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Consequence analysis for simulation of hazardous chemicals release using ALOHA software

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Abstract: Consequence analysis for simulation of hazardous chemicals using ALOHA has been evaluated in the present investigation. With the help of ALOHA, the PHAST results of the butanol main storage tank and source strength for butanol release have been obtained. From the scenario analyzed for Consequence analysis for n –Butanol Main storage tank 2" leakage for duration of 1hr the comparison between PHAST (Process Hazard Analysis Software Tool) and ALOHA (Arial Location Hazardous Atmosphere) suggest that PHAST results are more realistic as it predicted actual scenario based on the real inputs.
Keywords: simulation, hazardous chemicals release, ALOHA software.

1. Introduction:

ALOHA (Arial Location Hazardous Atmosphere) 5.0 allow the user a choice of several accident scenarios, then uses an appropriate source algorithm to inject material into the air over a limited time [1]. The source emission time may vary between limits of one minute to one hour. A flat, homogeneous earth is assumed. For purposes of solar radiation and day/night decisions, time is fixed at the moment the leak begins. In this study, simulation of hazardous chemical release using ALOHA 5.0 software has been carried out.

2. Methods

ALOHA 5.0 provides for the following source options

Direct

The user selects this option when dealing with an (a) instantaneous or (b) continuous release of material from a point source.

Puddle

This option is selected when the source is a liquid puddle of constant radius. The liquid can be either (a) normal evaporating liquid, or (b) boiling (includes cryogenic LNG).

Tank

This option is selected when the source is a horizontal or vertical cylinder, or a spherical tank at ground level with a single hole. The tank initially contains a gas, a liquid, or a liquefied gas. The contents can change phase as a result of temperature and/or pressure changes.

Pipe

This option is selected when the source is a pressurized pipe containing gas with a single hole at ground level.

Direct

Direct injection of a gas is the simplest of all algorithms, and the most hypothetical. The direct source is a point release and can be either a continuous emission of rate Q (kgs-I) or an instantaneous release of total mass, *M* (kg).

The following data must be provided for a direct release: (a) type: instantaneous or continuous release, (b) total mass, M, or the mass flow rate, Q, and (c) source height.

For tanks and pipes the hole height is assumed to be close enough to the ground that for dispersion algorithms, considering the ground-release equations.

PHAST

We have carried out simulation of hazardous chemical release using Process Hazard Analysis software tools PHAST 6.6 software. Using the PHAST it is possible to analyse more detailed scenario study and specific analysis is possible.

3.0 Consequence Analysis Model

Source model are used to compute discharge rate (kg/s) and dispersion model are used to estimate air borne concentration (ppm or mg/m^3). Finally, fire and explosion model are used to compute thermal heat flux calculation. Liquid release rate from a storage tank can be calculated using fluid mechanics formulaes.

Discharge of pure (i.e. non-flashing) liquids through a sharp-edged orifice /nozzle is given by Equation (1)

$$G_L = C_d A \rho_l \left(\frac{2(p - p_a)}{\rho_l} + 2gH \right)^{1/2} \tag{1}$$

Where, G_L= liquid mass emission rate (kg/s); C_d= discharge coefficient (dimensionless); A= discharge holoe area (m^2); ρ_l= liquid density (kg/m^3); p = liquid storage pressure (N/m^2 absolute); p_a = downstream (ambient) pressure (N/m^2 absolute); g = acceleration of gravity (9.81 m/s^2); H = height of liquid above hole (m)

Flash fraction from a superheated liquid can be calculated using Equation (2)

$$F_V = C_p \Delta T / H_{vap} \qquad \Delta T = (T - T_b)\ ^oK \tag{2}$$

Where T is process line/vessel temperature and T_b is normal boiling point temperature, H_{vap} is the heat of vaporization at normal pressure.

Air Borne concentration of a chemical due to Dispersion from a continuous release source using Gaussian Dispersion Model using Equation (3)

$$C(x,y,z) = \frac{G}{2\sigma_y \sigma_z u} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma y}\right)^2 \right] \left[\exp\left(-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2 \right) + \exp\left(-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2 \right) \right] \tag{3}$$

Where x,y,z = distance from source, m (x = downwind, y = crosswind, z = vertical) c = concentration (kg/m^3) at location x, y, z; G= vapour emission rate (kg/s); H = height of source above ground level plus plume rise (m); σ_y, σ_z = dispersion coefficients (m), function of distance downwind; u = wind velocity (m/s)

