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## **Evaluation beyond a consequence-only approach: When is it really needed?**

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### **Abstract**

The basic consequence analysis is the initial step for any facility siting analysis. It turns out, however, that many studies quickly demonstrate that the impact to buildings can be more significant than what have been defined as acceptable. For such cases, the analysis unfolds a set of more sophisticated approaches that should be considered; explosion exceedance curve, quantitative risk analysis, likelihood of building failure, among others. The current paper addresses a comprehensive methodology that comprises computational fluid dynamics (CFD) technique in the early stage of the analysis without compromising the time schedule and the budget. The more accurate results obtained with CFD modelling lead to cloud sizes which are mainly less conservative than traditional methods. The benefit of the analysis lies on the fact that it may be sufficient to show an acceptably low level of risk right at the initial stage. Therefore, it may avoid extra costs associated with a more detailed quantitative analysis.

**Keywords** Computational fluid dynamics (CFD), siting, gas dispersion

### **Introduction**

The concept of facility siting studies have gradually matured in the past 20 years, whether in the perspective of problem understanding (recognizing limitation of the simplified consequence modelling approach) and the advancement of technology, which enable a more refined consequence analysis (such as Computational Fluid Dynamics-CFD) to be conducted within acceptable budget and schedule [1]. However, despite the improvement in the study or theory understanding,

traditional practice of facility siting study is usually still the preferred option for most facility owners. A typical traditional facility siting study may start with a consequence only assessment of potential fire, overpressure and toxic hazards without considering the event frequency. It is not surprising if most of these consequence based studies will eventually point out that the area of interests (such as occupied and critical buildings) design capacity is not adequate to meet the calculated hazard load [2]. In addition, any building retrofit recommendations that surface out of this consequence only assessment tend to be more costly than what the facility has budget for. Therefore, it is very common for facility owners to expand the study scope beyond the consequence only approach; for example by conducting Quantitative Risk Analysis (QRA).

There have been previous attempts to use CFD in facility siting studies. Shaikh et al. [3] have considered the application of CFD for explosion modelling addressing factors such as; obstacles, mitigation measures and DDT (Deflagration to Detonation Transition). Hansen et al. [4] have called attention to scenarios where the flammable cloud can be extrapolated beyond the battery limit, as in Buncefield accident. The authors also emphasized that DDT scenarios should not be ruled out. Therefore, one of the recommended procedures is to incorporate the CFD for explosion modelling [3,4] in the facility siting analysis.

This paper in particular highlights the importance of CFD gas dispersion modelling in estimating flammable cloud size in facility siting study in accordance with PSM, OSHA 29 CFR Part 1910.119 - Process Safety Management. The influence of the wind direction and leak direction in the cloud size is investigated. The results indicate that there is a preferable wind direction that leads to the largest cloud. The dilution of the cloud is also addressed and the results show that the increase of the ventilation does not necessary necessarily yield a smaller flammable cloud. Comparison between the flammable clouds calculated using the Integral Model and CFD shows significantly different cloud volumes. The increase of the wind speed led to different trends as far as the Integral and the CFD approaches are considered. Analysis of the results also show that the release pointing downwards led to cloud sizes about three times greater than the cloud sizes calculated when the leak direction was horizontal.

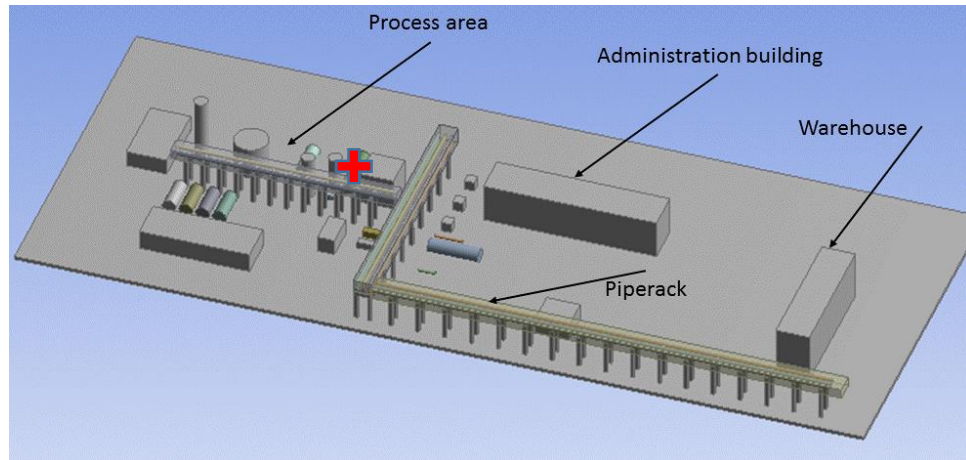
Finally, one case study is conducted using the same explosion model for two different cloud sizes. One of the cloud sizes was calculated using the Integral Model while the other cloud size was calculated via CFD technique. The outcome of the explosion modelling leads to the impairment (for a pre-established criterion) of the selected administration building when the Integral model is considered during the dispersion analysis. On the other hand, the results show no impairment of the building when the cloud volume calculated via CFD is considered.

The paper is organised as follows. In the next section the gas dispersion modelling using computational fluid dynamics and the Integral model is presented. The section following the modelling discusses the results and the case study. The last section of the paper provides the conclusions that have been drawn.

## **Gas dispersion modelling**

### CFD Modelling

The current study considered a typical onshore facility for gas processing. The geometry has been built based on previous experience considering the main equipment and buildings normally present in a process plant. Figure 1 shows the 3D model used in the CFD calculations.



**Figure 1: 3D model used in the CFD simulations. The release was placed at the edge of the process area near the pipe rack as indicated by the red cross.**

The computational domain was 600 m x 300 m and 50 metres high. The process area was about 253 metres long by 105 metres wide. The boundaries of the computational domain were placed far enough from the process area in order to ensure no influence on the numerical results.

#### Mesh sensitivity

In order to verify the grid independency, the simulations were performed for three different mesh sizes (coarse, base and refined). The number of cells used in the simulations are presented in **Table 1**.

