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Original Article

Modelling of a Propylene Leak on the Premises of Synthomer Plc, in Sokolov

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Abstract *- This paper deals with setting up a system of safety regulations and crisis management at Synthomer plc, in Sokolov, the Czech Republic, with regard to a potential leak of a hazardous substance (propylene) from the warehouse of a chemical company. The program ALOHA (Areal Locations of Hazardous Atmospheres) was used to describe two realistic operating variants of a massive propylene leak, which predict the consequences of an accident for the immediate vicinity of the chemical plant. The modelling result subsequently verifies the software tool's hypothesis as an effective addition to modern crisis management. This analysis and research demonstrate that the program for predicting emergency situations is an effective tool in crisis management and planning to prevent emergency events in the chemical industry.*

Keywords *– Aloha program, Crisis situation modelling, Hazardous substance leakage, Propylene, Warehouse management.*

1. Introduction

In the developed industrial world, which also includes the industrial production of chemical compounds, preventing accidents and protecting public health and values are integral parts of a quality management strategy. Professionally prepared crisis management plans are a tool for overcoming crisis situations and minimizing the potential effects of unexpected operational situations. These include procedures from the stage of their recognition, through their management, to the removal of resulting consequences. Strategic crisis documents monitor purely technical measures, leading to the prevention and control of business processes, based on which additional measures can be implemented in the company's crisis strategy system, such as a software tool for predicting the risk of a dangerous substance leak that will allow simulating variations of a dangerous substance leak, taking into account the specific situational disposition of the company's operation [1]. Today, computer technology is used very effectively to model security risks. The issue of modelling the dispersion of hazardous substances in the atmosphere is a challenging area, the mastery of which requires perfect knowledge of a wide range of aspects. However, the results of a well-conducted dispersion study can be well worth the effort. It makes it possible to demonstrably detect the conditions under which the resulting cloud will disperse the slowest and, above all, to establish safe zones where people will not be endangered by the hazardous substance [2 – 7].

A propylene leak from a storage tank in a chemical plant is dealt with in this paper [24], in which the authors modelled a propylene leak in the ALOHA program. However, they do not address the specific situation that could cause a hazardous substance leak. The paper also fails to address storage tank technology security and crisis management precautions. Only danger zones are included in the map, but they do not indicate the number of persons directly at risk and evacuated persons in the event of an emergency. However, the authors provide an overview of various programs and models, including theoretical analysis, experimental research and practical application for modelling the consequences of chemical accidents.

The modelling of a hazardous substance leak in the ALOHA program is presented in papers [9 – 11]. Here, the authors deal with the leakage of a specific hazardous substance from a stationary source in a chemical plant with regard to the toxic threat to the population. Specific potential crisis situations that may occur in the storage of a dangerous substance are selected here as the source of the leakage. The hazardous substance release modelling results are subsequently incorporated into emergency and crisis plans. Preventive measures and recommendations for emergency services are also provided. The authors conducted very different research in their paper [12], which dealt with modelling the consequences of a traffic accident, an automobile tanker carrying LPG, in the ALOHA program.

The disadvantage of this research is that the authors can choose the area of potential leakage depending on a very different number of people at risk (highway, populated area, city center). In this case, it isn't easy to establish a security measure afterwards. In this type of emergency, rescue services must proceed according to predetermined activities and procedures, which depend on the specific situation.

The paper [13] deals with preventing high-risk situations, focusing on detecting the leakage of hazardous substances. The authors address the installation of detectors at vulnerable points in the system. When a gas leak is detected, these special detectors forward this information to the equipment operator. It may also trigger other security features in the system, making it possible to quickly prevent risky situations and subsequent emergency events that may impact the surrounding population. In the event of a crisis situation that may be dangerous for the operator of the equipment or in which detection systems are damaged, a mobile device may be used. The aim of the authors' paper [14] was to build a tracking robot that is technically, operationally and economically independent. The robot requires minimal maintenance, and because it is autonomous, it does not require any maintenance. The robot is equipped with detectors for the leakage of hazardous substances and a thermometer for measuring the current temperature in the room. It can forward the measured data and values to the selected device, operator or control room. Given the above factors, it can replace chemical operation workers in very dangerous situations and prevent emergencies in time.

The above-prompted research aims to implement a software tool in the crisis management processes at Synthomer plc to demonstrate the positive contribution of computer modelling as a sophisticated addition to increasing the level of safety and protection against high-risk events in the propylene operation of the investigated company. The program simulation will help coordinate the components of the integrated rescue system more precisely in the event of a sudden crisis situation and will allow the prediction of broader aspects of the impact of the risk to the population and the environment that accompanies these events. The above issue of propylene leakage is not comprehensively dealt with in the Czech Republic. Most research and modelling of the release of hazardous substances focus on the release of ammonia from winter stadiums or tank cars, as well as on the release of LPG from stationary tanks or in traffic accidents during its transport. However, special chemical companies with a specific type of hazardous substance are an exception.

