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CFD Based Reproduction of Amuay Refinery Accident 2012

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Amuay refinery accident 2012 is the recent follower of similar nature accidents happened in Buncefield, UK (2005), Jaipur, India and Puerto-Rico, USA (both in 2009), respectively. The failure of a mechanical part i.e. valve or piping led to the escape of a flammable dense-than-air cloud. Approximation of size of such clouds depends on the density of the dispersed gas, atmospheric turbulence (wind, temperature and humidity), gravity and their mutual interactions. Since experimental reproduction of such accidents are not always possible numerical simulations help a lot to understand and replicate the scenarios on qualitative basis. In the present work Amuay refinery accident (2012) is reproduced with a CFD (Computational Fluid Dynamics) model which takes into account the heaviness of the gas (LPG here), wind and gravity driven spread. The extent to which the dispersed gas could travel is specified as LFL (Lower Flammability Limit) criterion. It is assumed that the running vehicles on the street across the plant were the major source of ignition.
Scenarios for different atmospheric conditions are considered and compared. For validation purposes also a reproduction of the Thorney Island Trial 26 is conducted.

1. Introduction

Industries globally still heavily rely on hydrocarbon energy resources. Therefore there is a tremendous need for exploiting, processing and storing such substances in order to ensure their global distribution. In future years the demand for energy will constantly increase (Exxon, 2015), (BP, 2015). Two of the most important hydrocarbon fuels are natural gas and petroleum gas which are usually transported and stored liquefied in cryogenic tanks. The demand of natural gas is expected to rise by 65 % in 2040 as compared to 2010 (Exxon, 2015). Due to the high flammability of liquefied natural gas (LNG) and liquefied petroleum gas (LPG) they become extremely hazardous when accidentally spilled onto land or water, if for example a leak in a pipe or vessel occurs. LPG is stored near its boiling point (propane 231 K, butane 273 K) (Mannan, 2015).
The spillage of LPG occurs in different stages. After release spilled LPG forms a pool and vaporized LPG starts dispersing. The cold LPG vapor mixes with the warmer surrounding air creating a denser-than-air cloud that is negatively buoyant thus staying at ground level. During this stage the cloud is characterized by horizontal movement where at the same time vertical turbulent mixing with the overlying air is dampened which leads to a stable stratification of the cloud (Koopman, 1989), (Havens, 1985). As the cloud propagates mixing of gas and air increases behind the cloud surface, caused by a Kelvin-Helmholtz instability (Koopman, 1989). Due to mixing the air temperature around the cloud surface remains low (Luketa-Hanlin, 2007). As mixing increases cloud temperature rises and the cloud gets dominated by atmospheric flow. In the third stage the mixture reaches ambient temperatures and the gas will dilute in the atmosphere as trace gas (Havens, 1985).
Due to the delayed dilution of the LPG vapor, LPG spills bear a significant risk as the distance between source and lower flammability limit (LFL) can be drastically increased, depending on ground structure, spill rate and atmospheric conditions (Luketa-Hanlin, 2007).
On 25th August 2012 around 1.11 AM (GMT) such spill caused a violent explosion at Punto Fijo refinery (commonly known as Amuay refinery) in northwestern Venezuela (Google Maps, 2015). It is run by the state-owned company Patróleos de Venezuala, S.A. (PDVSA) and is one of the largest refineries in the world with an output of 645,000 barrel-per-day. The refinery mainly handles crude oil, LPG and LNG. The disaster officially cost 47 lives and caused a financial damage of more than 1 $ billion. The explosion was caused by leaking flammable liquid. The specific substance that caused the explosion is still unknown though reports

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name olefins, LPG or LNG as possibilities (Petroleum World, 2015), (Global Barrel, 2015). All of them form denser-than-air vapor clouds when released in to the atmosphere. The source of the leakage was probably near a number of spherical tanks (Mishra, 2014). The cloud than propagated under wind influence and most likely was ignited by vehicles passing by on a nearby street (Mishra, 2014), (Petroleum World, 2015).
For the present investigations LPG is considered as causing substance. The aim is to investigate the potential and possibilities of computational fluid dynamics (CFD) to reproduce a possible course of events of the Amuay accident which could help identifying errors that caused the severity of events and to aid for further safety relevant measures to reduce the risk of accidents for future scenarios. Different dense gas dispersion scenarios that could have happened at the Amuay refinery are simulated. For validation of the numerical model available data on dense gas experiments was used from the Thorney Island trial series (1982-1984) (Puttock, 1985).

