chemical that may escape from a tank or pipeline.

In this paper, the ALOHA program was applied to assess the potential chemical accidents that could result from ammonia tank releases in the fertilizer industry, including the possible development of such accidents, the resulting threat zones, and their potential impact on the environment.

3. Simulation results and Discussion

To predict the potential hazards of a chemical spill or leak, One will need to gather a wide range of data - everything from the specific chemical compound involved, to the location of the accident, to the current weather conditions. All of this information is crucial for accurately modeling and simulating the potential consequences of the chemical dispersion.



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SOURCE STRENGTH:
  Leak from hole in horizontal cylindrical tank
  Flammable chemical escaping from tank (not burning)
  Tank Diameter: 3 meters                Tank Length: 29 meters
  Tank Volume: 205 cubic meters
  Tank contains liquid                   Internal Temperature: -33° C
  Chemical Mass in Tank: 139 tons        Tank is 90% full
  Circular Opening Diameter: 2 inches
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Fig -2: Source strength of ammonia

The specific scenario being investigated in this paper is the diffusion of gas from a horizontal ammonia tank in the fertilizer industry, which can be caused by any one of the reasons that were mentioned earlier. The dimensions of the damage are provided, as well as the volume of the tank and the percentage to which it is filled in the Figure 2. To simulate the potential release of gas, the most unfavorable meteorological conditions are taken into account, such as wind speed, temperature, humidity, and atmospheric stability. This information is retrieved from the India meteorological department's website.

Finally, the modeling process involves determining the boundaries of zones that could be affected by the hazard, as well as defining a safety zone for people and objects. This includes assessing the potential impact of demolition, over-pressure of impact waves, and thermal energy effects.

In this study, the researchers investigate the potential dangers of a damaged tank storing ammonia. The tank is pressurized and kept at a very low temperature, and if it is damaged, a significant amount of ammonia gas could be released into the atmosphere in a vapor form. Ammonia is both slightly flammable and explosive, which could lead to a variety of accidents scenarios. However, the focus of this study is on the risks associated with fire and explosion, as these present the greatest danger from the release of ammonia. The study examines various models of how the gas could spread and ignite, including the spread of vapor clouds, jet fires caused by ignition in the cylinder, and liquid expanding vapor explosions. The ultimate goal is to estimate the potential risks posed to people and objects in the plant and surrounding areas.

Figure 3 illustrates how in each of these scenarios, ammonia was released from the storage tank at a speed of 47 g/s in the form of an aerosol. Ammonia was released for a total of 60 seconds.

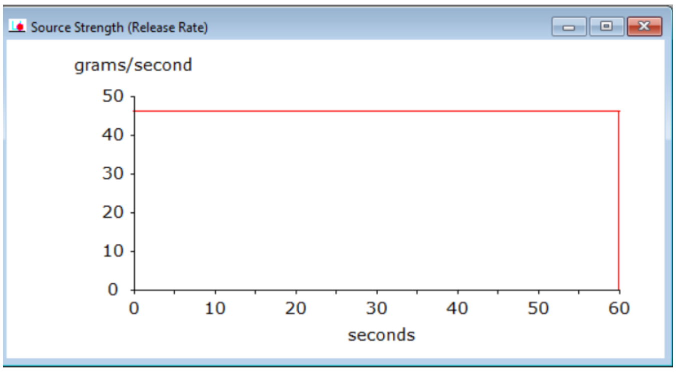

Fig -3: Release Rate of ammonia

The first scenario, given in Table 2, includes the release of non-burning ammonia forming a flammable vapor cloud.

Table -2: Conditions in Scenario 1

Scenario	weather		Releasing substance
Ammonia release without ignition with formation of flammable cloud	Temperature	30^{0}C	Ammonia
	Wind	5 mph	
	Humidity	50%	
	Stability class	B	
	Cloud cover	5 tenths	

Upon conducting the chemical accident simulation, the areas with gas vapor air concentration that falls within flammability limits and is prone to starting a fire were identified with precision. These findings are outlined in detail in Figure 4, which depicts the results of the simulation. According to the findings, the gas concentration in the atmosphere at a distance of 0.2 miles from the hazard location spot in the wind direction exceeds 1100 ppm, thereby presenting an extremely high risk of fire (marked in red). The workers who are present at their jobs and the area of the factory nearby are at the greatest risk in this area. The yellow and orange zones are important areas to consider when assessing the potential hazards associated with the storage and handling of ammonia. These zones extend from 0.2 miles to 1.25 miles in the wind direction from the source of the hazard. The yellow zone is characterized by a gas concentration of more than 30 parts per million (ppm), while the orange zone has a higher concentration of over 160 ppm. It is essential to take adequate safety measures in these areas to protect personnel and the environment from the potential dangers posed by ammonia exposure. This may include the use of protective gear and clothing, as well as the implementation of evacuation procedures in the event of an emergency.