2. Description of the Industrial Enterprise

Synthomer plc consists of a worldwide network of branches and companies owned by the multinational manufacturing company Synthomer, headquartered in London, Great Britain. The branch in Sokolov produces acrylate monomers, but the company's production plants are scattered worldwide. The conglomerate's production includes an extensive range of products such as carpets, adhesives, chemical compounds, reagents and packaging [15]. Synthomer plc is an essential regional employer in the Sokolov region. It employs about 370 employees, some in very narrowly specialized positions. Synthomer plc is a modern and safe enterprise that strictly complies with legislative standards and technical regulations governing the field of chemical production. In the area of safety and technological processes of chemical production, it has implemented management control systems aimed at increasing the safety and protection of health and the environment in all activities related to business, in accordance with the voluntary Responsible Care program. The establishment of corporate control entitles the company to use the Responsible Care® logo (since 1996), an environmental management system according to ČSN ISO 14001 (year 1997). The company is also certified to comply with ČSN ISO 50001 Energy Management System (2016). Since 2007, the company has been a Serious Accident Prevention System member according to the law [16].

2.1. Description of Propylene

Propylene is a colorless, highly flammable gas (flash point: < -40 °C, ignition temperature: approx. 455 °C to 465 °C), which is heavier than air in its gaseous state. This causes it to accumulate in lower places and form an explosive mixture with air (explosive limits: lower: 2.0%, upper: 10.3%). Its general formula is C3H6, and its systematic name is propene. Propylene is chemically stable under normal conditions. Propylene is used as a raw material for further processing in the chemical industry for producing polypropylene (plasticizers for PVC, solvents). It is used to produce acrylic acid and acrylates, propylene oxide. Propylene is stored in tanks made of low-temperature steel, cooled below the boiling point of propylene, or under pressure in pressure vessels.

When released into the air under normal atmospheric pressure, evaporation occurs by boiling at temperatures up to -45 °C, posing a risk of frostbite when the substance comes into contact with the skin. Propylene vapors at higher concentrations have a narcotic effect. They cause headaches and stomach upset and irritate the eyes and respiratory tract—the suitable extinguishing agent for extinguishing a propylene fire extinguishing foam, extinguishing powder, and CO2. Water is not a suitable extinguishing agent (H2O). Propylene vapors form an explosive mixture with air, burning with a sooty flame and simultaneously releasing carbon monoxide (CO). Emergency protective clothing is required when the fire is extinguished to prevent contact with the skin and eyes, and a self-contained breathing apparatus is required. It is always necessary to limit the fire area and prevent further leakage of the substance into the sewer, water and soil. Propylene should be disposed of by absorbing it into a porous material or pumping it off, then disposing of it according to applicable legislation [17].

3. Modelling the Spread of Toxic Substances

There are many modelling programs in the field of modelling hazardous substance leaks in chemical accidents. Specially programmed tools are not freely available, and the price of an investment in acquiring a program is up to tens of thousands of euros, depending on the program's sophistication. Each of these software programs has its own specifics, and their modifications are 'tailor-made' according to the requirements of industrial enterprises and their operating conditions, the location of enterprise products, and the technologies used. Software tools for simulating the release of toxic substances use predictions of different situations adapted to real conditions. The output of the simulation is a verified mathematical model [18]. Models can generally be classified as discharge, evaporation, dispersion, fire, explosion and vulnerability models. One software tool for modelling and estimating the consequences of industrial accidents with the release of hazardous substances is the computer program ALOHA. Based on a number of input data and external influences, the functions of the ALOHA program can model the danger zone, where the properties of the leaked substance pose a risk. Modelling software tools create a scenario of an emergency event according to the specifications and characteristics of the company's industrial production. The basic parameters of the emergency are entered, such as meteorological data (temperature, wind speed and direction, altitude, relative humidity, cloudiness, season), the place of the accident, the type of equipment involved in the accident, the type of accident and the time of the accident. The model subsequently presents the processed data in a clear output, in which the specified parameters of the scenario are processed. The solution includes activated emergency response units, the transmission of information about the accident, the method of warning the population in the area, the calculation and evaluation of the extent of the leak, the completion of the accident solution and the restoration of the affected area [25].