**Table 1: Computational unstructured mesh sizes used in the mesh sensitivity analysis.**

Unstructured Mesh	Size
Coarse mesh	1,331,255 cells
Base mesh	9,642,963 cells
Refined mesh	14,518,088 cells

There was no significant difference between the results calculated for the base mesh and the refined mesh as listed in **Table 1**. Since the number of cells were still large, a fourth analysis was conducted. The optimal mesh was then selected to be 2,337,110 cells. Comparison of the results from the optimal mesh have shown minor difference from the results calculated using the base mesh as reported in **Table 1**.

It should be noted that the mesh size will vary slightly from case to case. The slight variation was due to the refinement of the jet near the release. Overall, it can be stated that the “production mesh” was around 2 million elements.

The full set of averaged Navier Stokes equation was solved using the finite volume method. The mass fraction transport equation is also solved for the chemical species transported. The simulations were run in the steady state mode as the investigation was not concerned with the dynamics of the cloud. The convective terms were solved using the upwind scheme whenever possible. For the cases presenting numerical instability or significant false diffusion, a higher order discretization scheme was considered.

The Reynold stress was modelled using the Boussinesq approach and the k-epsilon turbulence model has been considered.

The jet release has been modelled using a pseudo leak approach where the subsonic leak velocity was prescribed at the boundary. This is a reasonable approach as the jet velocity will decay fairly quickly when the distance from the leak orifice increases.

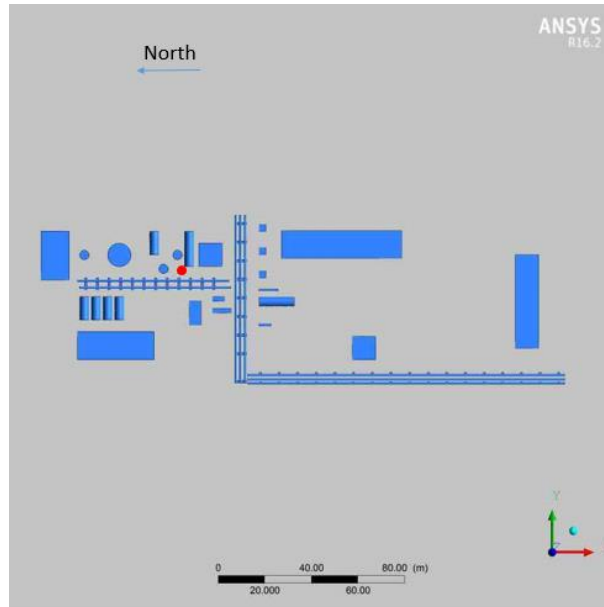
The wind has been modelled using the Monin-Obukhov theory and the atmospheric stability was taken into account via the Monin-Obukhov length. Solid surfaces were set as non-slip surfaces. In the outlet boundaries, the gradient in the direction normal to the outlet surface were equal to zero.

### Integral Model

For Integral Model comparison purpose, a set of Methane jet release scenarios were modelled using Phast. The same source boundary condition applied in the CFD modelling was considered in Phast. An equivalent of 3 inches release scenario at velocity of 200 m/s was created using user defined source model and the same atmospheric conditions were applied. Both horizontal and down release scenarios were observed in this comparison. The explosion cases were modelled using the TNO – Multi Energy approach and the strength 7 was applied in the entire volume of the flammable cloud.

Plan view snapshot of the plant are taken from the CFD model geometry and presented in **Figure 2**. **Table 1** comprises Phast scenarios varying the leak direction and weather conditions. The simulation was set based on the following segment characterization:

- Pressure: 95. bar
- Temperature: 37.5 C
- Hole size 3 inches
- Leak elevation: 2 m



**Figure 2: 2D snapshot used in the Phast simulations. The release was placed at the edge of the process area near the pipe rack as indicated by the red dot.**

**Table 2: Integral Model (Phast) Scenarios with 2 Leak Directions and Weather Conditions**

Case no.	Material	Leak rate (kg/s)	Leak jet speed (m/s)	Leak jet direction	Wind Angle	Weather condition	Leak area (m <sup>2</sup> )	Volume (m <sup>3</sup> )
Phast_01	CH4	69.24	200	S	From N (downwind)	2F	0.45	280.14
Phast_02	CH4	69.24	200	Down	From N (downwind)	2F	0.45	372.80
Phast_03	CH4	69.24	200	S	From N (downwind)	6D	0.45	195.94
Phast_04	CH4	69.24	200	Down	From N (downwind)	6D	0.45	679.75

