ORIGINAL ARTICLE

Consequence Modeling of a Rupture of Methyl Diethanolamine (MDEA) Storage Spherical Tank (Catastrophic Rupture Scenario)

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ABSTRACT: The rupture of flammable materials is one of the significant hazards existing in huge industry. In this study, the rupture of methyl diethanolamine (MDEA) tank in Ilam gas treatment refinery was modeled by PHAST (Process Hazard Analysis Software Tool) software. Distances with high risk was determined in fire and explosion scenarios versus consequence modeling. The results revealed that the catastrophic rupture scenario of MDEA tank in summer climates is the worst case with the highest risk, since in this case, the affected distance is about 2,450 meters for explosion overpressure, and 840 meters for vapor release; thus, these distances should be nonresidential. By considering a bund wall around the tank, the abovementioned distance reduce to 1,860 meters for explosion overpressure and 780 meters for vapor release.

INTRODUCTION

Today, population growth has led to the expansion of chemical industry and has consequently increased the risks of chemical materials. The damages and hazards are inevitable, since they are not predictable in many cases. Combustible chemical release and vapor cloud formation align with a spark sources can cause the occurrence of an unbearable disaster such as Jaipur (India) and Viareggio (Italy) accidents [1]. Acquiring readiness to respond to these crises at the time and place of incidents requires recognizing and evaluating high-risk locations. The risks related to chemical industry have direct relationship with their fast growth and development. In addition to utility risks, inherent properties and hazards of chemicals such as their flammability, explosive capability, toxicity or corrosiveness should be considered.

Aqueous methyl diethanolamine (MDEA) is one of the solvents that can be used in the natural gas sweetening unit. Absorbing H_2S/CO_2 leads to corrosion and foaming in the process, leading to the decreased quality [2]. Irritating vapors and toxic gases like NOx and CO may be formed when involved in fire. Expert committees documented several instructions about exposure to hazardous chemicals in environment [1]. The users should be very careful when using toxic and flammable chemicals, because any leakage might cause their dispersion in atmosphere, leading to harm effects on the environment, animals and vegetation; in severe conditions, it can even cause human deaths [3], for example, the accident of chlorine-carrying train in South Carolina [4].

In previous contributions, the analysis and evaluation of fire and explosion accidents of gas storage facilities were considered using assessment methods [5-9]. Luo et al. published a comprehensive work on risk assessment method to analyze a gas storage tank fire and explosion accident, and quantitatively calculated its occurrence probability. In order to reduce the probability of an accident risk, they proposed a specific measurement with the highest probability [5]. Leem and Huh designed an intelligent decision-making system based on the safe distance specified in the safety standard levels to use it in gas storage tanks and prevent the caused damage in the field of explosions [6]. Tang et al. first investigated the fire and explosion risk factors related to 100,000 m^3 of a dry gas storage tank, and then applied the fault tree method to prediction of possibility occurrence accident and proposed the safety countermeasures [7]. The explosion behavior of gas tank was simulated and analyzed by Ren et al. who provided a scientific basis to prevent and control gas-related accidents [8]. Given the quantitative simulation calculation method for accident consequences, Fan investigated the consequences of gas poisoning, fire, and explosion due to gas leak in a blast furnace gas tank. He/she presented a theoretical foundation for hazard prevention in industries [9].

Therefore, this study is aimed at investigating the high-risk area near the around of MDEA tank, in the catastrophic rupture scenario in different seasons. The MDEA storage spherical tank is in Ilam gas treatment refinery around Ilam. In this work, the following parameters are calculated: distance to safety point, extension of hazardous area, and safe distance for the electrical enclosure installation. Finally, the storage tank was investigated using a bund wall assumption.

MATERIALS AND METHODS

The determination of initial conditions for instantaneous and continuous discharge models depends on the release and accidental event sources. In consequence model, the initial conditions for a release are adjusted through defining the release properties and the failed equipment. Vessel of the material is under pressurized conditions. Several parameters such as temperature, pressure, and MDEA phase are effective in the specification of initial conditions. Pressurized storage conditions are considered in the cases with the vessels including the pure saturated liquid phase or the gaseous material held in pressure vessels.