The ALOHA computer program can very effectively predict the dispersion of toxic clouds, the course and concentration of the chemical release of hazardous substances, and scenarios of fires and explosions based on realistically entered parameters. The program is designed to accurately and quickly simulate the level of danger and subsequent threats. These models subsequently serve as study materials for analysing crisis management documents. The latest versions of ALOHA are designed based on cross-checking the inputs of many real accidents to minimize errors and warn users in time. The simulation output predicts how quickly the chemicals will leak and the changing concentrations of the substances over time and under certain conditions. The model scenarios work with the specific properties of the specified substances, also considering the spatial conditions of the production destination. Depending on the scenarios, they evaluate the course of the leak, toxicity values, flammability, thermal radiation, overpressures, vapors and jet fires. The program can also model the atmospheric dispersion of chemical spills on a water surface. ALOHA's sophisticated user interface is designed to make it easy and intuitive. Each window contains help dialogue. The outputs of the simulations can be printed in many graphic, text and map formats [20].

4. Situational Analysis of the Propylene Storage Facility

The propylene storage facility is located on the northern side of the production site in an area roughly bounded by the Ohře River, a railway siding leading to the site, and the production facility itself. The propylene is stored in two above-ground 1000 m^3 spherical tanks at ambient temperature (under pressure). The propylene warehouse management facility is part of the production plant, and it is in charge of unloading propylene from tank cars, storing unloaded propylene in tanks and dispensing propylene. Regarding the project, warehouse management is divided into operating units and buildings. Propylene enters the warehouse management unit through the operating unit. The warehouse equipment allows for the smooth flow of propylene into the production process. Due to the nature of the medium, the entire propylene warehouse is fenced, and entry points are locked. A surveillance system monitors the whole premises. The activities performed in the propylene warehouse management aim to ensure the warehouse's trouble-free operation, the receipt of raw materials, and the dispensing of raw materials. Trouble-free operation of warehouse management is associated with regular inspections by operators, operation of machines (mainly pumps) and equipment located in warehouses, regular inspection of routes, devices, storage tanks, wastewater, safety measures, etc. Emphasis is placed on measuring devices and the system detecting malfunctions and emergency states.

5. Materials and Methods

The leakage of propylene during operation most often occurs when it is unloaded from a tank into a spherical storage tank, where the human factor plays an important role. The ALOHA program will model two operating situations. The first situation will simulate the leakage of propylene and its explosion, the so-called BLEVE phenomenon (Boiling Liquid Expanding Vapor Explosion). The BLEVE phenomenon occurs when a container suddenly ruptures due to its over-pressurization. In a container that is partially filled with a flammable liquid with a vapor space (e.g. liquefied gas under pressure, with the temperature of this liquid higher than its normal atmospheric boiling point), as a result of the action of heat (fire or flame), the liquid evaporates, the vapor heats, the pressure increases, and the strength of the material of this vessel changes. Continuous depressurization by the safety valve is insufficient. At a certain point, pressure destruction occurs, and the liquid evaporates instantaneously.

The explosion creates a shock wave, and fragments of the vessel are thrown into the surrounding area. The expanding mixture of the combustible substance and air ignites immediately, resulting in intense combustion that creates a fireball [21]. In the second case, the spread of propylene in the location of the production company will be modelled.

5.1. Propylene Explosion Modelling

For the purpose of modelling the case, it worked with a potentially real operational situation in which a propylene leak occurred due to the wrong connection of the dispensing hose to the dispensing valve. After the ball valve was opened, the control lever was damaged and could not be closed. This caused an uncontrollable leak of propylene gas through the fully open ball valve. The leaking propylene created an explosive concentration up to a distance of approximately 20 meters. The fire was initiated by coincidence by the warm engine of the foreman's vehicle, who arrived to inspect the scene. Upon initiation of an explosive concentration of propylene with air, an explosion approximately 50 meters in diameter occurred, and the leaking propylene continued to burn. The leaking burning propylene on the site heated the liquid propylene inside the tank car, and this heating led to the BLEVE phenomenon. The following input data were entered in the ALOHA program for modelling: The location's altitude was 400 m above sea level. In the 'Building type' tab, the option with value 1 is selected. Substance identification: propylene. All substance properties are listed in the CAMEO Chemicals database, which is part of the ALOHA program. Atmospheric data: Wind speed 6 m/s, easterly, measured 3 meters above the ground. The surrounding area is urban or forest. It was cloudy on the day of the accident. The air temperature was set at 8 °C. The stability class selected was 'D'. The weather was without inversion, with 50% humidity. The propylene is delivered in tank cars. The necessary source data for modelling were found in the catalogue of freight wagons of ČD Cargo plc [22]. According to the catalogue selected in ALOHA, the corresponding type of car was a cylinder tank with the following parameters: cylinder height of 2.9 m and cylinder length of 14.93 m. The ALOHA program calculated the volume of 98.6 m^3; the output of the program calculation is shown in Figure 1.

