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Consequence analysis for catastrophic explosion of solvent storage tank – A case study

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Abstract: Chemical plants, in particular, Solvent plants are potential threat to the environment safety and pollution. Research work on the safety measures studies has nowadays taken its whole new level as several precautionary measures have been taken while installing a plant. However, few plants are very prone to accidents thus causing damage to the environment by means of pollution and environmental contamination. In this investigation, the catastrophic failures of solvent plants have been studied using models and calculations have been made on the explosion of butanol storage tank.
Keywords: explosion; catastrophe; phosphoryl chloride; chemical plant;

1. Introduction

To study the effects, a sample chemical plant was chosen where Tributyl Phosphate plant (TBP) was synthesized for recovery of heavy metals. This plant uses N- Butanol and Phosphorus Oxy chloride in Storage Tanks as Tri-Butyl Phosphate facility at Solvent extraction plant is very important [1]. Moreover, TBP has other applications in the chemical industry. It is used for recovery of rare metal like Molybdenum or Uranium from nuclear industry by solvent extraction method. The entire TBP production facility consists of different units like reactors, storage tanks apart from control rooms. In this investigation, the catastrophic failures of solvent plants have been studied using models.

Consequence analysis is a necessary step for risk management. It covers rate of release in line with source models, calculation of concentration profiles (mg/m^3), heavy gas dispersion for the gases which are having density more than air, however for the lighter gases because of buoyancy of air it dilutes and disperses and subsequently the lighter gas goes to the top atmosphere. This phenomenon can be modelled using Gaussian Dispersion theory. Several authors worked on consequence analysis either using some software or carried out some case study. However very few literature is available on consequence analysis of both toxic and flammable substance using fundamental principles. Rigas et.al [4] studied different kind of explosive substances and various fire and explosion models were used to arrive thermal heat flux and subsequent damage. Thoman et.al [5] developed a code named “EPI code” to estimate the air borne concentration of chemical and results were validated using ALOHA software results. Reiners et.al [6] studied safety management aspects for different cluster of chemical industries and specific petrochemical industries. There is no literature available on consequence analysis of Phosphorous Oxy chloride and Butanol in a Tri-Butyl Phosphate Synthesis Plant.

Objective of this work is to carry out consequence analysis of solvent facility especially on its N-Butanol and Phosphorus Oxy Chloride Storage Tanks. Lower flammable limit (LFL) and Upper Flammable Limit (UFL) concentration determination is very important due to release from storage tanks that carries huge inventory which can pose potential threat of Vapor Cloud explosion in presence of ignition sources. Similarly, toxic concentration determination of $POCl_3$ is very important as above threshold limit value (TLV) may give rise to harmful health effect/fatality in excess concentration. TBP plant is a solvent synthesis plant used esterification process which has both raw material toxic and flammable. TBP is normally used to extract valuable metal or heavy metal from dilute aqueous solution.

2. Methodology of Consequence Analysis

Fire Model is used to estimate the thermal heat flux and effect model is used to predict possible injury / fatality due to postulated solvent fire.

Thermal heat flux due to Boiling Liquid Expanding Vapor Explosion (BLEVE) is estimated using following empirical formulaes

Peak fireball diameter (m), $D_{max} = 6.48\ M^{0.325}$ (1)
Fireball duration (s), $t_{BLEVE} = 0.825\ M^{0.26}$ (2)
Center height of fireball (m), $H_{BLEVE} = 0.75\ D_{max}$ (3)
Initial ground level hemisphere diameter (m), $D_{initial} = 1.3\ D_{max}$ (4)
Where, M = initial mass of flammable liquid (kg).

The initial diameter is used to describe the short duration initial ground level hemispherical flaming-volume before buoyancy forces lift it to a semi-steady height. The radiation received by a target (for the duration of the BLEVE incident) is given by

$$Q_R = \tau E F_{21} \tag{5}$$

Where, Q_R = radiation received by a black body target (kW/m2) τ = transmissivity (dimensionless); E = surface emitted flux (kW/m2); F21= view factor (dimensionless). The correlation formula for correction in transmissivity that accounts for humidity is:

$$\tau = 2.02(P_w x)^{-0.09} \tag{6}$$

Where, P_w= water partial pressure (Pascals, N/m^2); x = path length, distance from flame surface to target (m). Thermal heat flux can be calculated using Equation (7)

$$E = \frac{F_{rad} M H_c}{\pi (D_{max})^2 t_{BLEVE}} \tag{7}$$

$$F_{21} = D^2/4r^2 \tag{8}$$

Where, F_{21}= view factor between sphere and target surface; D = sphere diameter (m); r = distance from sphere center to target along the ground (m)

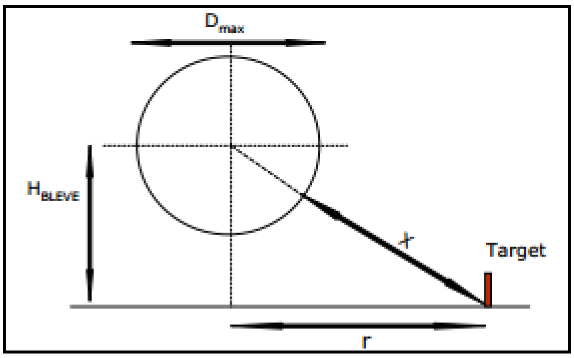

Fig1: BLEVE Schematic

The toxic/thermal effect of any chemical accident can be derived using effect following model

$$Y = k_1 + k_2 \ln V \tag{9}$$

Where, Y is probit (Probability Unit) and k1 and k2 are probit parameters for specific chemicals as shown in table 1. From the probit values, the percentage fatality can be calculated using probit correlation of error function.