Gaussian Model

Different parameters maybe affected by the discharge modeling of materials; i.e. full rupture diameter, material phase and its amount, etc. The prediction of dispersed concentration at specified distance and time is one of the main goals in the material release modeling. This model shows the acceptable constantly applied accuracy in the release modeling cases [10].

The model based on the following partial equation, called the Gaussian model, can be obtained through considering the mass conservation equation:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i}(u_i . C) = 0 \qquad (1)$$

where C shows the material concentration; u represents the wind velocity and i index is the direction of x, y and z. Concentration in the continuous release model is represented using:

$$[C](x,y,z) = \frac{Q_m}{2\pi\sigma_y\sigma_z}\exp\left[-\frac{u}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \times \left\{\exp\left[-\frac{u}{2}\left(\frac{z-H_r}{\sigma_y}\right)^2\right] + \exp\left[-\frac{u}{2}\left(\frac{z+H_r}{\sigma_y}\right)^2\right]\right\}$$
$$(2)$$

where H_r and σ stand for actual stack height and dispersion coefficient, respectively. In flash release, it is calculated by:

$$[C](x,y,z,t) = \frac{Q_m}{(2\pi t)^{1.5}\,\sigma_x\sigma_y\sigma_z}\exp\left[-\frac{u}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \times \left\{\exp\left[-\frac{u}{2}\left(\frac{z-H_r}{\sigma_y}\right)^2\right] + \exp\left[-\frac{u}{2}\left(\frac{z+H_r}{\sigma_y}\right)^2\right]\right\}$$
$$(3)$$

The maximum concentration can be calculated using the following equation:

$$[C]_{max} = \frac{2Q_m}{e\pi u H^2}\left(\frac{\sigma_z}{\sigma_y}\right) \qquad (4)$$

Simulation Background

PHAST software v.7.2 (Det Norske Veritas and Germanischer Lloyd (DNV, GL) company) was adapted to the accident model. This software is employed to identify and analyze the points with high probability in accident occurrence [11]. It is also used to analyze and interpret the accidents in chemical processes, including toxicity emission or vapor cloud formation, flammable chemical, rupture of a vessel, pool fire explosion, calculation of concentration dispersion, and overpressure [12].

The scenario described in this work is the catastrophic rupture of the storage spherical tank accident involving MDEA analyzed with the bund wall and then compared with it. The effects of overpressure damage are shown in Table 1 [13].

Table 1. Damage effect of the overpressure

Overpressure (bar)	Damage effect
0.01035	Typical pressure of glass window damage
0.0207	10% of the glass is broken
0.0345	Windows are damaged and the building structure is less damaged
0.0483	Upper limit of reversible impact on personnel
0.069	Part of the building is damaged, metal plates are twisted, and glass fragments are scratched
0.138	Part of the walls and roof collapses
0.1656	Eardrum ruptures of exposed workers
0.1725	Critical deaths of personnel
0.207	Distortion and foundation displacement of buildings with steel structures
0.345	Wood structure fracture
0.69	Almost all buildings collapse, and the lungs of personnel bleed
1.38	Direct shock waves cause 100% death

In the first episode, the storage tank without bund wall was considered; then, a bund wall is considered around the tank to identify what changes occur at the safety distance. Since the volume calculated from bund wall area should be more than the fluid volume in the tank, the length, width and height of the possible wall were 12 m and 12 m and 1.5 m, respectively. In addition, the wall is made of cement. All values of parameters used in this paper were estimated from the real condition of factory in case of incident occurrence. The volume of MDEA in the tank was 219.4 m^3; its properties are tabulated in Table 2.

Table 2. The attributes of MDEA in the vessel (storage tank).

Density	1.043 g/ml
Viscosity	101 MPa. Sec
Molecular weight	119.164 g/mol
Critical temperature	403.9 °C
Critical pressure	3.7 MPa
Normal boiling point	247 °C
Flammable/toxic	Flammable
LFL (Lower Flammable Limit)	6000 ppm
UFL (Upper Flammable Limit)	12000 ppm
Flash point	127 °C
Heat of combustion	34.7 KJ/mol
Appearance	colorless liquid

Values of the saturated liquid MDEA storage spherical tank, tank height, wall thickness, operational pressure and temperature, and ambient temperature were 6.3 m, 1 m, 3.18 mm, 1 bar, 88°C, and 40°C, respectively.