3. Result and Discussion

PHAST Results for Butanol Main Storage Tank through Release 2” hole

Assumption Weather criteria: Stability Class D , wind velocity 4.9m/s , Temp 30 deg C

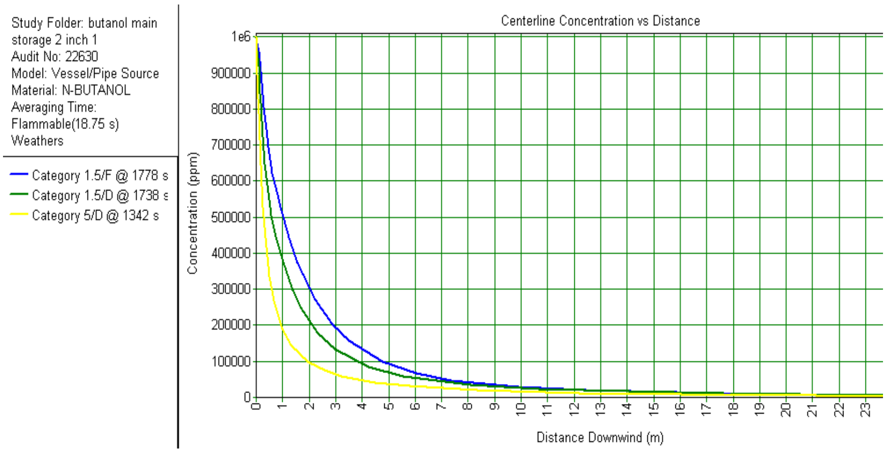


Figure 1: Centre Line Concentration of Butanol Vapour vs. distance

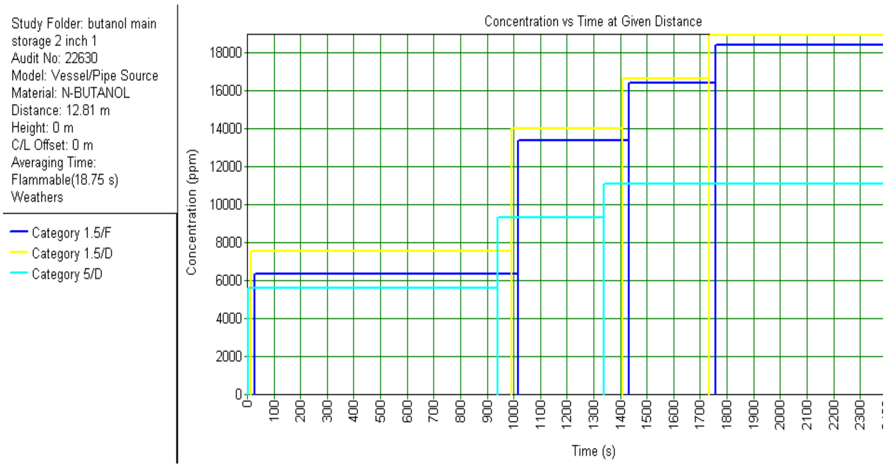


Figure 2: Concentration of Butanol Vapour Vs. Time at a given distance

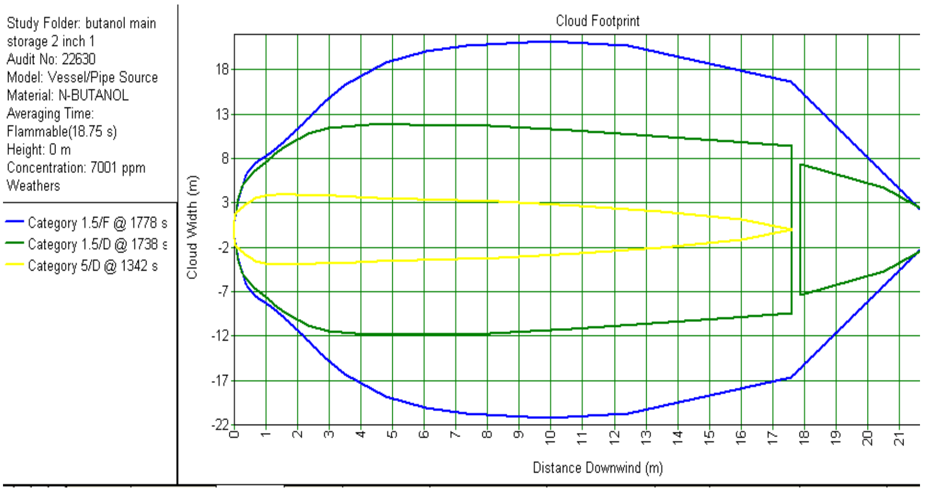


Figure 3: Butanol Vapour Cloud footprint

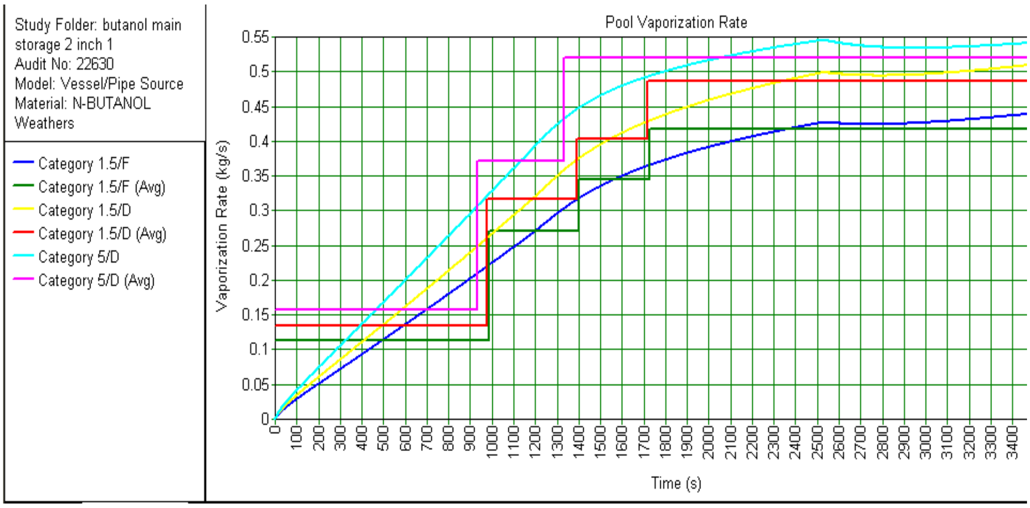


Figure 4: Butanol release and pool evaporation

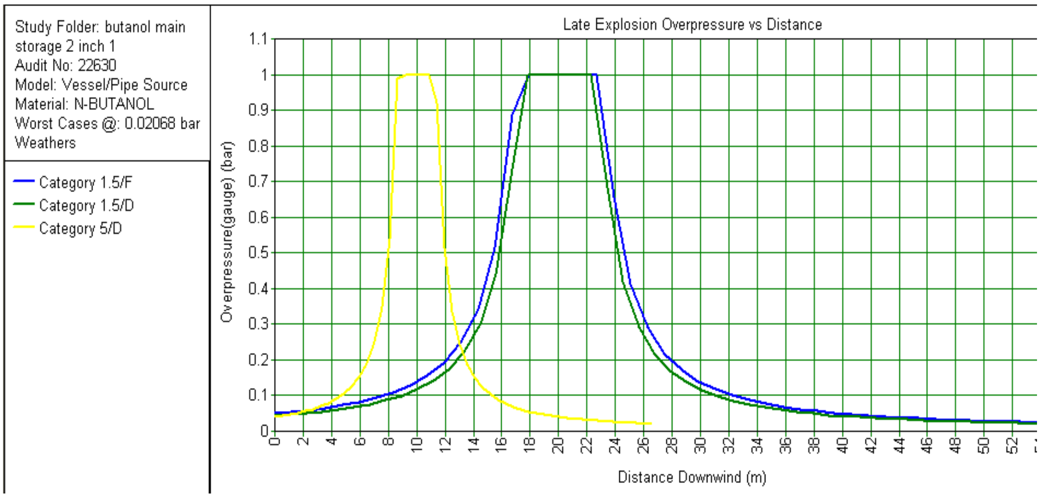