The tank contains a liquid substance that is stored at ambient temperature. The intervention card indicates that the tank was 100% full at the start of the unloading. The valve was open for 47 minutes from the opening of the valve to BLEVE. It takes 240 minutes to unload the tank. The original volume of liquid propylene was 98.6 m^3. This means there were 79.5 m^3 of propylene in the tank at the time of the BLEVE phenomenon, which is 80.6% of the total amount, indicating that 19.1 m^3 of propylene was unloaded. The rest of the volume was propylene in a gaseous state. The calculation of the volume of propylene in the tank is shown in Figure 2.

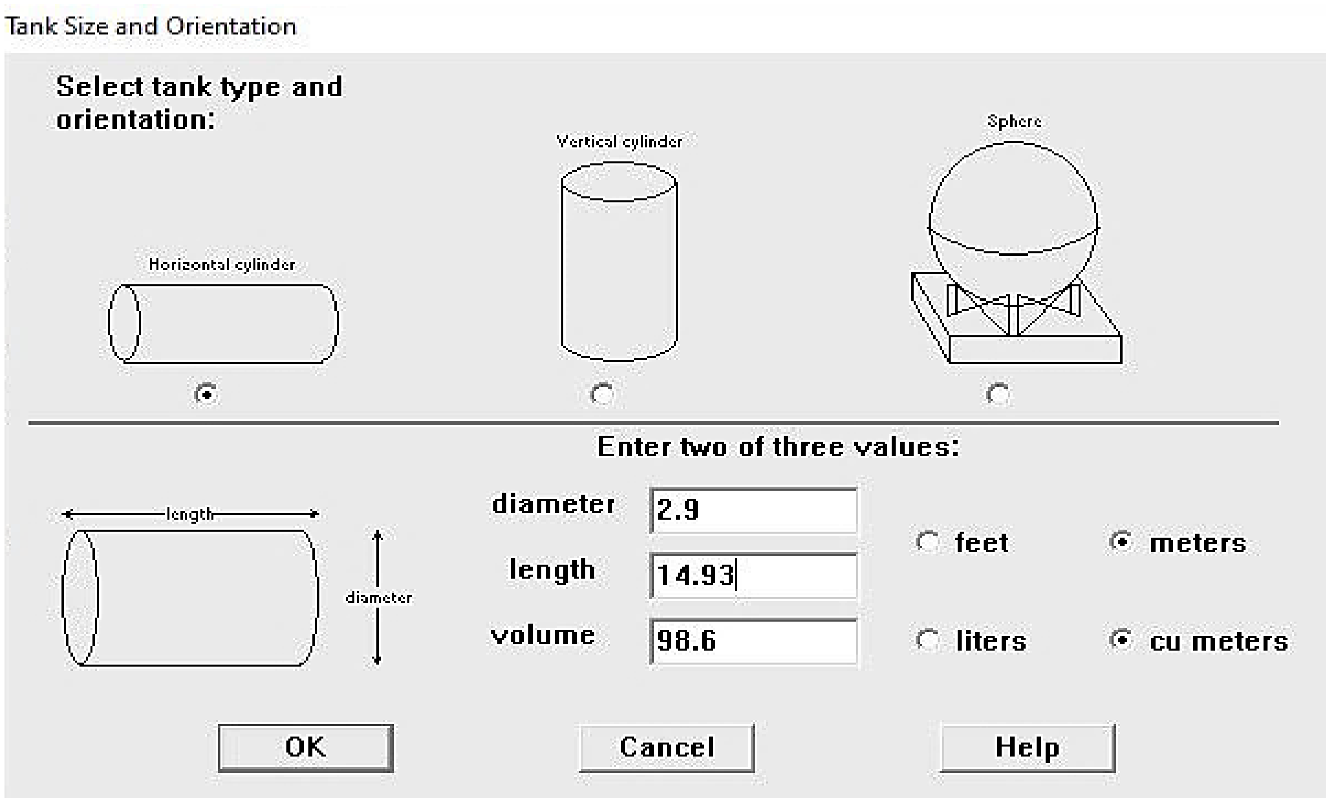

Fig. 1 ALOHA output – tank information [20]