RESULTS AND DISCUSSION

The prediction behavior of a flammable chemical propagation, formation of vapor cloud, and its concentration in different portions allow making reasonable guesses for incurred damage on human and environment in order to take appropriate safety measures [1, 14].

This modeling is aimed at consequence modeling of the MDEA release, thermal radiation of burning and the explosion overpressure in different climates. In the present paper, this is the first risk concept and consequence modeling is described briefly; finally, consequence of MDEA emission in Ilam refinery is analyzed by PHAST software. Bottom corrosion causes the rapture in a vessel containing 219.4 m^3 MDEA and entire discharge of the cargo; apart from MDEA evaporated and consequently, a vapor cloud began to form. The electrical closure was adjacent to the vessel and a spark in the flammability area may lead to occurrence of pool fire.

Figure 1 shows maximum concentration footprint (Cloud width vs. Distance Downwind) in different areas from the above perspective. Limited area between UFL and LFL is a flammability area that may cause a spark to cause a fire. Moreover, as observed in this figure, various site sections with any concentration maybe observed.
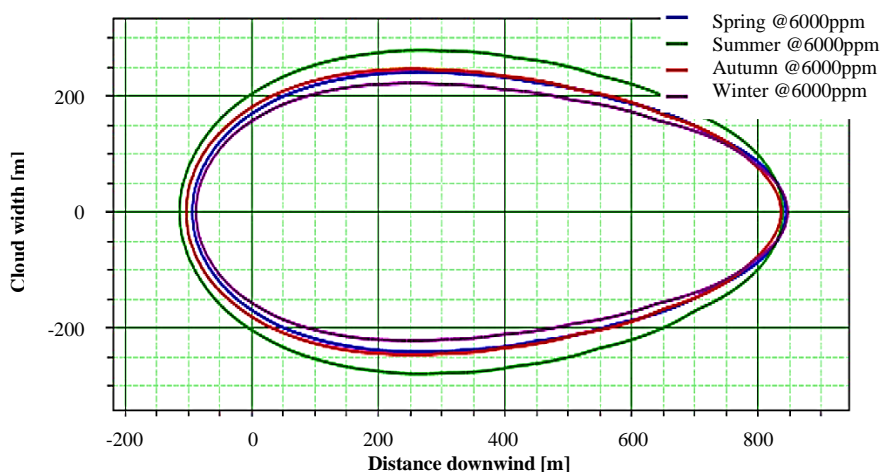

Figure 1. Maximum concentration footprint (Cloud width vs. Distance Downwind) at averaging time: flammable 18.75 s

The PHAST simulation results (when bund wall existed) show that maximum concentration (6,000 ppm) distance in real and with bund wall are 850 m and 780 m, respectively. According to the results of Hosseini on *The Chlorine Release in Urban Area* (a case study in the water supply of Eyvan city, Iran), it has been showed that the progression of the concentration profile in summer with the same temperature conditions as our research is more than that in other seasons [10].