## Results

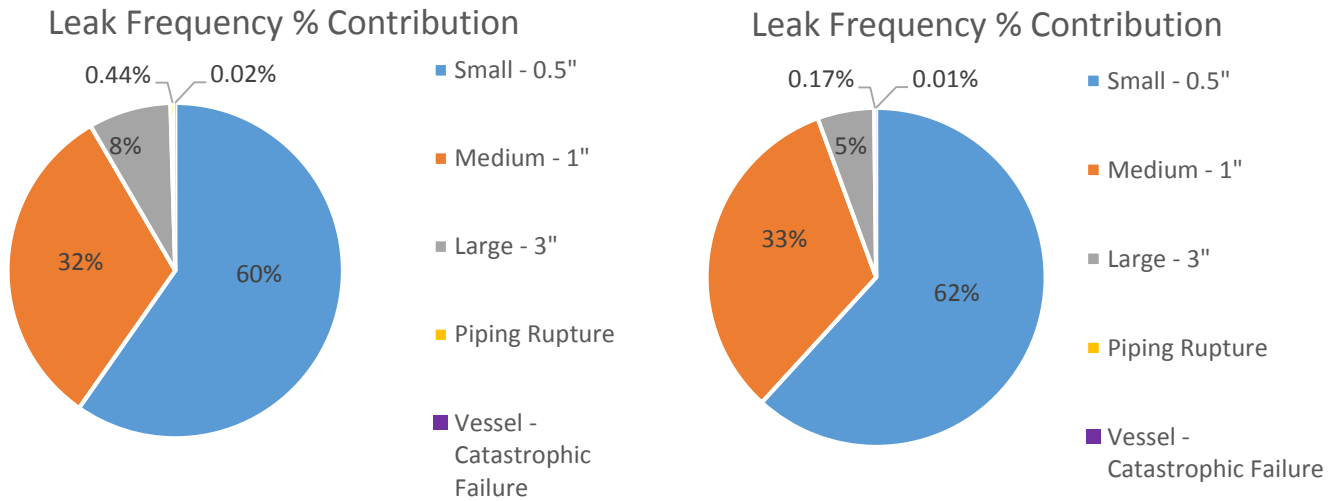
### Computational Fluid Dynamics – CFD

**Table 3** comprises all gas leak scenarios varying the leak direction and the wind direction. The CFD cases were set based on the following segment characterization:

- Pressure: 95.15 bar
- Temperature: 37.78 C
- Hole size: 3 inches

The CFD leak scenarios were set focused on the variation of wind direction and wind speed in order to verify how the ventilation in the process area and the orientation of the wind can influence the flammable volume of the cloud.

The leak size used in the current analysis was selected based on the leak distribution documented in the HSE data base. **Figure 3** presents the leak frequency distribution observed for two projects performed by the authors. The two charts indicate that most of the releases occur for leak sizes smaller or equal to 3 inches. Previous work [5] has also documented that the two-inch leak represents about 95% of the accidental releases. The API RP 752 guidance, as also reported by [5], recommends the utilisation of the “Maximum Credible Event” (MCE).



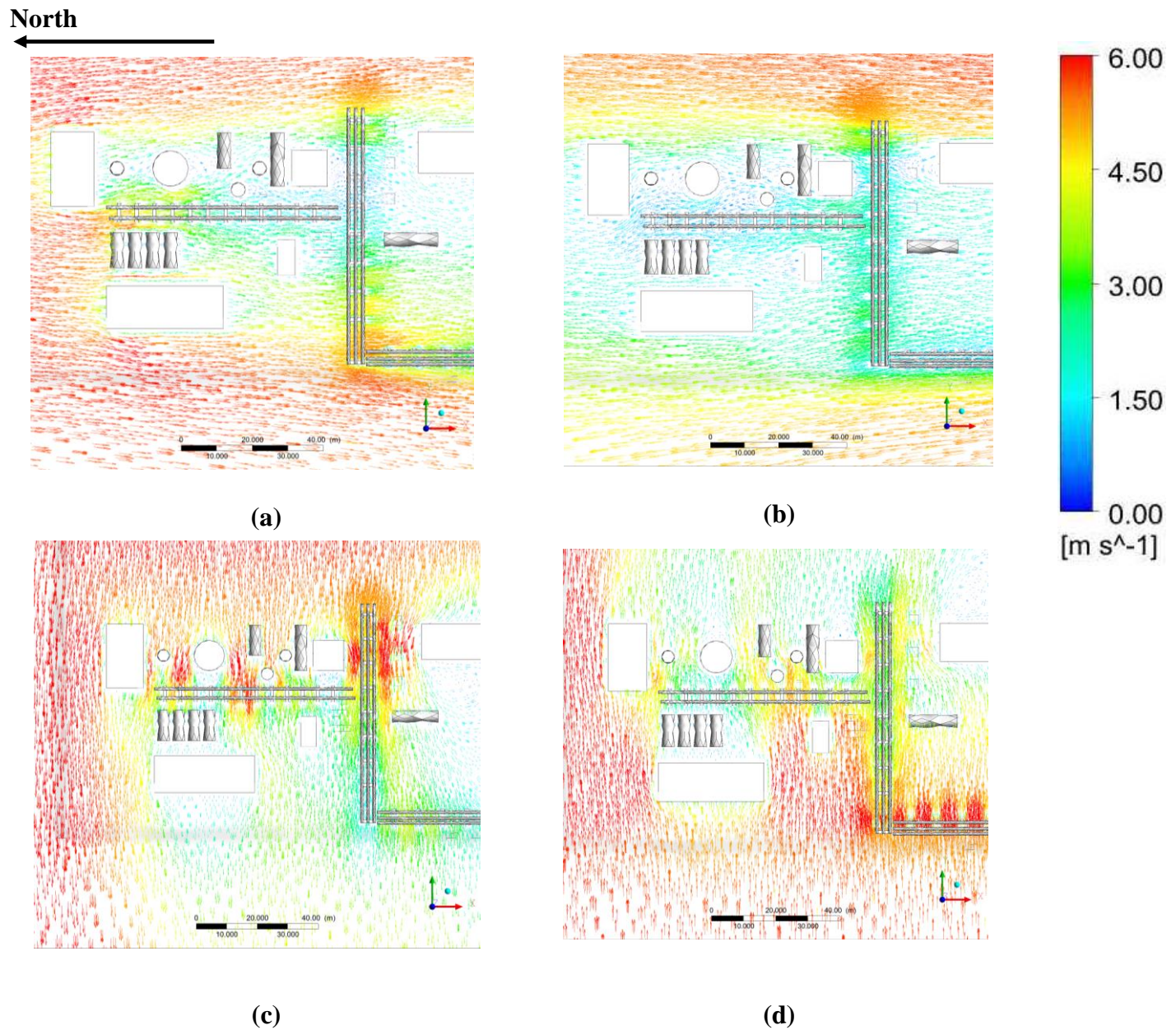
**Figure 3: Leak frequency contribution from various leak sizes in typical industrial installation.**