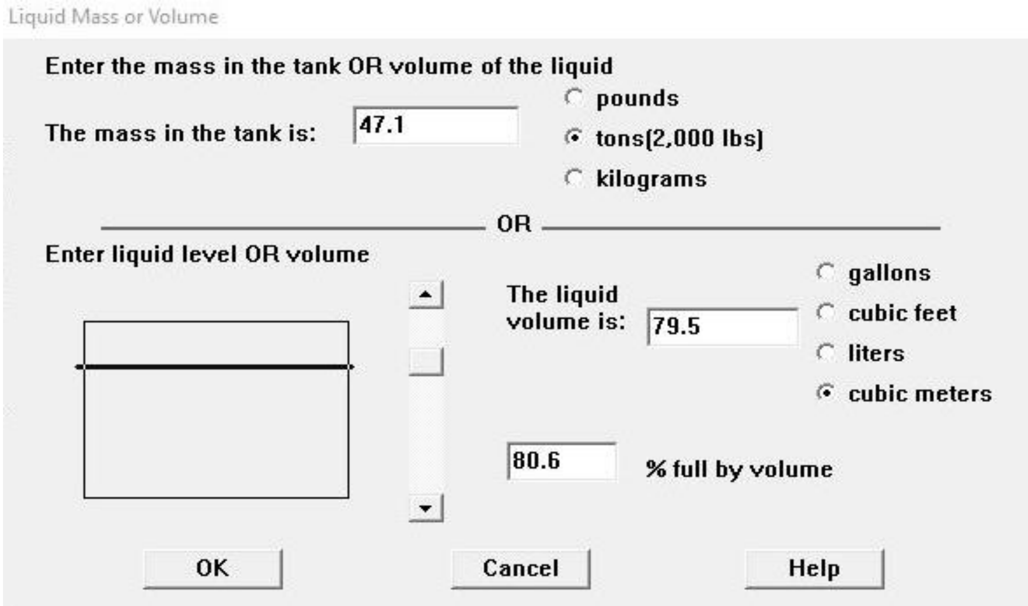

Fig. 2 ALOHA output - calculation of the amount of the substance [20]

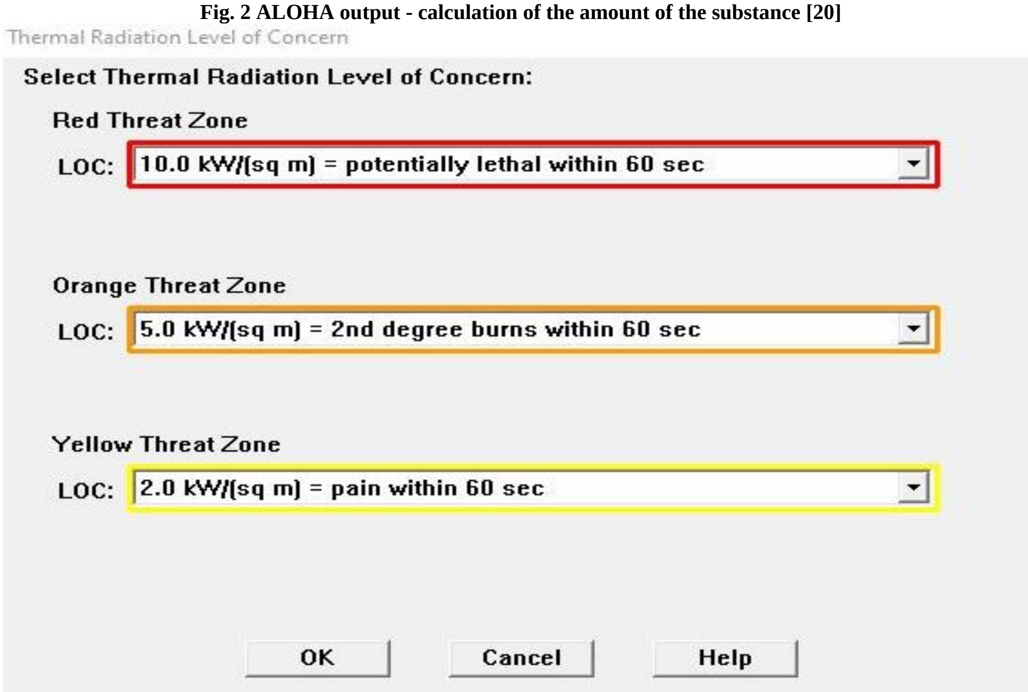

Fig. 3 ALOHA output– critical values of thermal radiation [20]

In the next step of the simulation, the possibility of all the liquid escaping at once was chosen. In the main menu in the 'Display' tab, 'Threat Zone' was selected. The ALOHA program offers three-level modelling of thermal radiation hazard zones, shown in Figure 3.