Concentration of MDEA in terms of time for a given distance is shown in Figure 2, and with the wall is shown in Figure 3. The concentration increases in a few seconds and then decreases. As observed in Figure 3, in summer climates, the maximum gas cloud concentration in 40 seconds is 30,000 ppm that is much less than 207,000 ppm in non- wall conditions at 15 seconds. Haghnazarloo et al. argued that the concentration increases in the first few seconds and then suddenly decreases in the consequence of real rupture modeling for toluene storage tank [1].
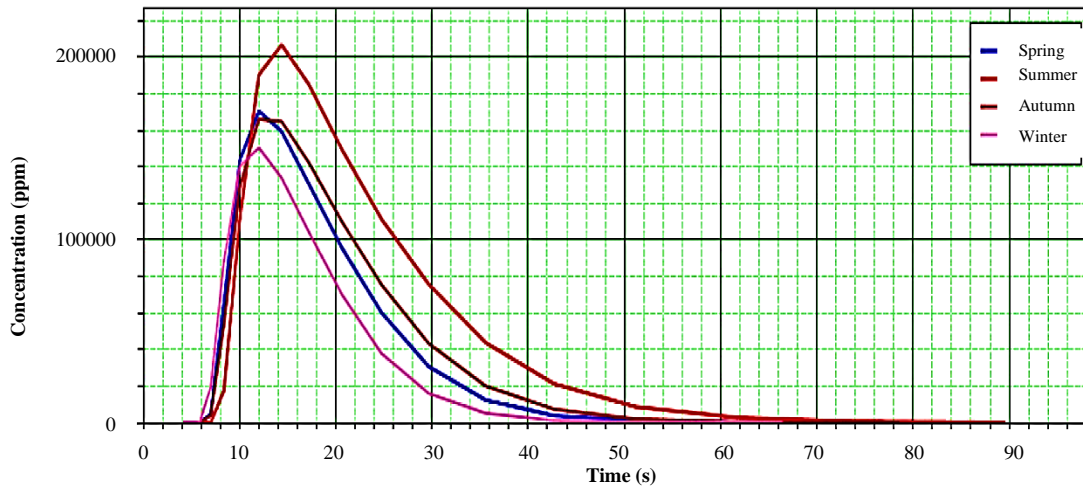
Figure 2. Concentration vs. Time at given distance at downwind distance of 141 m.
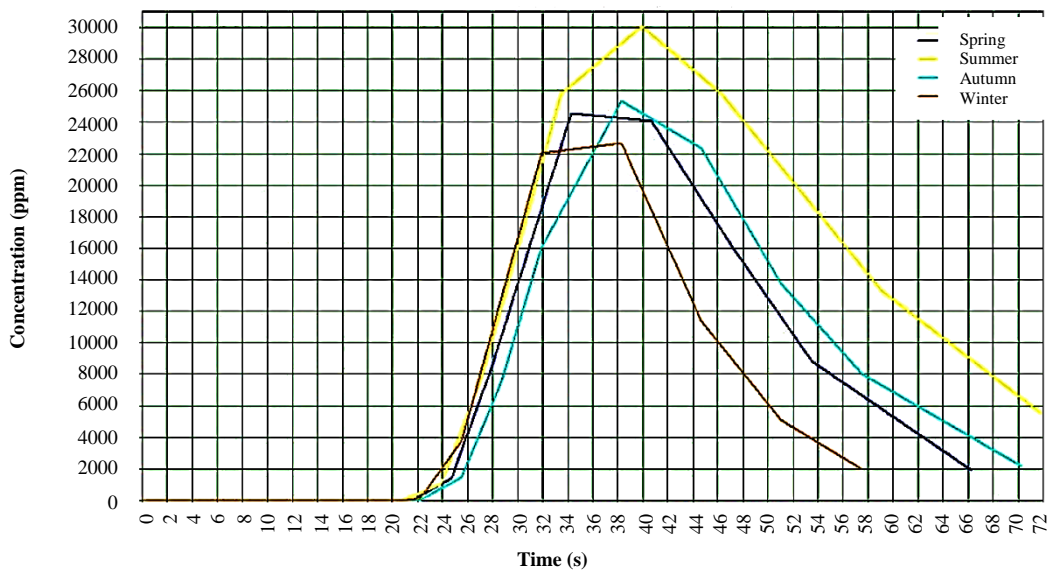

Figure 3. Concentration vs. Time at given distance of 473.5 m (with bund wall)