2. Methodology

2.1 Theoretical Background

The present simulations are carried out using the commercial software code Ansys CFX 15.0 (ANSYS, 2015). It uses the Finite Volume Method to solve the Navier-Stokes equations on a discretized computational domain. The equations are integrated over all control volumes such that mass, momentum and energy are conserved within each control volume. The obtained linearized system of equations is solved with a pressure based coupled solver.
Modeling turbulence correctly is essential for obtaining reasonable results in flow simulations, especially for cloud dispersion modeling. Turbulence is a main reason for fluid mixing in shear layers of adjacent fluid phases and is important for the spreading and dilution of gas clouds. The development of the atmospheric boundary layer in which the cloud dispersion is taking place is also influenced by turbulence (Luketa-Hanlin, 2007).
The simulations are conducted using the $k-\omega$ SST model which combines the advantages of the $k-\varepsilon$ model for flow regions outside the boundary layer and of the $k-\omega$ model for near-wall flow regions (Menter, 2003). This is achieved by the use of a blending function.

2.2 Computational Domain

The topology of the refinery has been reconstructed using images from Google Maps. The origin of the leak was reported to be located near a number of spherical tanks. The ignition source was on a nearby street (Mishra, 2014). Therefore a rectangular part of the refinery containing the location of leakage and ignition was considered as computational domain (Figure 1). The road is located at the eastern boarder of the refinery. The area contains spherical and cylindrical tanks of different sizes. The height of the tanks was estimated due to a lack of available data. The diameter was extrapolated from the available image data. Further, a grid of walls is located between a number of tanks. The total domain has a size of 750 m x 400 m x 50 m. An unstructured mesh was created using tetrahedral elements with prism layers at the ground to improve mesh quality in the boundary layer. The mesh has a total number of 775 686 cells.

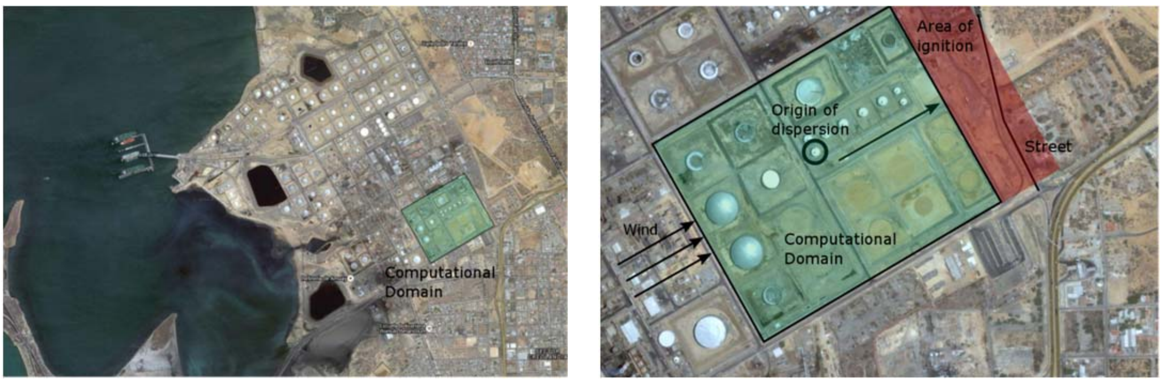

Figure 1: Satellite image of the refinery and its surroundings (Google Maps, 2015)

2.3 Boundary Conditions

At the left domain boundary an air inlet is posed to account for the influence of wind. The wind velocity shows a vertical profile that is influenced by the stability of the atmospheric boundary layer. The stability can be categorized according to the Pasquill-Gifford stability classes (A-F) where A corresponds to extremely unstable and F corresponds to stable conditions (Pasquill, 1983). The wind profile is modeled using an empirical power law

$$u(z) = u_0 \left(\frac{z}{z_0}\right)^{\lambda} \tag{1}$$

where u_0 is the velocity at reference height z_0 (10 m), λ is depending on the stability class and can be calculated with the Monin-Obukhov theory (Luketa-Hanlin, 2007). For the present test cases λ = 0.1 is chosen, which corresponds to stability class "C" (slightly unstable) (CCPS, 1999). Three different wind speeds (0.5 m/s, 2 m/s, 5 m/s) are simulated to investigate their influence on the dispersing cloud.