**Table 3: Gas leak CFD cases run varying the leak direction and wind direction.**

Case no.	Leak location	Geom.	Material	Leak rate (kg/s)	Leak jet speed (m/s)	Leak jet direction	Wind Angle	Wind speed (m/s)	Leak area (m <sup>2</sup> )	Leak width (m)	Volume (m <sup>3</sup> )
Case_01	Facility site	Built	CH4	69.24	200	S	E	2.0	0.45	0.67	64.13
Case_02	Facility site	Built	CH4	69.24	200	S	S	2.0	0.45	0.67	122.16
Case_03	Facility site	Built	CH4	69.24	200	S	N	2.0	0.45	0.67	88.52
Case_04	Facility site	Built	CH4	69.24	200	S	W	2.0	0.45	0.67	79.54
Case_05	Facility site	Built	CH4	69.24	200	Down	S	2.0	0.45	0.67	378.70
Case_06	Facility site	Built	CH4	69.24	200	Down	E	2.0	0.45	0.67	375.89
Case_07	Facility site	Built	CH4	69.24	200	Down	N	2.0	0.45	0.67	309.68
Case_08	Facility site	Built	CH4	69.24	200	Down	W	2.0	0.45	0.67	359.38
Case_09	Facility site	Built	CH4	69.24	200	Down	N	6.0	0.45	0.67	404.53
Case_10	Facility site	Built	CH4	69.24	200	S	N	6.0	0.45	0.67	100.16
Case_11	Facility site	Built	CH4	69.24	200	E	W	2.0	0.45	0.67	122.37
Case_12	Facility site	Built	CH4	69.24	200	W	E	2.0	0.45	0.67	103.16
Case_13	Facility site	Built	CH4	69.24	200	N	S	2.0	0.45	0.67	282.65
Case_14	Facility site	Built	CH5	69.24	200	Down	N	1.0	0.45	0.67	298.98
Case_15	Facility site	Built	CH6	69.24	200	Down	N	8.0	0.45	0.67	339.00
Case_16	Facility site	Built	CH7	69.24	200	Down	N	10.0	0.45	0.67	286.73

**Figure 4** presents ventilation patterns in the process area. Four wind directions have been considered (North, South, East and West). For the cases presented in **Figure 4**, wind speed was

set as 6.0 m/s. Analysis of **Figure 4** shows a significant variations in the wind pattern within the process area. Wind blowing from west (d) and east (c) generates a much higher wind speed in the process area. On the other hand, the wind blowing from north (a) and south (b) leads to a lower wind speed field in the process area. The latter is due to the large obstruction that are present at the north and south side of the process area as illustrated in **Figure 1**.



**Figure 4: Ventilation in the process area. (a) Wind blowing from north generating significant recirculation in the process area. (b) Wind blowing from south also generating zones of recirculation in the process area. (c) Wind blowing from east and (d) wind blowing from west. Regions of higher wind speed are noticed in the process area for the case in which the wind is blowing from east and west.**

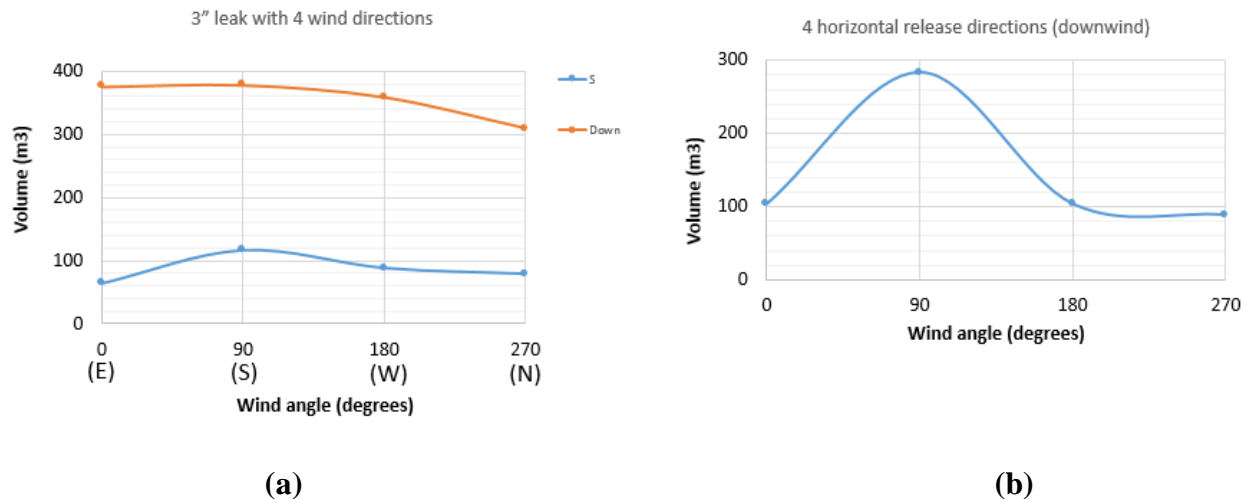
It is also observed that wind speed within the process area is lower when the wind is coming from the south, in comparison with wind blowing from the north. This difference is due to the fact that the buildings on the north face of the process plant are smaller than the building sitting on the south face. Therefore, they offer less obstruction to the wind flowing from the north.

In addition, for all wind directions considered in the analysis it is also possible to observe the formation of recirculation zones in the process area. The recirculation and flow associated with eddies can lead to significant mixing relative to the mean flow.

In the process area, the flow is governed by the dynamics of large eddies stirring and mixing the ambient fluid (air) into the plume. This turbulent mixing plays a very important role in the rate of air entrainment.

**Figure 5** below shows how flammable cloud size varies with varying wind direction. **Figure 5(a)** presents flammable volume as function of wind direction for two releases, namely South (S) and Down. The largest cloud is achieved when the wind is blowing from South (90 degrees as per **Figure 5**). There is also significant difference in the flammable cloud volume as far as the leak direction is concerned.

Analysis of **Figure 5** (b) shows the flammable cloud as a function of the wind direction aligned to the leak direction (i.e.: Downwind releases). The largest flammable cloud is also observed when the wind is blowing from South (90 degrees).