The characteristics comparing between the cloud formed in terms of the distance and height of the cloud and direction of the downwind from the side view is shown in Figure 4. As observed, the cloud will rise to 11.5 meters with a concentration of 6,000 ppm. In Figure 5, the area between the green and blue lines demonstrates the flammability concentration between UFL and LFL at summer weather. Moreover, it can be understood that a spark can lead to explosion of vapor cloud in this range. In fact, the extracted data from this figure are useful to set up sparkle equipment or electrical cables at a suitable distance from the MDEA tank.
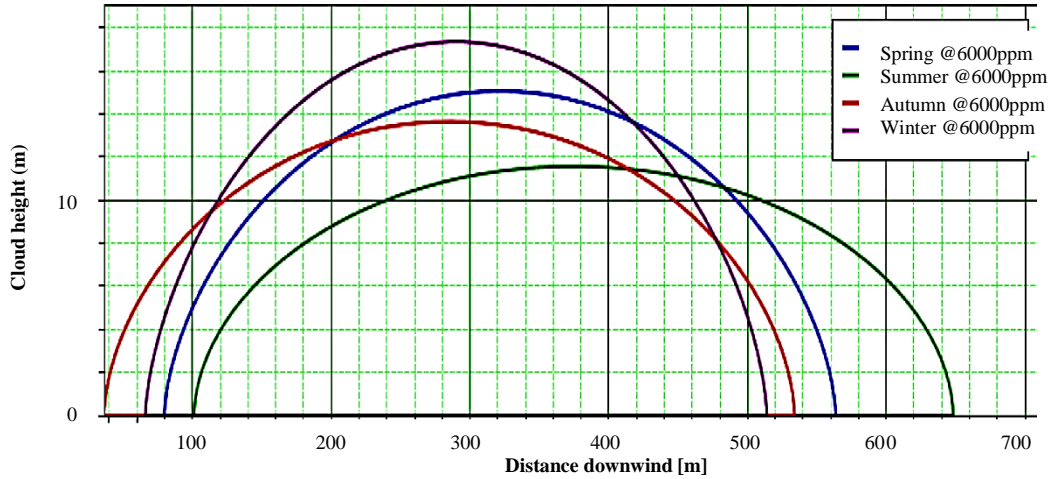
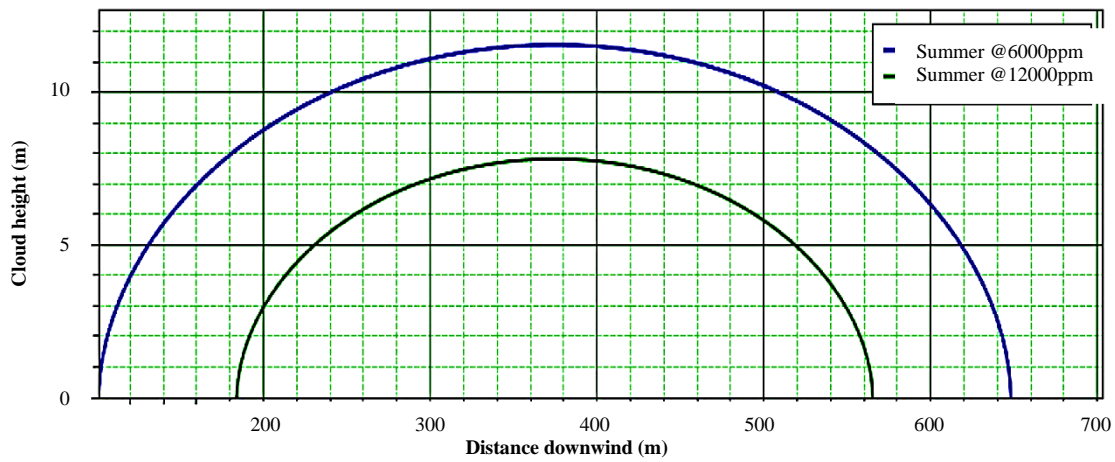**Figure 4.** Side view (cloud height vs. distance downwind)at averaging time: flammable 18.75 s

Figure 5. Side view (cloud height vs. distance downwind in summer)