The dense gas probably originated from a leaking pipe or tank. The pressurized liquefied gas spilled on the ground forming a pool from which the dispersing cloud developed. For the simulation it is assumed that the pool is formed in the dike of a spherical tank. The diameter of the dike corresponds to the tank diameter of 25 m. The dike is modeled as inlet condition where LPG is injected at a mass flow rate of 0.12 kg/(m^2s) which is the boil-off rate of LPG at ambient conditions (Hyatt, 2003). A similar approach has been used in (Tauseef, 2011).

The ground surface, tanks and walls inside the domain are modeled with no-slip boundary conditions. To take into account the influence of large obstacles on the atmospheric boundary layer a surface roughness height of 1 m was assumed corresponding to large refinery sites (CCPS, 1999).

For the top boundary best results have been obtained using a free slip wall boundary condition. This allows fluid flow parallel to the top boundary but not perpendicular to the boundary such that the atmospheric boundary layer profile is preserved throughout the domain (Luketa-Hanlin, 2007). The remaining boundaries correspond to open boundaries where normal gradients of all fluid quantities are zero.

2.4 Initialization

The initial wind profile in the domain is obtained by a steady state simulation with the dense gas inlet switched off. A time step of Δt = 1s is chosen to satisfy convergence criteria of 10^{-4} for all RMS residuals. The initial turbulence intensity is related to the free stream velocity U_∞ such that

$$k \approx 10^{-4} U_\infty^2 \tag{2}$$

$$\epsilon \approx 10^{-4} U_\infty^4. \tag{3}$$

This corresponds to a turbulence intensity of 1 % (Arntzen, 1998).

3. Results and discussion

The LPG evaporates from the circular dike under the lower spherical tank with an effective pool area of A = 490.87 m^2. This yields a mass flow of $\dot{m}$ = 58.9 kg/s. For estimating the flammable distance of the cloud from the source the lower flammability limit (LFL) is used which is approx 2.2 % of volume in air for LPG (CCPS, 1999). For safety reasons a threshold of 1/2 LFL is often applied to account for the possible ignition of flammable gas pockets outside the LFL border (CCPS, 2010). As the source of ignition in the Amuay accident reportedly was at the street at the downwind domain border the time from the initial release to the first contact of the vapor cloud with the domain border indicates the minimum ignition delay time. Table 1 shows relevant parameters of the vapor cloud for all three wind speeds.

The delay time is significantly influenced by the wind speed. At 5 m/s wind speed the delay time is approx. 1/3 of the delay time at 0.5 m/s wind speed. The shape and area covered by the flammable cloud are shown in Figure 2 for all three wind speeds.

It can be observed that the gas cloud remains negatively buoyant at all times due to the density of LPG. It forms a low profile on the ground due to reduced vertical movement. Instead the kinetic energy of the cloud results in wide horizontal spreading. The presence of tanks disturbs the downwind extent of the cloud as the gas cloud needs to move around the obstacles. Additionally, gas is accumulated in front of the tanks forming a stagnation area. The presence of walls bounds the cloud expansion as gravitational force hinders flow across them such that they only can be overcome when enough gas has accumulated around them. As a consequence gas that has flown across a wall can form detached flammable pockets in its wake. At high wind speeds the cloud predominantly propagates downwind because of its increased kinetic energy, while at lower wind speeds crosswind and upwind spreading are increased. Thus the cloud is of broader shape for low wind speeds and develops a lengthy shape for high wind speeds. Due to the changing wind conditions in reality the cloud expansion can be significantly altered in time such that the ignition time delay is raised so that for continuous releases it is conceivable that an ignition is delayed for hours or even days.

