Assessment of Toxic Gas Dispersion using Phast and Panache

Tejeswi Ramprasad[1], Madhavi Gaonkar[2], Diptendu Das[3]

[1] ME Research Student, Department of Chemical Engineering, Jawaharlal Nehru Engineering College, Maharashtra, India
[2] Assistant Professor, Department of Chemical Engineering, Jawaharlal Nehru Engineering College, Maharashtra, India
[3] Scientific Officer (F), Industrial Plants and Safety Division, Atomic Energy Regulatory Board, Maharashtra, India
Email id: tejeswi22@gmail.com

Abstract- Modeling of incidents which involve accidental toxic gas releases has been challenge in chemical industries from a long time. The impact of the toxic gas which is released is further aggravated by the domino effect of the chemical which is occurred due to the toxicity, flammability or the radioactivity of the chemical released. The atmospheric conditions at the time of release also play a major role in the dispersion. Hence it is necessary to estimate the effect of dispersion which will in turn help to implement safety guidelines in the plant. There have been many dispersion models which have been widely used in the past with the most primitive one being he Gaussian Plume Model. After this many models have been developed which were used to study accidental releases of chemicals specifically for heavy gases (SLAB, HEGADAS, DEGADIS)and for both light and heavy gases (PHAST, AERMOD) but the models are found to be in adequate to depict the actual scenario of the plant. Hence to enhance study the phenomenon of dispersion, Computational Fluid Dynamics Models is used which solve the Naviers Stokes Equation. In this paper, the CFD model PANACHE is used to study dispersion of a toxic chemical H_2S at two different atmospheric conditions and the results obtained are then compared with the results obtained from PHAST. The main aim is to discuss the discrepancies in the results obtained and also to determine the effect of dispersion on the buildings which are situated in the surrounding areas. This will then be formed as the guidelines for the safety of the plant.

Key Words: Dispersion, PANACHE, PHAST, Computational Fluid Dynamics

1. INTRODUCTION

Many industries dealing with chemical compounds are often prone to accidents of different kinds. The industries handle huge quantities of chemicals which may cause accidents depending upon the properties of the chemical (toxicity, flammability, corrosivity, explosivity etc.). Accidents may occur due to accidental leakage from the tanks where they are stored, release from the stacks or flares and damage during transportation of chemicals in the pipeline. Some of these errors may be caused due to human negligence also which releases large quantities of chemicals in to the environment. It is predicted that around 51% of the accidents occurring in chemical industries are caused due to toxic chemical releases [9]. In this study Hydrogen Sulphide (H_2S) gas which is predominantly toxic and also a heavy gas is chosen for assessment of consequence due to possible release scenario. The potential release of H_2S from a flare stack is considered here.

Failures of this nature can lead to dire consequences causing extensive damage to public, property and environment. Therefore it is a concern to evaluate risk by estimating consequence and probability of each scenario and accordingly risk reduction measures are taken for high risk events. The risk varies with physical property of chemical and different process condition. The risk may also vary for the same chemical used in the process in different process condition. Also many of the chemical releases have domino effects associated with them which amplifies the extent of damage caused by the release. A typical chemical plant is chosen where H_2S is used in the process. H_2S release from Chemical plants can affect adjacent plant/ public located in surrounding area. Therefore, to analyze the concentration plume of H_2S gas in the plant boundary will help emergence preparedness and follow regulatory guideline [8].

2. MAJETHODOLOGY ADOPTED

In the following case study, a process plant where hydrogen sulfide is used to manufacture heavy water by Girdler Sulfide process is considered. The typical process plant consists of a storage tank, series of 12 towers which are arranged in pairs where exchange takes place and a flare stack through which the effluents are released. The potential failure of the flare stack which results in the release of H_2S is considered as the possible scenario. This is then modelled using the CFD software PANACHE and also PHAST under two different atmospheric conditions. Thus assessing the risk associated with dispersion is to be estimated.

2.1. *The CFD model*

The Fluidyn software PANACHE is used for the real time simulation of the considered scenario. This model is specifically used for atmospheric dispersion cases [6] [7]. This model simulates the 3D wind field as well as the dispersion taking in to account all the installations which are present in the scenario [10]. This model solves the Navier Stokes equations in a Reynold's Averaged form. It includes mass, momentum and the enthalpy calculations. k-differential, k-L and k-€ models solve for turbulence and micro meteorological model is used for wind, turbulence and temperature profiles which is based on the Monin Obhukov theory [2]. The forms of governing equations which are used in PANACHE are given below [1]:

Conservation of species equation:

$$\frac{\partial(\rho y_m)}{\partial t} + \nabla(\rho U y_m) = \nabla D_m \nabla(y_m) + S_m \quad (1)$$

Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla(\rho U) = S_p \quad (2)$$

Navier Stokes equation

$$\frac{\partial(\rho U)}{\partial t} + \nabla(\rho U U) = \nabla \tau - \nabla p + S_u \quad (3)$$

2.2. *PHAST model*

PHAST can model all of the release type models (vessel type, scenario and phase of material). Discharge data can be input directly for any scenario. The procedure adopted in the consequence module of PHAST is to calculate the physical parameters of the cloud (dimensions, density, temperature, concentration, liquid fraction) at regular intervals away from the release point. At each step, the program considers both the dispersion processes and the phenomenology (instantaneous or continuous, liquid or gas), selecting the most appropriate models for each, given the current state of the cloud [5].Thus the models used for rates of entrainment and spread may change as the cloud evolves; this is done in such a way as to make the transitions as smooth as possible

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2.3. *Processing options*

In order to model the scenario and determine the effect of meteorology on the dispersion of a toxic chemical, two different atmospheric conditions are chosen [4].
The simulation options for both the cases are tabulated below:

Table 1: Simulation options for Case 1

Input data	Value
Stack height (m)	125
Stack diameter (m)	0.3
Temperature (^{0}C)	40
Wind velocity (m/s)	5
Wind direction (^{0})	315
Pressure (mb)	1000
Stability class	D
Relative humidity (%)	34
Roughness Parameter	0.45
Mass flow rate (kg/s)	0.1
Turbulence model	k-L

Table 2: Simulation options for Case 2

Input data	Value
Stack height (m)	125
Stack diameter (m)	0.3
Temperature (^{0}C)	10
Wind velocity (m/s)	2
Wind direction (^{0})	315
Pressure (mb)	1000
Stability class	F
Relative humidity (%)	15
Roughness Parameter	0.45
Mass flow rate (kg/s)	0.1
Turbulence model	k-L

3. RESULTS AND DISCUSSION

The considered scenario is simulated in PANACHE and the results obtained are then compared with those obtained in PHAST.
First, the wind field has to be stabilised for the proper run of the dispersion solver. Once the residuals are obtained in the range of 10^{-3}, the wind field is said to be stabilized [2] [3]. Once this is done, the dispersion solver is started. The geometry and meshing of the scenario are given below:

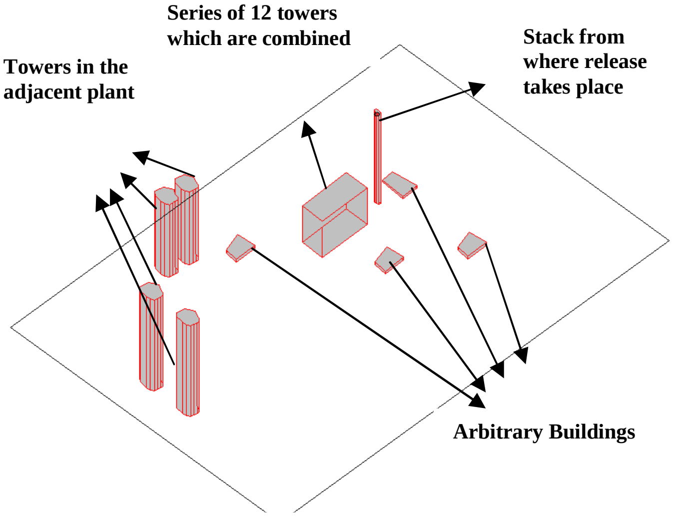

Fig 1: The geometry of the scenario

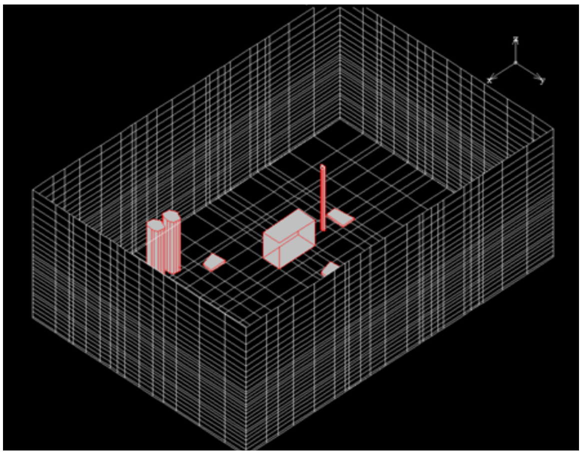

Fig 2: Meshing

The release of H_2S is at a height of 125 meters. But our area of concern is at the ground level. Hence, we need to monitor the concentration at the ground level at different downwind distances.