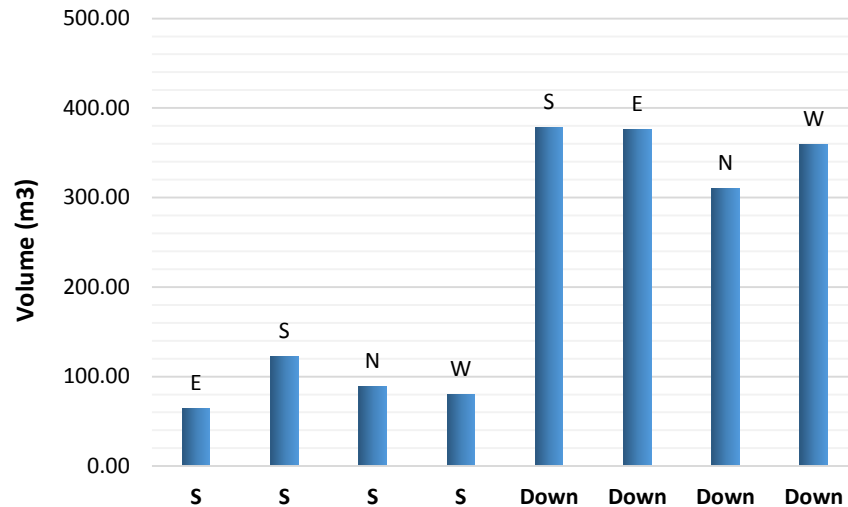
**Figure 5: Flammable gas cloud as a function of wind direction. (a) Horizontal and downwards releases varying with wind direction. Significant difference in the cloud size volume is noticed for different leak directions. (b) Four horizontal leak releases (North, East, West and South) aligned with wind direction (downwind). Wind blowing from South (90 degrees) led to the largest cloud in all cases.**

**Figure 6** presents cloud size as a function of leak direction considering four wind directions (North, South, East and West). Both **Figure 5** and **Figure 6** indicate significant differences in the flammable cloud volume with varying leak direction (down or South). The cloud volumes calculated for downward leak direction is more than 3 times greater than the cloud volumes when

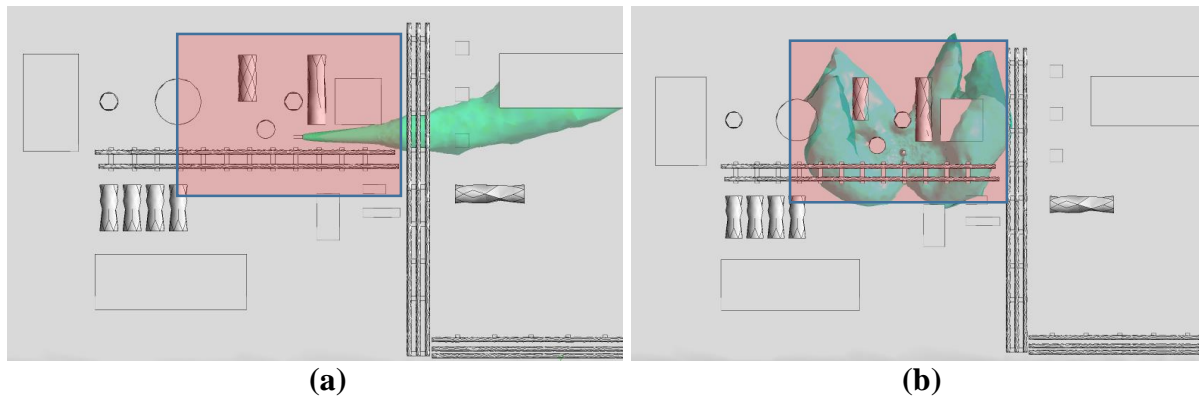


the leak is pointing horizontally toward the South. The leak impingement on the floor reduces the jet momentum allowing for the increase of the air entrainment rate. The rich part of the cloud is diluted yielding a larger flammable cloud than the scenario where the leak direction is horizontal.

**Figure 7** (a) shows the iso-contour at the lower flammable limit for the horizontal release. **Figure 7** (b) shows the leak pointing downwards. Analysis of **Figure 7** (a) and **Figure 7** (b) shows a significant higher cloud in the process area when the leak is pointing downwards (**Figure 7- b**).



**Figure 6: Cloud size as a function of leak direction considering four wind directions (North, South, East and West).**

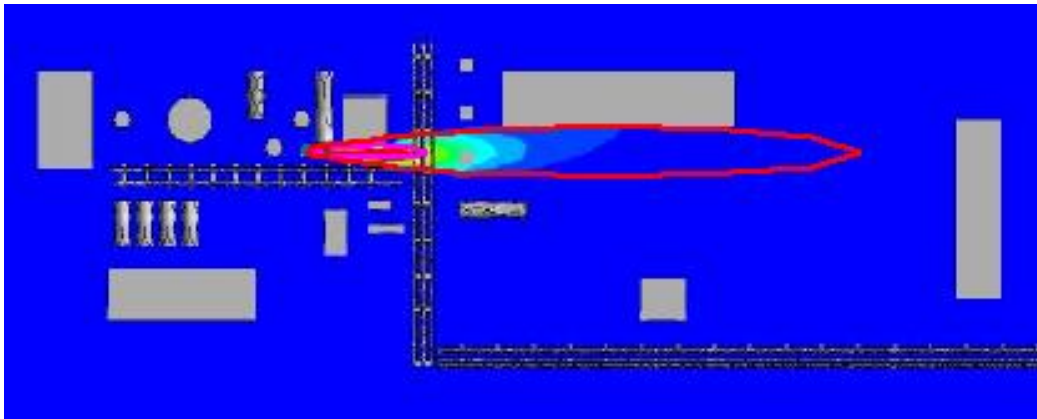


**Figure 7: CFD flammable cloud iso-surface for horizontal release (a) and downwards release (b). A significant larger cloud is observed in part of the process area (red indicated region) when the release is pointing down.**