Table 1: Properties of flammable cloud (LFL) for different wind speeds at the possible time of ignition

Wind speed [m/s]	Ignition delay time [s]	Cloud size [m^2]	Max. down-/upwind extend [m]	Max. crosswind extend [m]	Cloud volume [m^3]	LPG released (rel. density 2.0) [kg]
0.5	595	115,800	505	353	739,800	1,479,600
2	215	55,500	480	271	45,000	90,000
5	190	31,700	443	232	37,000	74,000

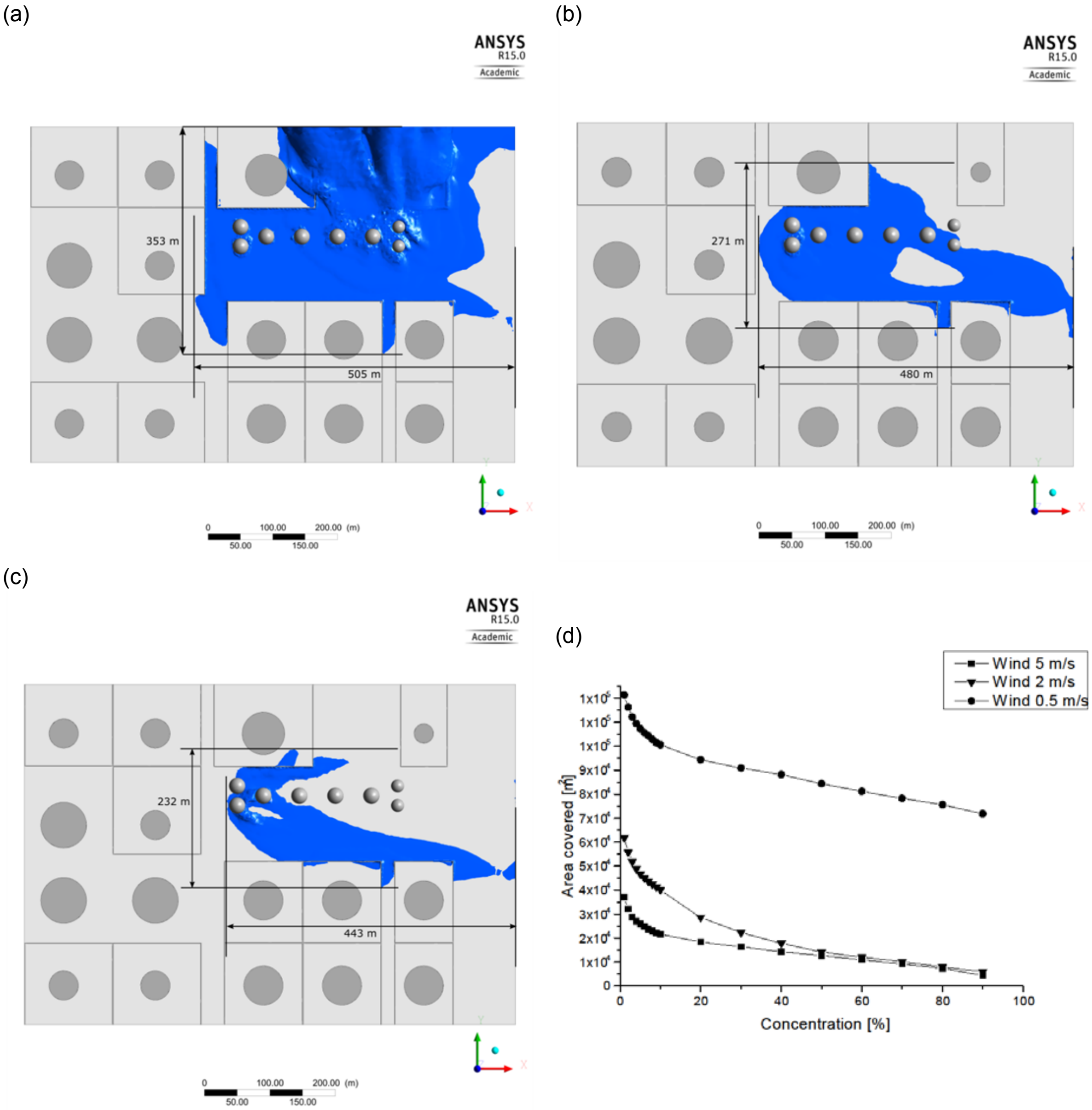

Figure 2: Area covered by flammable cloud (LFL) at the ignition delay time. Wind speed 0.5 m/s (a), 2 m/s (b), 5 m/s (d), Comparison of concentrations and area covered (d)