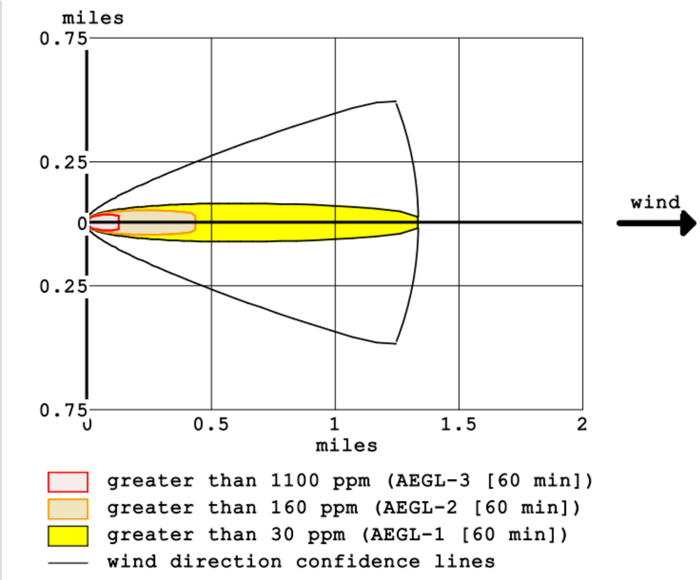

Fig -4: Simulation of scenario 1

The second simulation estimates the probability of forming an explosive zone caused by over-pressure, i.e., it defines the areas on which explosion of the formed ammonia cloud releasing into the atmosphere can occur, even though the second scenario, shown in Table 3, refers to the simulation of the accident under the same conditions.

Table -3: Conditions in Scenario 2

Scenario	weather		Releasing substance
Ammonia release without ignition with formation of explosive cloud	Temperature	30^{0}C	Ammonia
	Wind	5 mph	
	Humidity	50%	
	Stability class	B	
	Cloud cover	5 tenths	

The simulation was performed for the detonation ignition occurred in the time period of 60 seconds after the gas release.

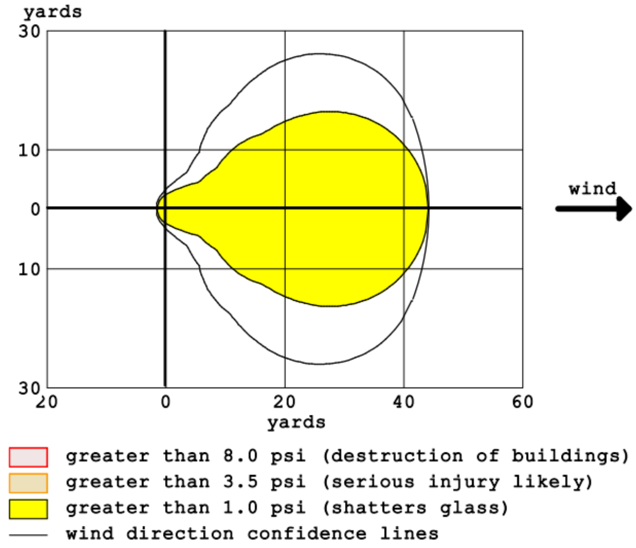

Fig -5: Simulation of scenario 2

Figure 5 shows that the yellow zone is the area where there is a pressure of more than 1 PSI. In this area, there have been reports of minor human injuries as well as minor structural issues like cracked windows and glasses.

The release of ammonia from a hole in a horizontal storage tank in flame was predicted in the third scenario, shown in Table 4.

Table -4: Conditions in Scenario 3

Scenario	weather		Releasing substance
Release of burning ammonia (Jet fire)	Temperature	30^{0}C	Ammonia
	Wind	5 mph	
	Humidity	50%	
	Stability class	B	
	Cloud cover	5 tenths	

The software warns of a potentially dangerous threat: thermal radiation. This scenario also includes three dangerous zones, as shown in Figure 6.

The software predicted a jet flame 11 yards long that would last 60 seconds. Thermal radiation with an energy greater than 10 kW/m2 is expected in the 11 yard radius red zone. This zone is potentially lethal and can cause severe burns in as little as 60 seconds.

