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MODELING ISOBUTANE UNCONTROLLED RELEASE FROM A STORAGE TANK

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Abstract: This work represents a modeling isobutane uncontrolled release from a classic horizontal cylindrical storage tank of 141 m^3 and its negative aspect on the environment. Accident modeling is a key part of risk assessment in the chemical industry. Risk assessment in the chemical industry is a prerequisite for reducing or avoiding possible accident situations. By recognizing and identifying the critical points of a system and its proper and safe management, the risk is reduced to the lowest possible probability and extent of consequences.
Key words: isobutane, storage leaking, accidents, chemical industry

INTRODUCTION

Isobutane (C_4H_{10}), an isomer of n-butane, is often used as a raw material in petrochemical industry, a refrigerant, a component in aerosols, and as a fuel. However, precisely because of its low vaporization point and wide explosive range in air, it poses a significant safety challenge. Uncontrolled release of isobutane, especially from large storage tanks, can lead to the formation of flammable clouds and serious incidents, including fires, explosions and chemical contamination of the environment. Therefore, it is necessary to develop methodologies for the prediction and analysis of such scenarios, in order to reduce the risk and protect human lives and resources.
For this purpose, software tools have been developed that enable the simulation of chemical accidents and the assessment of consequences in controlled conditions. Among them, ALOHA (Areal Locations of Hazardous Atmospheres) stands out – an advanced software that enables the visualization and quantification of potentially hazardous zones resulting from chemical leaks. ALOHA, developed by the United States Environmental protection agency (EPA), uses input data on the physicochemical properties of the substance, atmospheric conditions and location characteristics to generate realistic projections of the spread of pollutants and the extent of the hazard.

MATERIAL AND METHODS

Characteristics of isobutane

Isobutane (C_4H_{10}) belongs to the group of saturated hydrocarbons, alkanes. Under standard conditions (25°C, 1 atm) it is a colorless gas with a characteristic odor, with a pronounced flammability and a low boiling point. Its molecular weight is 58.12 g/mol, while the boiling point is −11.7°C, which means that isobutane is in a gaseous state even at room temperature. The density of gaseous isobutane is about 2.7 kg/m^3, which is approximately twice the density of air. Due to this property, isobutane is classified as a so-called "heavy gas" and tends to remain on the ground in the event of a leak, especially in adverse atmospheric conditions.
Isobutane is extremely flammable. It will be easily ignited by heat, sparks or flames. Will form explosive mixtures with air. Vapors from liquefied gas are initially heavier than air and spread along ground [1,2].
The main physical and chemical characteristics of isobutane are listed in the table 1.

Table 1. *Physical and chemical characteristics of isobutane [3]*

The parameters	Units	Values
Molecular mass	g/mol	58,12
Boiling point	°C	-11,7
Melting point	°C	-159,6
Density (gas at 0°C, 1 atm)	kg/m³	2,67
Relative density (relative to air)	–	2,01
Lower Explosive Limit (LEL)	% vol.	1,8
Upper Explosive Limit (UEL)	% vol.	8,4
Flash point	°C	-83
Self-igniting temperature	°C	460
Heat of combustion	kJ/mol	2877
Specific heat	kJ/kgK	1,67

Due to its physical and chemical properties (low evaporation point, high flammability and tendency to remain on the ground), isobutane poses a serious hazard in case of release or accidents. Accidents involving isobutane can have far-reaching consequences for people, property and the environment, especially in industrial areas with close residential houses.