3.1. Stack release at D class stability

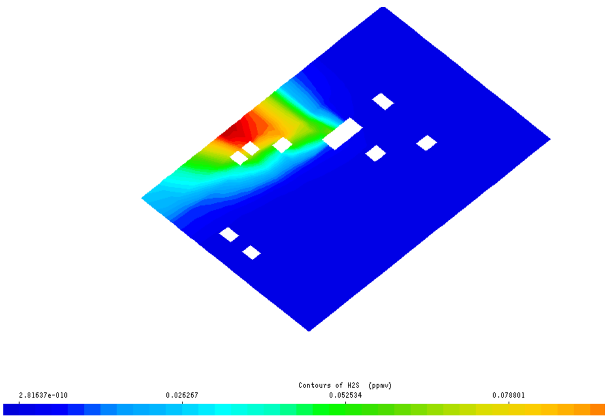

Fig 3: Ground level concentration at D class

It is seen that the maximum concentration reached at the ground level is at a distance of 50m which is 0.3 ppm as obtained from the CFD model. The concentration at the various distances is noted down and these values are then compared with the results obtained from PHAST. The results are tabulated and the graph is shown:

Table 3: Comparison between PANACHE and PHAST

Downwind distance (m)	PANACHE	PHAST
50	0.8	1.3
100	0.18	1
200	0.15	0.7
400	0.1	0.54
600	0.078	0.23
800	0.06	0.15
1000	0.055	0.1
1200	0.04	0.07
1400	0.021	0.04
1600	0.015	0.022
1800	0.01	0.016
2000	0.009	0.01

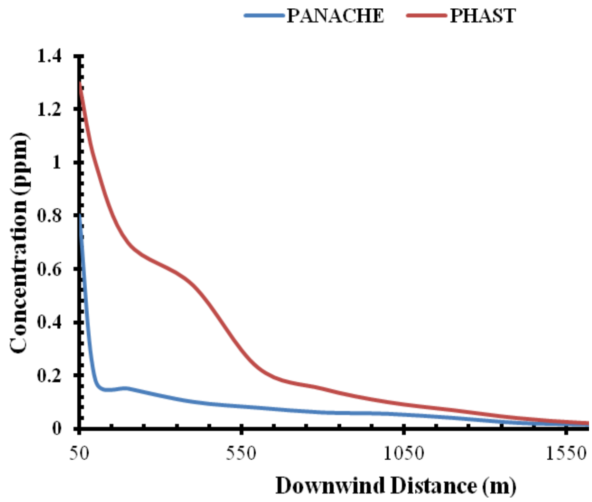

Fig 4: Comparison between PANACHE and PHAST at different downwind distance

It is observed the concentrations predicted by the PHAST model are on the higher side as compared to the CFD model and hence account for the conservative cases. The discrepancy in the results between these models is due to the fact that in PANACHE we consider the entire geometry of the plant whereas in PHAST only the system where the release occurs is considered i.e. it does not account for the effect of obstacles. Also the CFD model accounts for the turbulence which is generated to the gas dispersion in the system which is solved using the Navier Stokes equation and the turbulence models. However it is also observed that at longer distances i.e. after 1200m, the concentrations estimated by both the models is similar. This is due to the absence of obstacles after this distance.

3.2. Stack release at F class stability

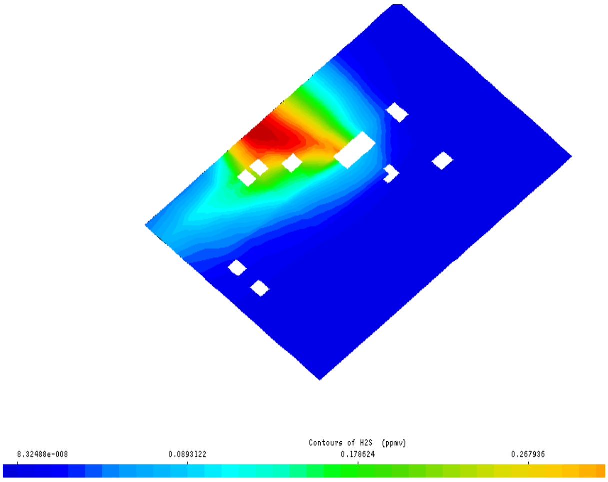

Fig 5: Ground level concentration at F class

It is seen that the maximum concentration reached at the ground level is at a distance of 50m which is 1 ppm as obtained from the CFD model. The concentration at the various distances is noted down and these values are then compared with the results obtained from PHAST. The results are tabulated and the graph is shown:

Table 3: Comparison between PANACHE and PHAST

Downwind distance (m)	PANACHE	PHAST
50	1	2.1
100	0.9	1.7
200	0.35	1.34
400	0.27	1.2
600	0.2	1
800	0.17	0.87
1000	0.15	0.75
1200	0.1	0.59
1400	0.078	0.4
1600	0.046	0.31
1800	0.021	0.22
2000	0.01	0.16

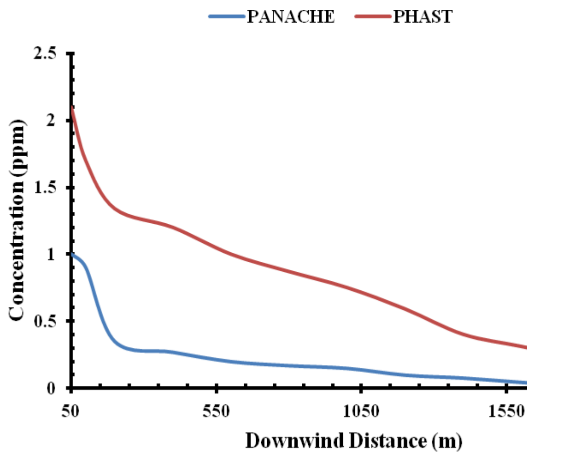

Fig 6: Comparison between PANACHE and PHAST at F class stability

The concentration profiles obtained using the two models are shown in the above graph. It can be seen from the graph that PHAST gives a higher value of H_2S concentration at the same distances as compared to the CFD model. It is due to the fact that in PANACHE, we consider the entire geometry of the plant whereas in PHAST only the system where the release occurs is considered i.e. it does not account for the effect of obstacles. Also the CFD model accounts for the turbulence which is generated to the gas dispersion in the system which is solved using the Navier Stokes equation and the turbulence models.
It is also observed that when the release of the gas when occurs at a stable condition, gives the maximum concentration at the larger distance than at neutral conditions. It can be accounted for the fact that at stable conditions, the vertical motion is restricted of the dispersed plume is restricted and therefore the plume travels much in the downwind distance giving higher concentrations at different downwind distances compared to the neutral class of stability [11].

4. CONCLUSION

From the results obtained, the following conclusions can be made for the dispersion of H_2S in this case study:
1. As compared to the dispersion at neutral conditions, the dispersion at extremely stable conditions gives higher values of concentration because of the atmospheric phenomena of restriction of vertical motion of the gas in the stable conditions. Hence, the dispersion at stable conditions is the conservative case of all.
2. The PHAST model always gives conservative result and hence it can be used to Emergency Regulatory and Response in chemical industries since it is faster compared to the CFD model.
3. Considering the worst case, the concentrations obtained at 700m where the flare stacks are present are

0.19 ppm and 0.93 ppm in D class and F class respectively. This is below the permissible limit of H_2S exposure and hence it can be said to be safe.

4. Considering the worst case, the concentrations obtained at 1200m where the flare stacks are present are 0.07 ppm and 0.59 ppm in D class and F class respectively. This is below the permissible limit of H_2S exposure and hence it can be said to be safe.

REFERENCES

[1].Bird.R.B.,Stewart.W.E.,Lightfoot.E.N.,Transport Phemnomena, John Wiley & Sons,2002

[2]. Ferziger.J.H.,Peric.M.,Computational Methods for Fluid Dynamics, Springer,2002

[3]. Fluidyn Techincal Guide.,1996

[4]. Fluidyn User and Reference Manual., 1996

[5]. Henk.W., Harper.M., Validation of Phast dispersion model for USA LNG siting applications, UKELG Discussion meeting, 2012

[6]. Hill.R.,et.al.,Field and wind tunnel evaluation of CFD model predictions of local dispersion from an area source on a complex industrial site.,Proceedings of the 11th International Conference on Harmonisation within Atmospheric dispersion models for regulatory purposes.,2007.

[7].Mazzoldi.A.,et.al., CFD and Gaussian atmospheric dispersion models., A comparison of leak from carbon di oxide transporatation and storage facilities., Atmospheric Environment.,2008

[8]. Nevers.N, Air pollution control engineering, 2nd edition, Boston: McGraw Hill, 2000

[9]. Planas-Cuchi E., Montiel H., and Casal J.,1997, A Survey of the Origin, Type and Consequences of Fire Accidents in Process Plants and in the Transportation of Hazardous Materials, Trans IChemE, 75

[10]. Tripathi,S.,Evaluation of Fluidyn PANACHE on Heavy Gas Dispersion Test Case.,Seminar on evaluation of Models of Heavy Gas Dispersion Organized by European Commission.,1994

[11]. U.S. Environmental Protection Agency, 2005, Basic Air Pollution Meteorology, Air Pollution Training Institute Course 409