3.0 Catastrophic case

3.1 Scenario: Catastrophic failure of$POCl_3$ Drum

Facilities at the Plant

Chemical: $POCl_3$
Inventory: Cylindrical drum, 200 kg

Ambient conditions

There is no flash point evaporation as boiling temperature is much greater than the surrounding temperature. The calculation for CEI and HD follows as:

Chemical Exposure Index (CEI) Calculation:

Phosphorus Oxy Chloride is very much toxic in nature and chemical exposure index was calculated to evaluate its hazard distance.

Around a concentric distance of 600 m the plant is unsafe after the catastrophic leakage of toxic Phosphorus Oxychloride. Hence, all other units like administrative and control rooms must be located accordingly.

$W_T = 200$ Kg $\quad F_V = 0$ as $T_B > T_S$
$\rho = 1645$ Kg/m^3 of $POCl_3$

Area of pool formed:

$$A_P = 100 * \frac{W_P}{\rho_1} = 100 * \frac{200}{1645} = 12.15 \text{ m}^2$$

Airborne Quantity:

$$AQ_P = 9 \text{ X } 10^{-4} A^{0.95} \frac{(MW)P_V}{(T+273)} = 9 \text{ X } 10^{-4} 12.15^{0.95} \frac{(153.33)(5.3)}{298}$$

$$CEI = 655.1 \left(\frac{AQ}{ERPG-2}\right)^{\frac{1}{2}}$$

For ERPG-2 value:

$$ERPG\text{-}2 = \left(\frac{ppm \times MW}{24.4}\right) = \left(\frac{0.479 \times 153.33}{24.4}\right) = 3.01 \text{ mg/m}^3$$

$$\therefore CEI = 655.1 \left(\frac{AQ}{ERPG-2}\right)^{\frac{1}{2}} = 655.1 \left(\frac{0.026}{3.01}\right)^{\frac{1}{2}} = 60.8$$

$$\text{Hazard Distance, HD} = 10 \times \text{CEI} = 608 \text{ m}$$

Flux calculation for N-Butanol fire:

Thermal Flux calculation for 50 % fatality from N-Butanol Main storage tank fire

Assumptions

Fatality = 50% (Probit 0.5 considered)
Exposure time:
a) 10 s
b) 100s

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a) 10 s
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$$Y = -14.9 + 2.56 \ln\left(\frac{10 I^{\frac{4}{3}}}{10000}\right)$$

a) For t=10 s,

I = 59.46 ≈ 60 kW/m² < 85.16 kW/m² (threshold)

b) For t=100 s

I = 10.76 ≈ 11 kW/m²

The exposure time used here in calculation of thermal flux show that the intensity of heat radiation is much lower than the first degree of burn. Hence a safer environment in case of N-Butanol fire explosion exists.

3.2 Bleve Calculation For n-Butanol Main storage tank

Calculation of the fireball diameter, time of duration of fireball and height of the centre of the fireball from the ground for N-Butanol [2]

Inventory: N-Butanol Main storage tank (60 kL)
Height: 8.9 m
Assumption: Cylindrical tank with liquid is filled up to 90 % of the maximum height.
Mass of Butanol released in catastrophic case = $810 \times 0.9 \times 60 \times 1000 \times 1000$
= 43.74 k Kg

$$t_{BLEVE} = 2.6 m^{\frac{1}{6}} = 2.6 \times (43740)^{\frac{1}{6}}$$

$$D_{\max} = 5.8 (43740)^{\frac{1}{3}} = 204.35$$

$$H_{BLEVE} = 0.75 D_{\max} = 153.26$$

Receptor distance = $\left(153.26^2 + (7.08 + 50)^2\right)^{\frac{1}{2}} = 163.5m$

3.3 Thermal POOL FIRE Calculation For n-Butanol Main storage tank failure

Radiation calculation from a burning pool:

Inventory: N-Butanol main storage tank (60 kL)
Assumptions: Catastrophic leakage. Windless day with 50 % relative humidity and dyke is not provided. [3]

Liquid catch fire.
Receptor distance =50 m

Data required:

Heat of combustion of n-Butanol = −2670 kJ/mol

Heat of vaporization of n-Butanol =5.95$\times 10^5$ J/kg
T_b =391 K
Ambient temperature=298 K
Density = 810kg/m^3
Heat capacity of liquid =176.86 J/mol-K

$$\Delta H^* = \Delta H_V + \int_{T_a}^{T_b} C_p dT = 5.95\times 10^5 + \int_{298}^{391} 176.86 dT$$

$$= \frac{5.95\times 74.12\times 10^5}{1000} + (391-298)\times 176.86$$

$$= 44101 + 16448$$

$$= 60.549 \text{ kJ/mol}$$

Vertical burning rate

$$Y_{max} = 1.27\times 10^{-6}\times\frac{\Delta H_C}{\Delta H^*} \qquad = 1.27\times 10^{-6}\frac{2670}{60.546} = 56\mu m/s$$

Mass burning rate

$$MB = \rho y_{max} = 810\times 56\mu m/s$$

$$= 0.453 \text{ kg/m}^3$$

Maximum steady state pool diameter

$$D_{max} = 2\left(\frac{\dot{V}_L}{\pi y}\right)^{\frac{1}{2}} \text{(not used)}$$

$$= 14.17 \text{ m (catastrophic case)}$$

$$A_{pool} = 157.68 \text{ m}^2$$

$$\text{Flame height} \Rightarrow \frac{H}{D} = 42\left(\frac{m_B}{\rho\sqrt{gD}}\right)^{0.61}$$

$$\frac{H}{D} = 42\left(\frac{0.0453}{(1.2 kg/m^3)\sqrt{9.81\times 14.17}}\right)^{0.61}$$

$$\frac{H}{D} = 1.26$$

$$H = 1.26\times 14.17 = 17.9m \approx 18 \text{ m}$$

Point Source Model

$X^2 = 9^2 + (7.08+50)^2$

$X = 57.78$ m

$$F_P = \frac{1}{4\times 3.14\times x^2} = \frac{1}{4\times 3.14\times 57.78^2} = 2..38\times 10^{-5} m^{-2}$$

$$P_w = \frac{RH}{100}\exp(14.14114 - \frac{5328}{T_a}) = 1580\,Pa \text{ at } 298\text{ K}$$

$$\tau_a = 2.02\left[(1580)(57.78)\right]^{-0.09} = 0.723$$

$$E_t = \tau_a \eta m_B \Delta H_C A F_P$$

$$= 0.723\times 0.35\times 0.0453\times 2670\times 10^3$$

$$= 1.55 \text{ kJ/m}^2\text{s}$$

Solid plum model:

$$E_{av} = E_m e^{-SD} + E_S(1-e^{-SD})$$

$$= 140\ e^{(-0.12)(14.17)} + 20(1-e^{(-0.120)(14.7)})\text{kW/m}^2$$

$$= 25.698 + 16.328 \approx 42.026$$

$$\tau_a = 2.02(1580\times 50)^{-0.09} = 0.732$$

$$\frac{X}{R} = 8.06\ ,\quad \frac{H}{R} = 2.52$$

F_{12} =0.015

$E_r = \tau_a E_{AV} F_{21}$

= 0.732×42.026×0.015=0.461 kW/m^2

Butanol dispersion calculation - Dispersion Model

Calculation of maximum concentration after dispersion from pool using Gaussian distribution
Assumptions:
Release height =0.3 m
Wind speed (10 m from ground) = 4.9 m/s
TLV = 61 mg/m3
For $x = 100m$
Concentrations of butanol vapour calaculated:

$$C(x,y,z) = \frac{G}{2\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma y}\right)^2\right]\left[\exp\left(-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right)\right]$$

U = 4.9 m/s H=0.3m

$$C_{\max} = \frac{2G}{\pi u H^2}\left(\frac{\sigma_z}{\sigma_y}\right)$$

$$= \frac{2\times 0.0136}{3.14\times 4.9\times 0.3^2}\times\frac{0.2x}{0.22x+(1+0.0004x)^{\frac{-1}{2}}}$$

$$C_{\max} = \frac{G}{\pi\sigma_y\sigma_z u}$$

$$C_{\max} = \frac{0.0136}{3.14.\times 22x\times(1+0.4x)^{\frac{-1}{2}}\times 0.2x\times 4.9}$$

$= 2.04\times 10^{-6}\, kg/m^3$

$= 0.002\, kg/m^3$

TLV for n-Butanol = 61 mg/m3

$$61\times 10^{-6} = \frac{0.0136}{3.14.\times 22x\times(1+0.0004x)^{\frac{-1}{2}}\times 0.2x\times 4.9}$$

Safe distance

$x = 18m$

Conclusion

Consequence analysis of a solvent synthesis plant has been analyzed for safety and studied using models. In this case, catastrophic failure of $POCl_3$ drum has been studied and the hazard distance has been calculated using chemical exposure index found to be 608 m. Similarly, thermal flux calculation for 50 % fatality from n-butanol main storage tank fire proved a safer environment exists for the explosion. Likewise, thermal pool fire calculation for n-butanol main storage tank failure also calculated using solid plum and dispersion model.

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