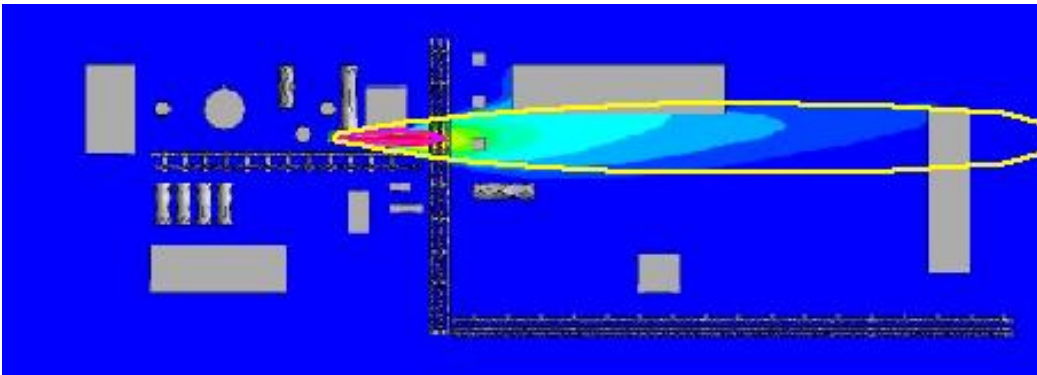
## Integral Model versus CFD

Horizontal and downward releases have been simulated using the Integral Model (Phast) and computational fluid dynamics (ANSYS- CFX). In all cases, the same wind direction and wind speed have been considered.

**Figure 8** (a) compares the length of the lower flammable and the higher flammable limit contour for a horizontal jet release pointing South. **Figure 8** (b) shows the contour for the same case. However, the length is based on half of the LFL. Analysis of **Figure 8** (a) shows that length calculated by Phast is longer than the length calculated using computational fluid dynamics. The difference is much more significant for the lower flammable limit concentration than for the upper flammable limit concentration.



(a)



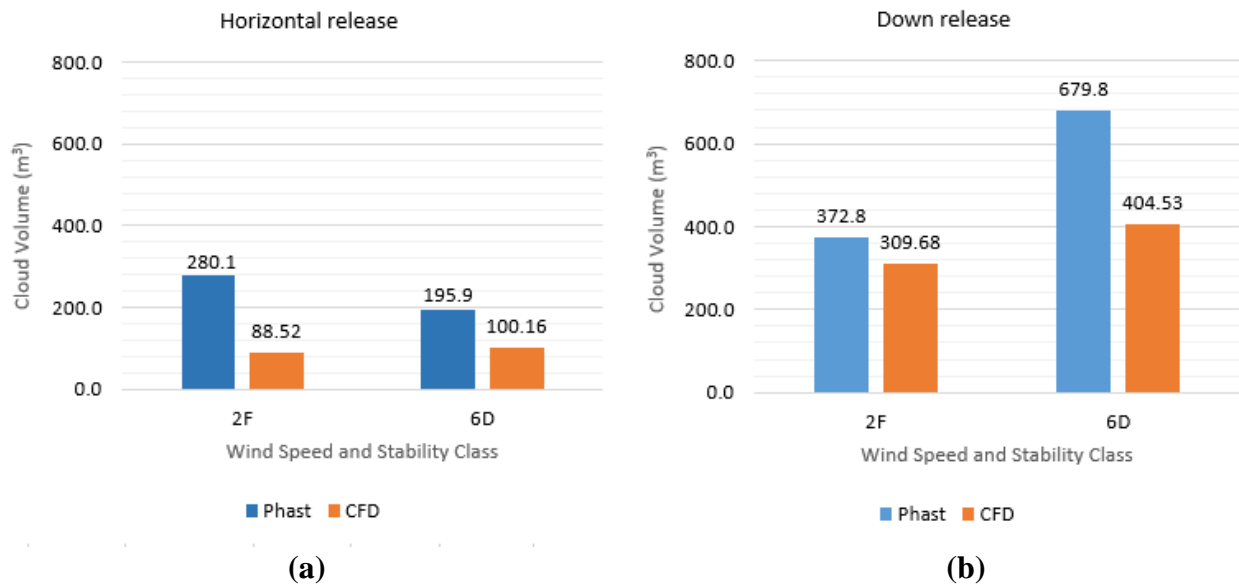
(b)

**Figure 8: Gas concentration contours calculated by Phast (solid line) and CFD. (a) LFL and (b)  $\frac{1}{2}$  LFL contour.**

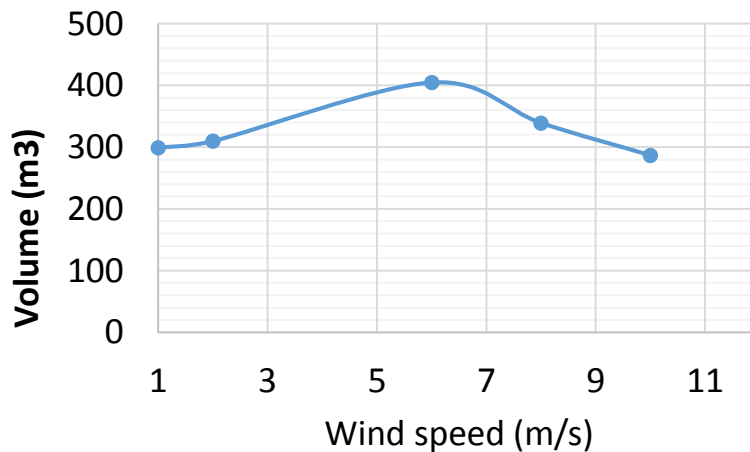
**Figure 9** presents the influence of the wind speed and the leak direction for gas dispersion. For the horizontal release, as the wind speed increased from 2 m/s to 6 m/s, the flammable cloud volume increased for the cases assessed using CFD. On the other hand, the flammable cloud volume calculated using Phast decreased by about 24%. The same trend was noticed when the CFD was applied for the simulation where the leak was pointing down. However, contrary to what was

observed in the horizontal release, the flammable cloud volume calculated using Phast increased as the wind speed increased.