The offered values were kept. The modelling resulted in a graphic and textual output. The graphic output of Figure 4 shows the respective zones bounded by the thermal radiation value. The red zone indicates the area where the thermal radiation reaches values of 10 kW/m^2 and more, which can result in human death if exposed for 60 seconds. In the orange zone, thermal radiation ranges from 5 to 10 kW/m^2, which causes 2nd-degree burns on unprotected parts of the human body when exposed for 60 seconds.

In the yellow zone, thermal radiation reaches values of 2 to 5 kW/m^2, which can cause severe pain when exposed for more than 60 seconds. The size of these zones depends on the surrounding area, the presence and distribution of buildings, and vegetation density. These circumstances can significantly reduce heat transfer.

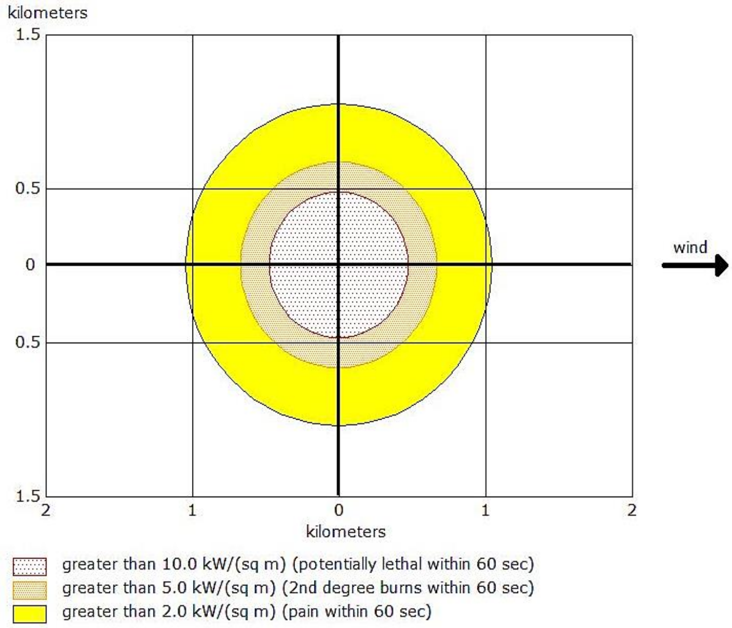

Fig. 4 Graphic output of ALOHA [20]

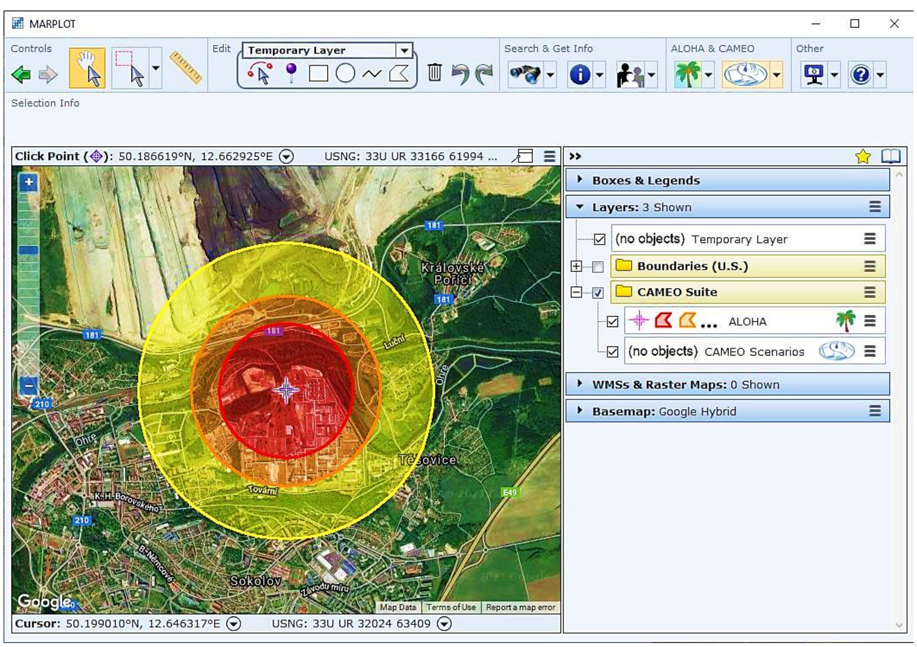

Fig. 5 Map with plotted explosion modelling

5.2. Propylene Leakage Dispersion Modelling

The premises of Synthomer plc are flat and fenced. The heat transfer after an explosion of the tank, as modelled by the output of the ALOHA program, would not be extremely affected. Figure 5 shows the results of the propylene explosion modelling plotted on the map of the location of the production company. The result clearly shows the consequences and scale of the accident. The red zone extends to a distance of 473 m, the orange zone to 668 m, and the yellow zone to a distance of 1000 m from the tank.