4. Validation

As modeling vapor cloud dispersion is a complex phenomenon that is sensitive to the correct application of the utilized models such as turbulence it is necessary to validate results to prove their plausibility. In the Thorney Island Phase II Trial No. 26 approx. 2000 m^3 of freon-12/nitrogen mixture (relative density 2.0) were

instantaneously released into the atmosphere. The gas was held inside a cylindrical tent (14 m diameter,13 m height) that was removed at the beginning of the test. The gas was left for dispersion under the influence of a cubical obstacle (9 m side length) 50 m downwind from the release point (McQuaid, 1984). The experimental findings are suitable for validating the present model as they represent both large scale dense vapor cloud dispersion and the influence of large obstacles. The simulation is conducted on a 225 m x 150 m x 50 m domain with 744,512 cells. For initialization the freon-12/nitrogen mixture is assigned to a part of the domain with the size of the experimental tent to account for an instantaneous release under ambient conditions. The wind speed is reported as u_0 = 1.9 m/s, λ = 0.07 (moderately stable) and z_0 = 0.005 m (Sklavounos, 2004).
The results are compared to experimental values at the front face of the obstacle at a height of 6.4 m (Figure 3). Additionally, Figure 4 shows the gas cloud 20 s after release. The present results are in good agreement with the experimental data. The peak concentration is 4.3 % as compared to approx. 4.84 % in the experiment. The simulation results show a slight shift of the peak value in time and small concentration fluctuations are not resolved. This is likely due to an idealization of the imposed boundary conditions. In the simulation a steady wind profile is assumed while in reality wind speed and direction are always fluctuating. Further, the modeling of turbulence introduces inaccuracies due to the averaging process. The validation study shows that the employed models are capable of accurately capturing dispersion behavior of dense gas clouds.

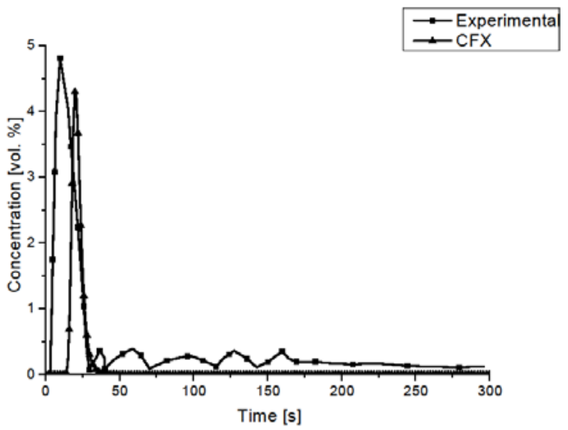

Figure 3: Comparison of simulation results and experimental values at a height of 6.4 m at the front of the obstacle (experimental data from (Sklavounos, 2004))

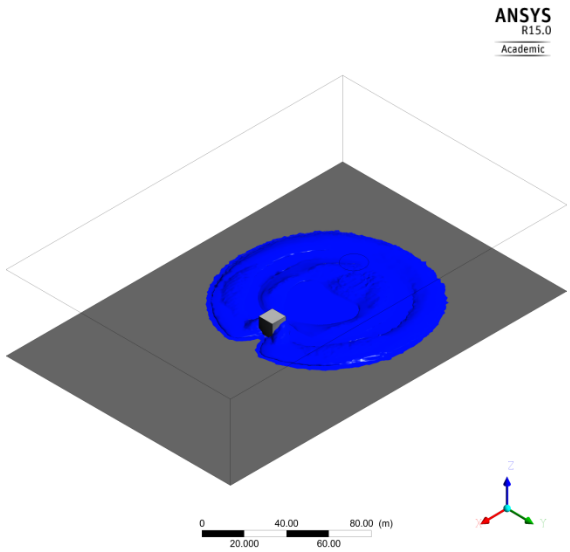

Figure 4: Gas cloud 20 s after release (isosurface 1 % vol.)