The larger flammable cloud calculated when the wind speed increased from 2.0 m/s to 6.0 m/s is due to dilution of the rich part of the cloud. When the rate of the dilution of the rich part of the cloud is greater than the rate of dilution of the lean part of the cloud, the net result is a larger flammable cloud. For the current case, the increase from 2.0 m/s to 6.0 m/s led to higher flammable cloud. For the facility layout considered in the analysis, the dilution of the cloud that led to smaller flammable cloud is not observed until the wind speed is higher than 7.0 m/s as presented in **Figure 10**.



**Figure 9: Flammable cloud volume for horizontal releases (a) and for downward release (b) using Phast and CFD.**



**Figure 10: Flammable cloud volume as a function of the wind speed.**

## Case study

The flammable clouds calculated using the Integral model and the CFD approach were used to calculate the vulnerable area related to the overpressure generated by accidental explosion. Two leak directions, two wind speeds and two instability classes were considered.

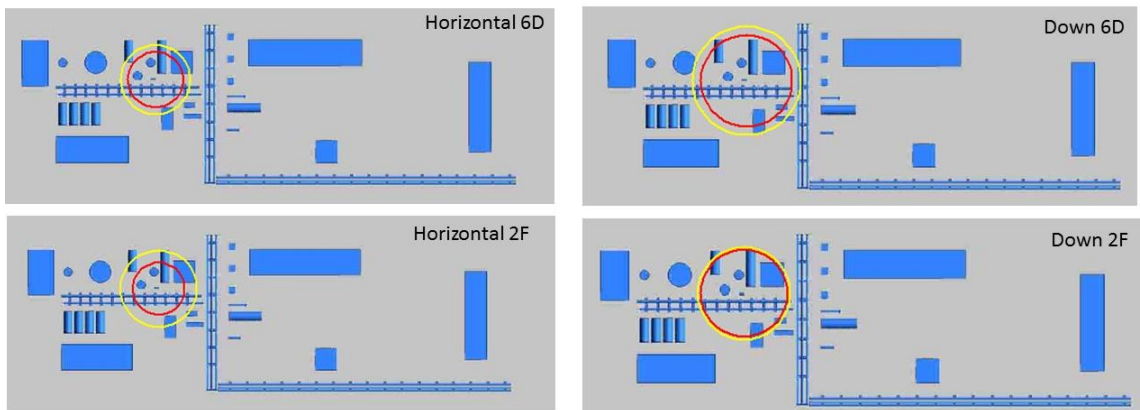
The case study investigated the impairment of the administration building indicated by the red arrow in **Figure 11** and **Figure 12**.

The impairment criterion selected for the current analysis was 1 psi. The overpressure criterion was selected based on the lowest physical effect that could lead to minor damage and possible breaking of glass windows. However, overpressure contours for 2 psi are also reported.

The explosion modelling considered that the flammable clouds calculated in the dispersion phase of the current investigation were placed in process area as indicated by the worst dispersion scenario in **Figure 7(b)**. The TNO Multi – Energy model was used in the simulations and the total volume of the cloud was considered as strength 7 in the scaled overpressure correlation.

**Figure 11** shows the 2 psi overpressure contours for cases considering flammable clouds from horizontal and down releases. The most significant difference between the overpressure contours was found to be for the horizontal releases where the 2.0 m/s wind speed was considered. For the 6.0 m/s wind speed, the difference is less significant.

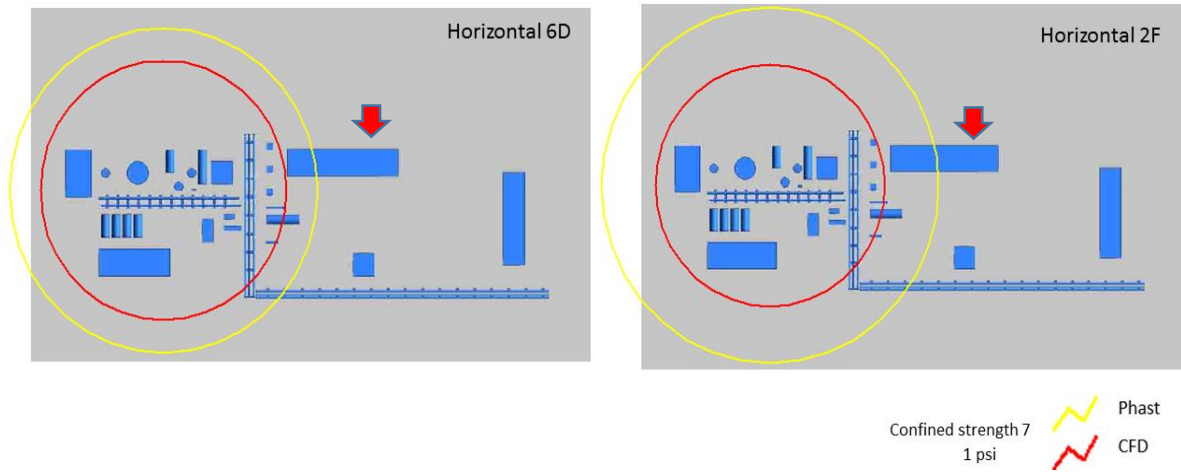
Considering the down releases, the results were similar when the wind speed was set to 2.0 m/s. The small difference is due to similar flammable cloud volumes. As the wind speed increases to 6.0 m/s, the difference between the cloud sizes is more significant, hence resulting in significantly different overpressure contours.



**Figure 11: Overpressure iso-contour for flammable clouds considering two leak directions and two wind speeds. The yellow contours are overpressure (2 psi) calculated using cloud volumes obtained using the Integral model. The red contours represent the overpressure 2 psi) calculated using the flammable clouds calculated via CFD.**

**Figure 12** shows the 1 psi overpressure contour for flammable clouds calculated considering 6.0 m/s and 2.0 m/s wind speed. Analysis of **Figure 12** shows that the administration building,

indicated by the red arrow, is exposed to an overpressure above the selected criterion when the flammable cloud volume calculated using the Integral model is considered.