In modelling the spread of propylene in a leak from a spherical storage tank, the BLEVE effect was not expected, but rather a dangerous toxic cloud of the leaked substance, threatening the residents of nearby settlements. The modelling follows the spread and contamination of the surrounding area of the production company with a dangerous substance. The simulation assumes that propylene leakage from the spherical tank can occur in the event of a pipe spigot defect. The quick-stop valve is located just behind a series of flanges from which the propylene escapes.

There is no way to stop the spread, and there is uncontrollable leakage of propylene gas. The sensor detects a dangerous concentration of propylene, and the vapor barrier is triggered. However, the concentration of the substance in the air is still saturated from a defect in the pipeline. The same data as in the first case were entered into the input data of the ALOHA program for modelling.

The leakage of propylene from the spherical storage tank in the amount of 430 t creates a cloud, which is blown by the wind over the populated area near the production plant. In Figure 6, the ALOHA program simulates the direction, movement and distance of the hazardous substance cloud in the surrounding area based on the specified parameters and wind direction.

The output of the accident simulation and the propylene spread in the ALOHA program is plotted on the map. The modelled simulation in Figure 7 indicates that the cloud of escaping propylene would hit the neighboring densely populated village of Královské Poříčí, endangering the lives of approximately 900 people.

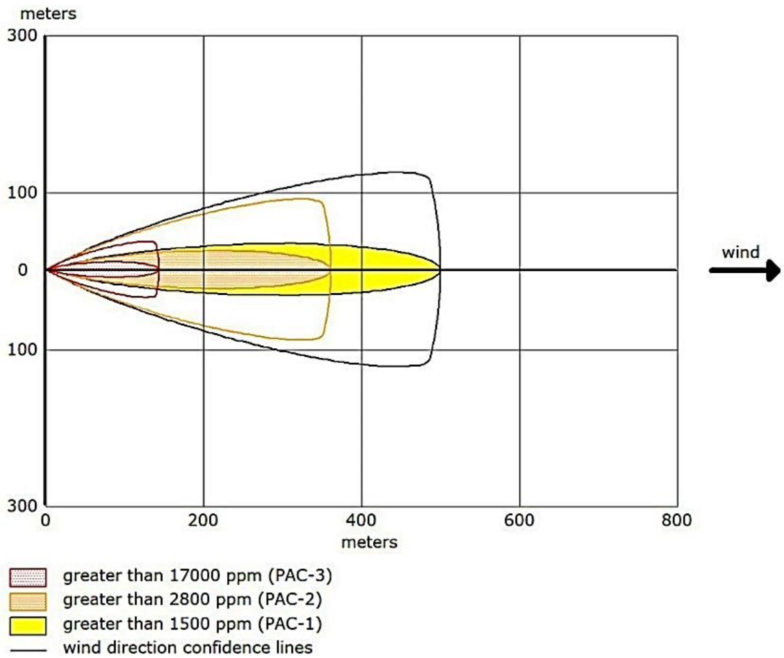

Fig. 6 Graphical output of ALOHA - substance dispersion [20]