Figure 5: Butanol release and Explosion over pressure

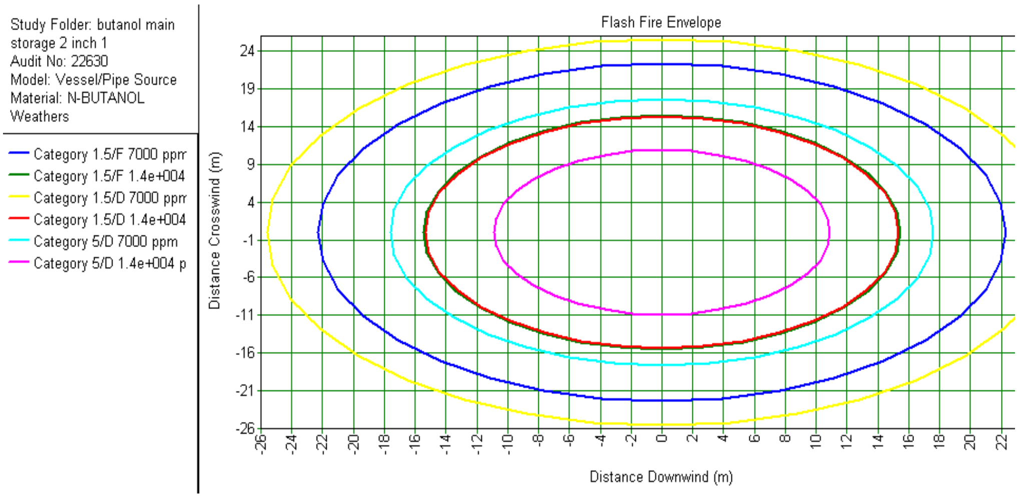


Figure 6: Butanol release and Flash fire Scenario

ALOHA Results for Butanol Main Storage Tank through Release 2" hole Assumption Weather criteria: Stability Class D, wind velocity 4.9m/s, Temp 30 °C

ALOHA considers 60 minutes releases and release scenario is shown below

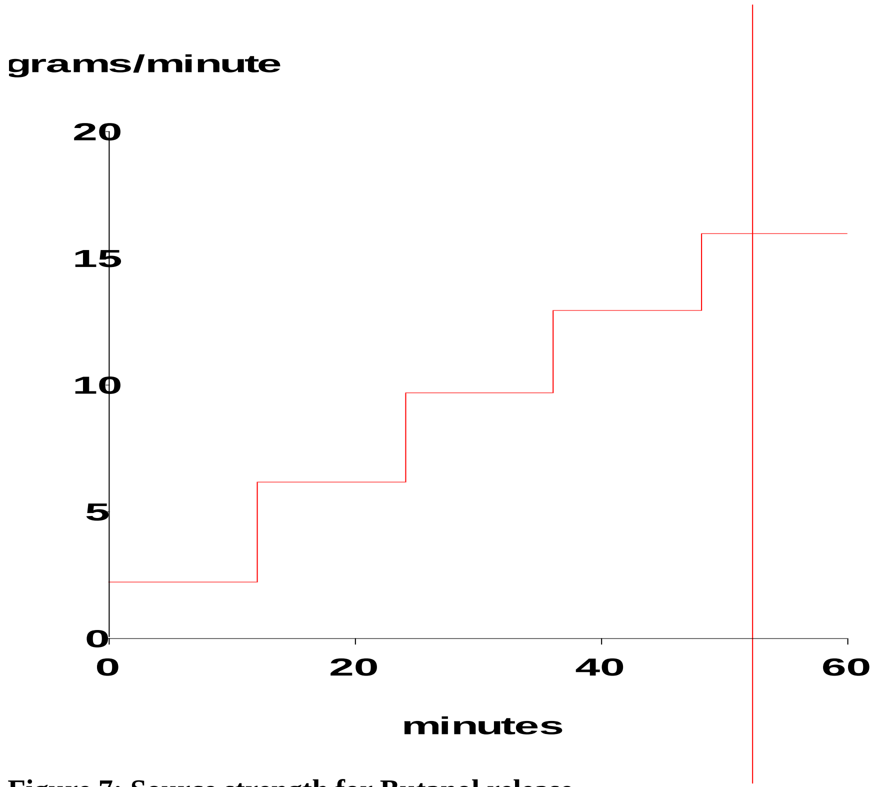


Figure 7: Source strength for Butanol release

ALOHA Results for Butanol Vapour Cloud

Threat Modeled: Flammable Area of Vapor Cloud
Model Run: Gaussian
Red : 19 meters --- (112000 ppm)
Note: Threat zone was not drawn because effects of near-field patchiness make dispersion predictions less reliable for short distances.
Orange: 19 meters --- (14000 ppm = LEL)
Note: Threat zone was not drawn because effects of near-field patchiness make dispersion predictions less reliable for short distances.
Yellow: 19 meters --- (7000 ppm)
Note: Threat zone was not drawn because effects of near-field patchiness make dispersion predictions less reliable for short distances.

From the scenario analyzed for Consequence analysis for n –Butanol Main storage tank 2" leakage for duration of 1hr the comparison between PHAST and ALOHA are given below.