**Figure 12: Overpressure contour for two flammable cloud volumes. (a) Horizontal release considering 6.0 m/s wind speed. (b) Horizontal release considering 2.0 m/s wind speed.**

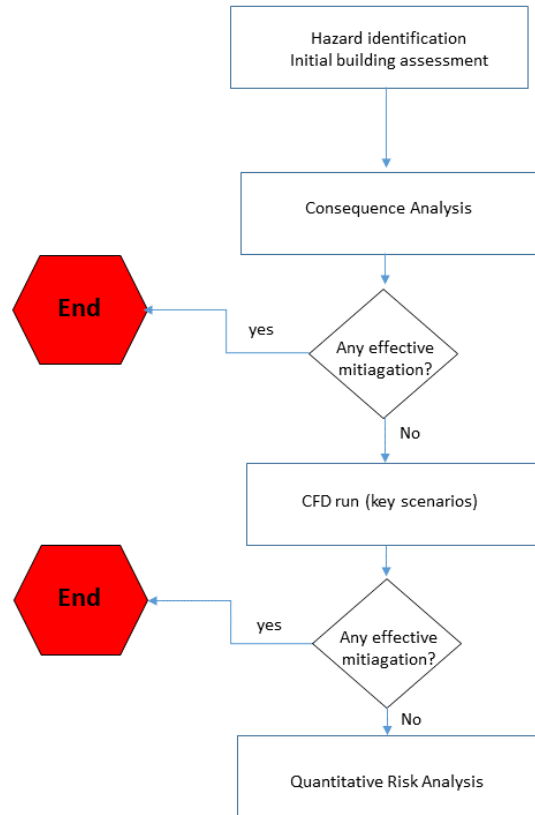
On the other hand, no impairment of the building is observed when the flammable cloud calculated via CFD is considered in the explosion modelling.

### Methodology

There seems to be indication that the application of CFD in the facility siting analysis can anticipate consequence scenarios which may not be noticed when empirical or semi-empirical approaches are applied.

The level of uncertainty of the model considered in the consequence analysis may suggest further evaluation (as presented in **Figure 12**) when it is not necessary. The utilisation of a more sophisticated tool can clarify if the necessity for a more detailed analysis is really necessary.

**Figure 13** presents a simplified diagram that illustrate the application of computational fluid dynamics prior to deciding to move ahead towards a Quantitative Risk Analysis (QRA), for instance.



**Figure 13: Methodology for facility siting analysis integrated with computational fluid dynamics.**

The first phase is focused on the identification of potential hazard scenarios determining which building must be considered in the analysis. The second step, namely the Consequence Analysis, evaluates the potential physical effects from the scenarios identified in the first phase. Should the facility present adequate protection and mitigation measures, the analysis can end at this stage.

Otherwise, before moving on to a risk based approach, the worst-case scenario or MCE scenarios, can be evaluated using CFD to confirm if the available mitigation measures are sufficient to protect the installation against the selected scenarios.

Bearing in mind the cost of computational fluid dynamics modelling, it is suggested to execute only the ventilation and dispersion modelling. Such approach, avoids the large number of hours required to model the small scale geometry required by the explosion modelling. Additionally, the cost of transient simulations can also be avoided as the steady state cloud is the main concern. Another important aspect is the application of pseudo source model for the release boundary condition. The “new” set of boundary conditions avoids the effects of compressibility speeding up the simulation with minimal impact in the cloud size, as the velocity decays rapidly with the distance from the leak orifice. In these lines, the application of the DESQr (Diameter of Equivalent Simulation for Quick Run) model, suggested by Ferreira and Vianna [6,7] is one of the alternatives that can be applied to overcome the burden caused by the compressibility effects near the jet leak.

## Conclusions

The gas dispersion simulations presented different results for the calculated flammable cloud sizes when the Integral model and CFD technique were considered. The cloud volumes calculated via CFD were smaller than the cloud sizes calculated using the Integral model. The rate of air entrainment in the cloud plays an important role in the dilution of the flammable volume. In any process area, the rate of air entrainment in the cloud is a function of the ventilation in the area. The wind pattern in the process area is mainly caused by interference of the large equipment and obstructions. The Integral model does not capture the dispersive effects as accurate as CFD techniques and therefore led to more conservative clouds.

The Integral model considers that the wind is blowing in the same orientation of the leak direction. The current analysis had shown that the wind direction that led to largest cloud is not aligned with the leak direction. In fact, it is related to the largest obstruction in the facility siting. The circulation zones in the wake of the largest obstruction is caused by the separation of the boundary layer along the bluff body surface. The recirculation pattern in the process area “traps” the gas in the area leading to larger clouds.

The leak orientation also seems to play a very important role as far as the flammable cloud volume is concerned. The leak releases oriented towards the ground (down releases) yielded a much larger cloud than the horizontal releases. Although the horizontal releases are important for the jet fire modelling, the down releases are recommended to be also considered in the explosion modelling.

A case study considering the explosion scenario presented significant differences as far as the overpressure effects are considered. For a pre-established criterion there was no impairment of the administration build for the flammable cloud size calculated via CFD. On the other hand, for the releases pointing down and for low wind speed, there was no significant difference in the flammable cloud volume/overpressure. The difference is better noticed when the wind speed increases. This is due to enhancement of the ventilation and consequent increase of the rate of air entrainment in the cloud.

The ventilation simulation also have shown that the increase of the ventilation does not necessarily reduce the flammable cloud size. There seems to be a critical wind speed when the flammable cloud size starts to reduce. For the investigated facility siting, the critical wind speed was above 6.0 m/s as shown in **Figure 10**.

A suggested methodology is presented in **Figure 13**. The approach suggests the application of the CFD simulations in the cases where the mitigation measures are not effective after the assessment using more traditional approaches. As shown in the current paper, the application of CFD may avoid the necessity of a more detailed risk based analysis. The cost of using CFD can be minimum as long as the set up discussed in the results section are followed and similar leak approaches, as suggested by Ferreira and Vianna [6,7], are considered.

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