5. Conclusions

It is shown that CFD based analysis of dense gas dispersion for industrial application is capable of yielding useful results for reconstruction and prediction of possible accidental scenarios. With the choice of appropriate boundary conditions and flow physics models it is possible to capture relevant aspects of vapor cloud dispersion behavior from the dispersion source to dilution of the cloud. It is further shown that the influence of wind speed is significant to the behavior of the cloud e.g. the time from release to possible ignition can be drastically reduced with increasing wind speed. For further research two-phase modeling of the leaking fluid could be investigated to take into account pool forming and additional phase interaction between liquid and gaseous phases.

References

ANSYS, 2015, ANSYS CFX-Solver Theory Guide 15.0, ANSYS Inc.

Arntzen B.J., 1998, Modelling of turbulence and combustion for simulation of gas explosions in complex geometries, Norges teknisk-naturvitenskapelige universitet, Trondheim, Norway

BP, 2015, BP Energy Outlook 2035

CCPS (Center for Chemical Process Safety), 1999, Guidelines for Chemical Process Quantitative Risk Analysis, Wiley, Hoboken (New Jersey), U.S.

CCPS (Center for Chemical Process Safety), 2010, Guidelines for Vapor Cloud Explosion, Pressure Vessel Burst, BLEVE and Flash Fire Hazards, Wiley, Hoboken (New Jersey), U.S.

ExxonMobile, 2015, The Outlook for Energy: A View to 2040

Global Barrel, http://globalbarrel.com/2012/08/30/amuay-refinery-disaster-syrian-naphtha-chavez-petroleum-revolution-in-flames/, accessed 07.08.2015

Google Maps, https://www.google.de/maps/place/Punto+Fijo,+Venezuela/@11.7206856,-70.184632,13z/data=!4m2!3m1!1s0x8e85ed24b8524353:0x18abea72d12fd565, accessed 07.08.2015

Havens J.A., The atmospheric dispersion of heavy gases: an update, 1985, Proc. 1985 European Federation of Chemical Engineers Conf. on the Assessment and Control of Major Hazards, The Institution of Chemical, 143-164

Hyatt N., 2003, Guidelines for Process Hazards Analysis (PHA, HAZOP), Hazards Identification, and Risk Analysis, CRC-Press, Boca Raton (Florida), U.S.

Koopman, R.P., Ermak, D.L., Chan, S.T., 1989, A review of recent field tests and mathematical modelling of atmospheric dispersion of large spills of denser-than-air gases, Atmospheric Environment, 23, 731-745

Luketa-Hanlin A., Koopman R.P., Ermak D.L., 2007, On the application of computational fluid dynamics codes for liquefied natural gas dispersion, 140, 504-517

Mannan, S., 2015, Lees' Loss prevention in the process industries: Hazard identification, assessment and control, Elsevier Butterworth-Heinemann, Oxford, UK

McQuaid J., 1984, Large scale experiments on the dispersion of heavy gas clouds, Atmospheric Dispersion of Heavy Gases and Small Particles, 129-138

Menter F.R., Kuntz M., Langtry R., 2003, Ten years of industrial experience with the SST turbulence model, Turbulence, Heat and Mass Transfer, 4

Mishra K.B., Wehrstedt K.D., Krebs H., 2014, Amuay refinery disaster: The aftermaths and challenges ahead, Fuel Processing Technology, 119, 198-203

Pasquill F., Smith F.B., 1983, Atmospheric diffusion, Ellis Horwood Ltd, Hemel Hempstead, UK

Petroleum world, http://www.petroleumworld.com/storyt13091001.htm, accessed 07.08.2015

Puttock J.S., Colenbrander G.W., 1985, Thorney Island data and dispersion modeling, Journal of Hazardous Materials, 11, 381-397

Sklavounos S., Rigas F., 2004, Validation of turbulence models in heavy gas dispersion over obstacles, Journal of Hazardous Materials, 108, 9-2

Tauseef S.M., Rashtchian D., Abbasi T., Abbasi, S.A., 2011, A method for simulation of vapour cloud explosions based on computational fluid dynamics (CFD), Journal of Loss Prevention in the Process Industries, 24, 638-647