Figure 6 shows the gas cloud density based on the distance between the direction of wind and the height of the cloud created from the side view in the presence of the wall and various weather conditions. As shown in Figure 6, in the worst cloud conditions, the cloud rises at a concentration of 6,000 ppm to a height of 13 meters. It has risen to 11.5 meters in similar conditions without walls; and as we know, increasing the height of the gas cloud will reducing the amount of concentration reached to a desired point. Haghnazarloo et al. reported that the cloud with a toluene concentration of 6000 ppm rises to a height of 9 meters in the same scenario [1].
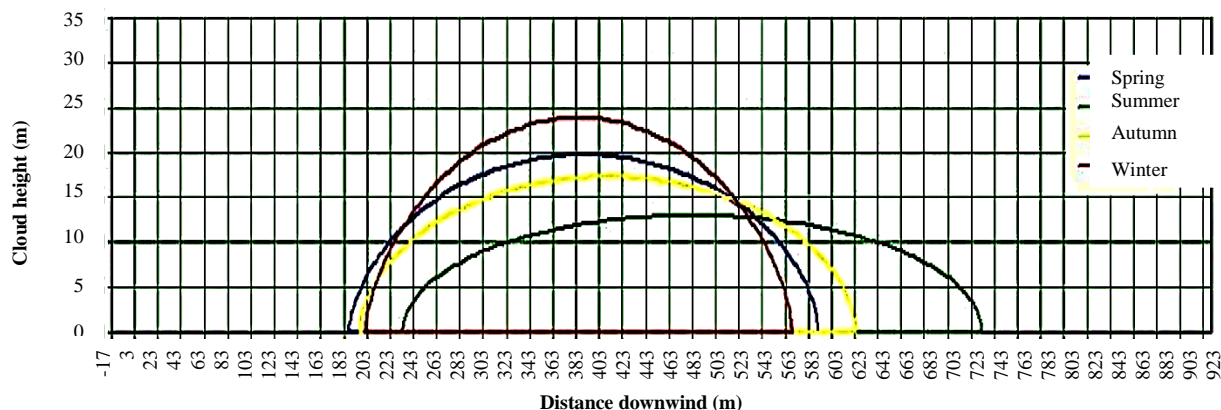
Figure 6. Side view (cloud height vs. distance downwind with bund wall) at averaging time: flammable 18.75 s

Figure 7 shows the radiation levels of the explosion in terms of distance in various weather conditions in a non-wall state. In Figure 7, the blue curve represents the region under pressure of 0.02 bar.

Due to the shock wave propagation during explosion, the structures and people can receive various damages. The damages on structures can be analyzed using the overpressure duration. The safe duration for positive pressure phase is predicted between 10 to 250 milliseconds, which markedly affected by same over pressure. From Figure 7 and Table 1, it can be observed that a compressive wave of 0.02 bar up to a distance of 2,450m causes the glass to break. The equivalent radius of serious injury by the DMEA-equivalent explosion model was 12m (overpressure = 0.69 bar) and the equivalent radius of foundation displacement of structure buildings was 112m (overpressure = 0.207 bar). By considering the personnel pulmonary hemorrhage as the equivalent value, the minor injury radius equivalent to the rupture of eardrum was equal to 215m (overpressure = 0.166 bar).