Table 1: Comparison of ALOHA and PHAST simulated results
Scenario: Main Butanol Storage tank 2 inch leakage.

Distance to concentration results

Concentration(ppm)	PHAST	ALOHA
UFL= 112000 ppm	1.77 m	Less than 19 m
LFL= 14000 ppm	10.90 m	Less than 19m
LFL frac = 7000 ppm	17.616	Less than 19 m

Distance to overpressure results

Overpressure	PHAST	ALOHA
0.02068	26.559 m	-
0.1379	14.28 m	-
0.2068	13.31 m	-

From the above analysis results it is understood that PHAST results are more realistic because it can predict actual scenario based on the real inputs [2]. Whereas ALOHA software is very easy to run and require very less inputs and therefore it assumptions are sometime deviate from practical scenarios. Though effect distance are more or less in similar range +/- 10%, which is acceptable. However using PHAST we can not only simulate Flash fire but also it is possible to simulate other scenarios such as pool fire, jet fire BLEVE etc. During training period also we have learnt to derive thermal heat flux, explosion overpressure calculation etc. the results of which found matches with the simulated results using PHAST.

Consequence Analysis Results of Chlorine leakage

In the Fuel fabrication Plant, Chlorine leakage from Tonner is considered the most probable scenario. Simulated results using PHAST of above postulated scenario for chlorine vapor release from 15 mm hole are shown below.

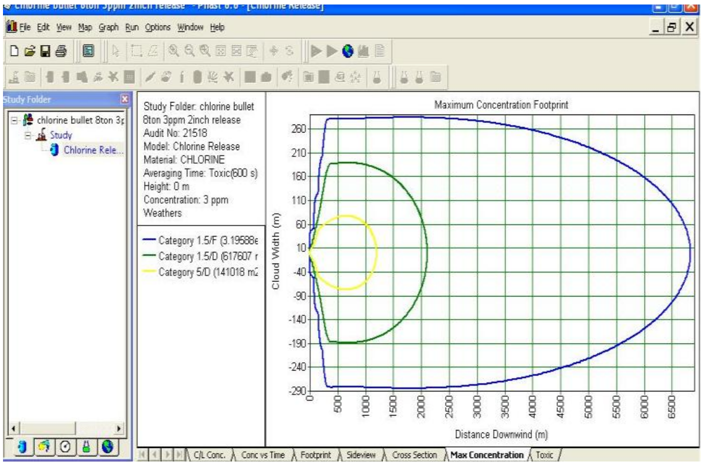
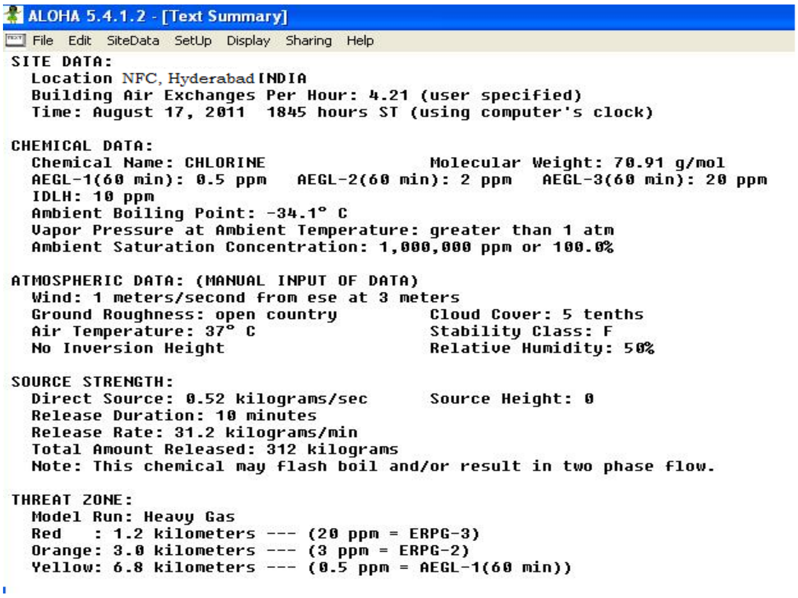


Figure. 8 ppm chlorine concentration at different downwind and cross-wind directions for D and F stability classes for different wind velocities in PHAST

Data input given in ALOHA:



ALOHA 5.4.1.2 - [Text Summary]