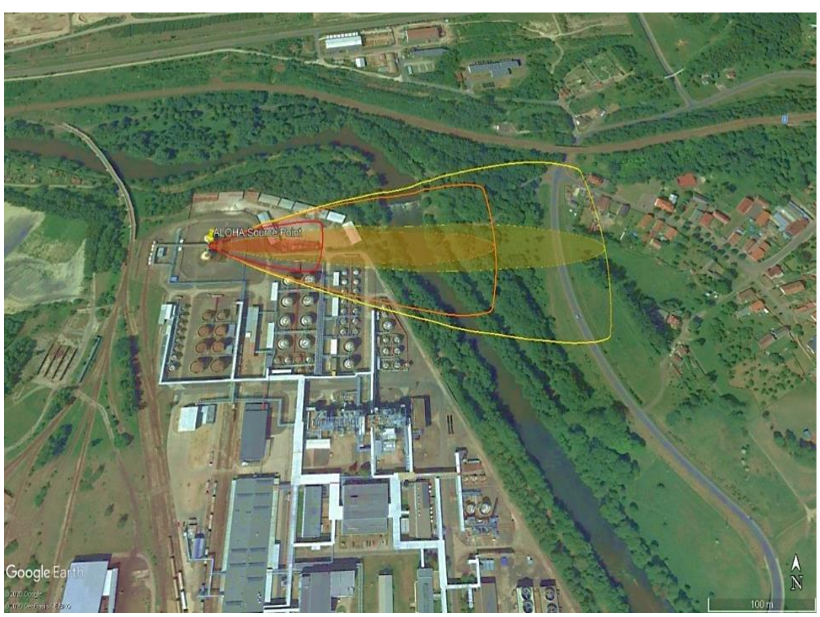

Fig. 7 Map of spreading model

6. Results and Discussion

The simulated outputs of the ALOHA program show that the first modelled accident could only occur if several safety measures were not observed. The explosion would require the ignition of leaked propylene. In contrast, warehouse management regulations strictly establish the type of clothing used in the defined area of warehouse management. Nevertheless, this situation cannot be ruled out in the event of failure of the human factor. In this case, the modelled accident would have catastrophic consequences, especially given the territorial location of the production in the middle of a medium-sized city. The zone of high heat radiation, calculated at a distance of almost 473 meters in diameter, would surely cause the death of all the people in the vicinity.

For this reason, evacuation of all people within a calculated radius is the primary task of emergency instructions. Although three-quarters of the company's premises consist of only greenery and grassy areas, the remaining one-fourth of the area is home to the production, technological and storage facilities of the Synthomer plc complex. Likely, an explosion caused by a fire during the release of propylene from a tank car would logically lead to a domino effect in the processing section. The consequences would be catastrophic. Data available in the CAMEO chemicals database [21] indicates that remote intervention is recommended if a large fire is in a tank transporting propylene. Portable monitors are recommended to extinguish the fire, and residents up to a distance of 800 m from the tank must be evacuated. The modelled result differs here because the modelling shows that the danger zone is 200 m larger. The results of the modelling of a propylene explosion show the need to inform the public in the danger zone of the potential danger and the evacuation of a zone with a radius of up to 1000 m to remove the consequences. The modelled results further show that in the event of a fire arising from a propylene leak, family and apartment buildings, manufacturing enterprises, essential civic services and a shopping center are located in the yellow zone. The graphically depicted area would be affected if an accident were to occur according to the modelled explosion and extent. The consequences would affect the daily lives of thousands of residents. According to the law [16], Synthomer plc is classified in group 'A', and an external emergency plan is developed for its operation.

In the second modelled case, the simulation is more realistic because the technology used on one of the two spherical tanks does not allow the leak to be immediately stopped in the event of a sudden propylene leak from the tank. This is due to the automatic shut-off valve located just behind the pipe spigot. The second spherical tank has already been modernized, and the automatic shut-off valve is located directly at the bottom of the tank. The automatic valve will immediately close the tank if a propylene leak at the flange occurs. With regard to the internal technical measures for detecting a propylene leak, this situation is secured by vapor barriers and other measures determined by the emergency plan. This is why the results of the second model are purely hypothetical to demonstrate the capabilities of the ALOHA program.

The propylene unloading process is the riskiest part of the handling process from an operational perspective. A human error can lead to a very dangerous accident in this case. Potential human factor errors could be eliminated by the installation of an unloading arm in this case. The unloading arm automatically connects to the transport tank. The technological control system of the unloading process minimizes unexpected situations. The unloading process includes a tightness inspection, testing and nitrogen flushing of transport vessels. The arms have parking position sensors so that the propylene unloading process can be done without manual operation.

7. Conclusion

This paper modelled a propylene leak at the Synthomer plc complex in Sokolov. The ALOHA program was chosen as a supporting means of the crisis management system, which can realistically simulate hazardous operational situations and predict their development. The paper provides an example of two propylene leak cases. The first simulates a propylene leak from a tank and shows the possible consequences of an explosion. The second case models the spread of a large amount of propylene through the air in the event of a leak from a spherical storage tank and the threat to residents in settlements surrounding the production company. Compared to other research conducted by the authors mentioned in this paper's introduction, this is a comprehensive modelling of a propylene leak from the warehouse of a chemical company.

The calculation of the case of a propylene tank explosion revealed that the evacuation perimeter should be 200 m larger than is established in the internal safety documents of Synthomer plc. The second modelled case vividly predicts the consequences of the spread of a toxic cloud over the residential area, making it possible to set up an emergency plan and its measures more effectively, leading to quick intervention and protection of the lives of residents. In conclusion, a technical measure to minimize human error in propylene unloading technology is presented. Handling hazardous substances is the riskiest part of the process regarding operational activities. Installing an unloading arm would automate the operational process and eliminate the dangerous situation. The result of the research further proves that the program for predicting emergency situations is an effective tool for crisis management and planning in the prevention of emergency events.

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