Figure 8 shows the radiation levels due to the explosion in the presence of the wall in terms of distance, influenced by a compressive wave pressure of 0.02 bar. This figure shows that, up to a distance of about 1860 meters from the site of the explosion, a compressive wave with an intensity of 0.02 bars is effective, which is lower than the non-wall state. Parvini and Gharagouzlou reported the hydrogen explosion radius in consequence modeling of the gas leak for buried gas pipelines [15]. They showed that the long spacing of the explosions might affect distance downwind. The highest radius was obtained on the overpressure of 0.02 bar and 0.13 bar involving a radius of 6.4 m and 1.6 m from dispersion zone, respectively.
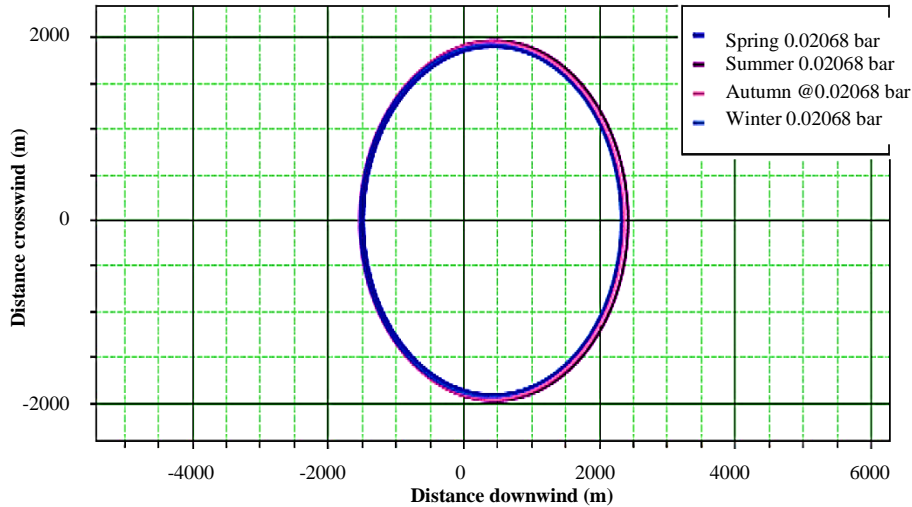
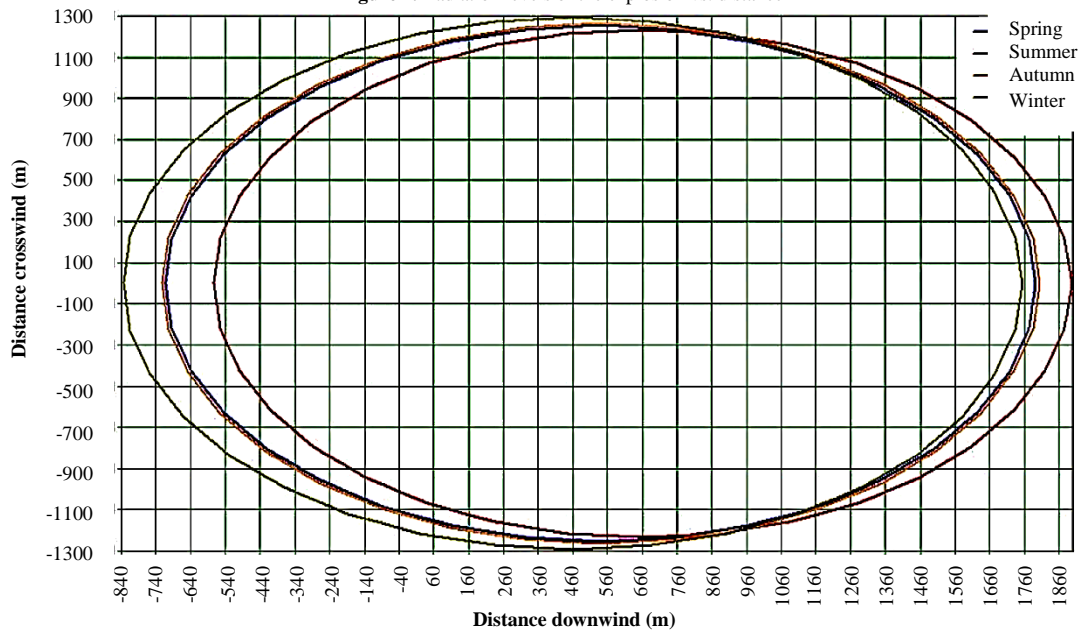**Figure 7.** Radiation levels of the explosion vs. distance

Figure 8. Radiation levels of the explosion vs. distance with bund wall

According to the results of this study, to prevent and manage accidents, some parameters such as safety education, safety awareness, and emergency skills should be considered as long-term risk control measures. The most effective prevention method is controlling any risk that may lead to an accident.

(1) The sealing system validity of a DMEA storage tank should be guaranteed. The sealing oil quality should be monitored regularly, and any undesired sealing oil should be replaced to prevent leakage. Furthermore, an alarm should be investigated to eliminate the risk of any accident.

(2) In the explosive risk, the area should be equipped by electrical instruments meeting the requirements of being at the explosion-proof level.

CONCLUSIONS

In this work, the consequence assessment of MDEA tank rupture has been studied to achieve an area with possibility of occurrence and spread of fire and explosion. Distances downwind of gas clouds in LFL conditions in real and with bund wall were determined as 850m and 780m, respectively. The maximum gas cloud concentration in 15 seconds was 207,000 ppm, which decreased to 30,000 ppm

in 40 seconds in the presence of the wall. Moreover, the maximum distance affected by the explosion wave 0.02 bar was 2,450m would break the window glass, reduced to 1860 meters with bund wall to secure the urban areas around the refinery.

The following recommendations can be used to prevent this type of accidents:

- Installing bund wall around the tanks containing MDEA
- Regular inspecting of the tank to prevent corrosion and erosion
- Installing sparkle enclosure in a secure location with safe distance from the equipment and tanks
- Considering minimum safety distance between equipment and storage tanks
- Regular inspecting for the power plant and power system shield of the site

ACKNOWLEDGEMENTS

Conflict of Interests

The authors declare no conflict of interest.

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