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SITE DATA:
   Location NFC, Hyderabad INDIA
   Building Air Exchanges Per Hour: 4.21 (user specified)
   Time: August 17, 2011  1845 hours ST (using computer's clock)

CHEMICAL DATA:
   Chemical Name: CHLORINE                 Molecular Weight: 70.91 g/mol
   AEGL-1(60 min): 0.5 ppm   AEGL-2(60 min): 2 ppm   AEGL-3(60 min): 20 ppm
   IDLH: 10 ppm
   Ambient Boiling Point: -34.1° C
   Vapor Pressure at Ambient Temperature: greater than 1 atm
   Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)
   Wind: 1 meters/second from ese at 3 meters
   Ground Roughness: open country          Cloud Cover: 5 tenths
   Air Temperature: 37° C                  Stability Class: F
   No Inversion Height                     Relative Humidity: 50%

SOURCE STRENGTH:
   Direct Source: 0.52 kilograms/sec       Source Height: 0
   Release Duration: 10 minutes
   Release Rate: 31.2 kilograms/min
   Total Amount Released: 312 kilograms
   Note: This chemical may flash boil and/or result in two phase flow.

THREAT ZONE:
   Model Run: Heavy Gas
   Red   : 1.2 kilometers --- (20 ppm = ERPG-3)
   Orange: 3.0 kilometers --- (3 ppm = ERPG-2)
   Yellow: 6.8 kilometers --- (0.5 ppm = AEGL-1(60 min))
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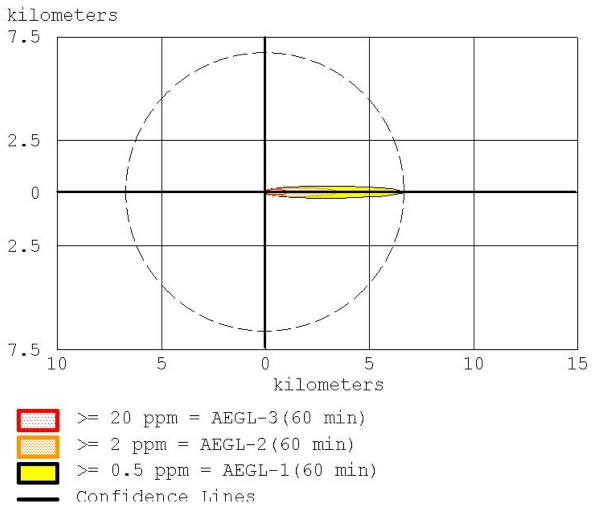

Figure. 9 ppm chlorine concentration at different downwind and cross-wind directions for D and F stability classes for different wind velocities in ALOHA

Conclusion

Case studies have been done taking different scenarios of release for both vapor and liquid leak for different orientation of storage bullet. Dike has also been designed considering different constraints. It is observed that for a 2″ leak liquid chlorine release rate is 15 times higher than that of vapor. It is also seen that vertical bullet has emptied out faster than that of horizontal one. From the DOW'S CEI calculation it is observed that liquid Ammonia is more dangerous than vapor Chlorine from toxicity point of view as per the inventory quantity and storage conditions. So, it should be handled carefully and proper emergency planning must be there.

Similarly, from the DOW'S F & EI calculation it is clear that though both LPG and Hydrogen storage facility falling in the range of intermediate degree of hazard, Hydrogen is posing more threat than LPG. So, storage facility should be properly designed (like good ventilation, separate storage area etc) and safety precautions must be there.

Chlorine vapor dispersion analytical calculations are carried out based on heavy gas dispersion model. For different ERPG values the corresponding distances are observed for various stability classes. The same situations are interpreted with software simulation. PHAST is showing more effect distances compare to ALOHA [3], because PHAST software considered more inputs on atmospheric data, geometric measures of chemical inventories; hence PHAST results are more realistic. Though hand calculation results show less effect distances due to dispersion model limitations.

BLEVE, Pool Burning and Vapor Cloud Explosion (VCE) models have been studied and thermal doses are calculated for different exposure time at different distances and finally safe distances are suggested for a particular inventory. Percentage deaths and percentage injuries are calculated for chlorine vapor dispersion taking a release scenario.

A HAZOP study has been done for vaporizer in NUOFP (O) ammonia storage yard and modification for automation of water supply to the vaporizer has been suggested.

So, future scopes are there in detail investigation for the causes of deviations in analytical results and corresponding Software results for dispersion, towards quantification of risk based on the failure data of the components of the storage facility, and in estimation of reliability of the facilities [4].

Acknowledgement:

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