Modeling isobutene leakage from a storage tank

Isobutane uncontrolled release from a storage tank in industrial plants can have serious consequences, especially when this gas is stored in large quantities under pressure. Pipeline failures, tank cracks, leaking gaskets, flanges, unreliable valves, or mechanical damage due to the corrosion typically causes this accident. In addition to physical damage to the system, releases can also occur during filling, emptying and equipment maintenance operations, especially if the procedures are not carried out in accordance with prescribed standards. Isobutane, as a gas with a higher density than air, tends to spread and keep close to the ground, collecting in depressions, ducts and closed spaces. Thus increasing the risk of forming an explosive mixture in contact with a flammable source.
ALOHA (Areal Locations of Hazardous Atmospheres) is a specialized software tool developed for modeling the atmospheric dispersion of hazardous chemicals, primarily in emergency situations. The software is developed by the US Environmental Protection Agency (EPA) and the National Oceanic and Atmospheric Administration (NOAA). The goal of its development was to enable a quick and reliable assessment of the potential spread of dangerous clouds in the atmosphere after a chemical leak, whether it is an accidental industrial accident or a terrorist incident. ALOHA allows you to enter details about a real or potential chemical release, and then it will generate threat zone estimates for various types of hazards. Threat zones can also be shown in Google Earth or Google Maps using ALOHA's KML export feature.
ALHOA models have three hazard categories: toxic gas dispersion, fires, and explosions. ALOHA employs several different models, including an air dispersion model that it uses to estimate the movement and dispersion of chemical gas clouds. From this model, ALOHA is able to estimate the toxic gas dispersion, the overpressure values from a vapor cloud explosion, or the flammable areas of a vapor cloud. ALOHA uses additional models to estimate the hazards associated with other fires and explosions.
When a gas that is heavier than air is released, it initially behaves very differently from a neutrally buoyant gas. The heavy gas will first "slump," or sink, because it is heavier than the surrounding air. As the gas cloud moves downwind, gravity makes it spread; this can cause some of the vapor to travel upwind of its release point. Farther downwind, as the cloud becomes more diluted and its density approaches that of air, it begins behaving like a neutrally buoyant gas. This takes place when the concentration of heavy gas in the surrounding air drops below about 1 percent (10,000 parts per million). For many small releases, this will occur in the first few meters. For large releases, this may happen further downwind [4].

All of the accidents that can be modeled in the ALOHA software are based on the physical and chemical characteristics of substances and weather conditions that are present at the time of accident. The weather conditions that are entered as input parameters for modeling of accidents are the most common temperatures, wind speeds and directions in the last decade. Sometimes, in real situations opposite weather conditions occur than those predicted in risk assessments but that are the limitations of the software tools.

RESULTS AND DISCUSSION

In this paper will be presented the modeling of isobutene uncontrolled release from a concrete tank with a volume of 141m^3 using the ALOHA software. In the following table 2 are given the input data used in the software.

Table 2. *Input parameters for isobutane uncontrolled release simulation in ALOHA software*

Category	Parameter	Value/Description
1. Chemical substance	State of substance	Compressed gas under pressure
	Chemical temperature	22°C
	Tank pressure	2.5 bar
2. Tank and hole	Tank type	Horizontal cylindrical tank
	Tank dimensions	Diameter: 3 m, Length: 20 m
	Opening type	Round hole
	Opening dimensions	3 cm
	Opening orientation	Lateral, west side of the tank
	Opening angle to the direction of the wind	0° (directly in the direction of the wind)
	Duration of release	Continuous / until empty
3. Meteorological conditions	Wind speed	5 m/s
	Wind direction	North
	Air temperature	25°C
	Relative humidity	50%
	Cloudiness	7
	Time of day	Day / Sunny

The results obtained from the ALOHA software show the formation of three danger zones corresponding to different concentrations of isobutane in the air. The most critical is the red zone (LEL × 60%), which represents an immediate danger of the formation of pockets of flame and possible instantaneous ignition. In this case, that zone extended 34 meters from the point of leakage. Next is the orange zone, which indicates the area where the concentration reaches the lower explosive limit (LEL) up to 26m, and then the yellow zone, which extends up to 104 meters from the source, with a concentration of 10% LEL, and indicates the area of possible inhalation, odor and presence of flammable vapors. Threat zones are presented on the following figure 1.