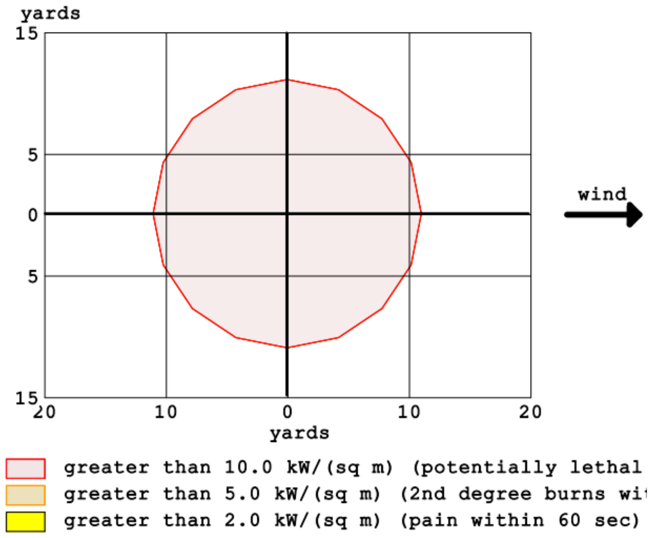

Fig -6: Simulation of scenario 3

The fourth scenario, shown in Table 5, was modelled for the Boiling Expanding Vapour Explosion (BLEVE). Thermal radiation (surface heat flux of flame) of the burning tank is the danger predicted by the software.

Table -5: Conditions in Scenario 4

Scenario	weather		Releasing substance
Boiling expanding vapour explosion	Temperature	30^0C	Ammonia
	Wind	5 mph	
	Humidity	50%	
	Stability class	B	
	Cloud cover	5 tenths	

Scenario 4 was created to model the Boiling Expanding Vapour Explosion (BLEVE) and the software predicts the danger of thermal radiation from the burning tank. The characteristics of the threat zones in Scenario 4 are shown in Figure 7. The software predicts that in Scenario 4, a fire with a diameter of 120 yards will occur in just 3 seconds. The red zone, where the fireball originates, has an energy flux greater than 10 kW/m2 and is potentially fatal to humans. The radius of this zone is almost 120 yards. The orange zone, which occupies the band from 120 to 190 yards, is characterized by a thermal energy of 5 kW/m2 and can cause fires in buildings and serious burns to people. The yellow zone is situated in the subsequent band, which lies at a distance of 190 to 300 yards from the accident, and the energy of the thermal flux in this band reaches 2 kW/m2, resulting in minor burns.

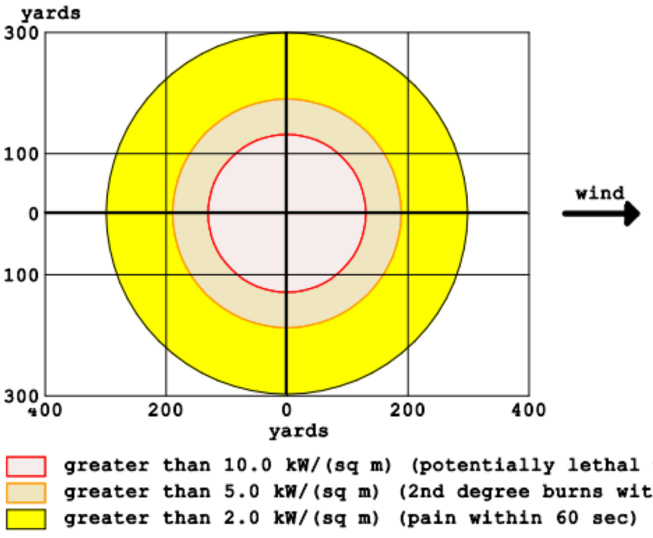

Fig -7: Simulation of scenario 4

4. CONCLUSIONS

The use of the ALOHA software for accident simulation has proven to be an effective tool in assessing the potential consequences of ammonia release from a horizontal storage tank in a fertilizer industry. The software provides a comprehensive analysis of the dispersion and impact of hazardous materials, including fire, explosions, and toxic gas releases. By simulating potential accidents and their consequences, safety professionals can better prepare emergency response plans and mitigate the risks associated with hazardous material storage and transportation.

The accuracy and reliability of ALOHA have been well established through numerous validations and tests, making it a widely recognized and accepted tool within the safety industry. However, the software is not a substitute for careful planning and adherence to safety regulations. It is only one of many tools available to safety professionals to help them make informed decisions and manage risks associated with hazardous materials.

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