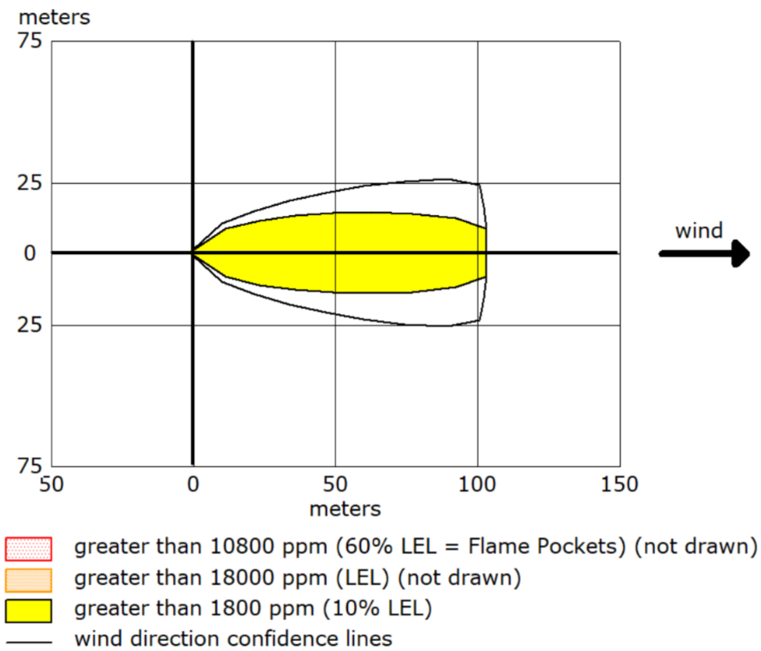

Fig. 1. *Threat zones of simulated accident*

Figure 2 shows a graph representing the simulation of isobutane concentration at a distance of 150 meters downwind of the release site. This analysis was performed using the ALOHA software package, with the aim of showing the influence of time on the accumulation of flammable gases both in open (outdoor) space and inside closed buildings. The model enables a quantitative assessment of the dynamics of gas expansion and its penetration into objects, which is of particular importance for making operational and safety decisions in real time during chemical incidents.

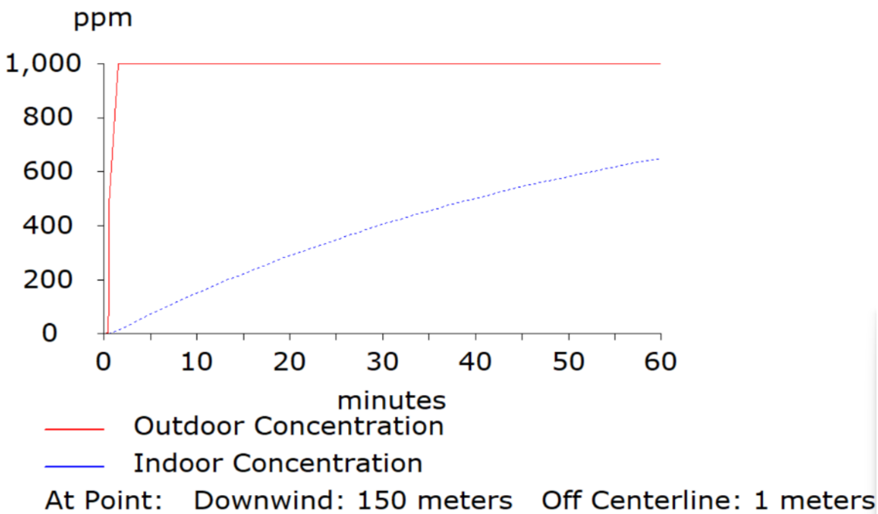

Fig. 2. *Graphic representation of isobutane concentration at a distance of 150m from the point of release*

The x-axis at the figure 2 shows time in minutes, while the y-axis is reserved for isobutane concentration in ppm (parts per million). The two curves give a comparison between:

- Red lines (Outdoor Concentration) - concentration of isobutane in the external atmosphere. It can be observed that the concentration suddenly reaches a maximum (~1000 ppm) already in the first minutes after the start of the leak, which indicates a very fast dispersion of the gas in the direction of the wind. This value remains stable, because it is a constant release of the substance during the simulated time period.

- Blue lines (Indoor Concentration) – concentration of isobutane inside a closed space, at the same distance of 150 meters, but with a minimal shift from the wind axis (1 meter on the side). This line shows the gradual increase in concentration in a closed facility, due to slower gas penetration through the structure of the facility (windows, doors, ventilation). After 60 minutes, the indoor concentration reaches about 600 ppm, which is significantly lower than the outdoor value, but still poses a serious risk.

The results from a modeling indicate that even in a relatively short period of time, it is possible to form a significant amount of flammable mixture in the atmosphere, especially in zones with slow ventilation. It is important to emphasize that in real situations the duration and rate of release may vary, and the actual values may be lower, but simulations of this type are used as a tool for designing protection systems, including automatic valve closing, sensor activation, evacuation and plant zoning.

CONCLUSION

In this paper ALOHA software was used to model uncontrolled release from a concrete storage tank, with input of realistic parameters such as pressure, opening size and weather conditions. The obtained results are presented through figures that define the danger zones, with a special emphasis on the range of the flammable mixture and the potentially endangered population or property.

Effective management of the risk of isobutane uncontrolled release requires an interdisciplinary approach - combining engineering knowledge, information technology, legal framework and industrial practice. Software simulations, such as ALOHA, are necessary for the preventive identification of potentially dangerous zones, while the application of laws and standards are the basis for a legally and technically correct response in the case of an accident.

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