# THE TNO – MULTI-ENERGY METHOD COMBINED TO MATHEMATICAL PROGRAMMING AND COMPUTATIONAL FLUID DYNAMICS FOR OPTIMISATION OF GAS DETECTORS

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## ABSTRACT

Gas leakage is a matter of concern for several industries such as oil and gas, mining, food, and healthcare. Usually, the difference is due to the type of gas. While oil and gas companies deal mostly with methane, hydrogen sulphide; food and beverages companies are concerned about ammonia. In all cases, the gas detector is the main tool used to avoid accidents and disasters, like an explosion. When the industry considers gas detectors, the main questions are: How many gas detectors are required? Where is the best location to install them? To answer those questions Computational Fluid Dynamics (CFD) simulations and optimisation procedures are employed to calculate the plume location and plume volume to better position the gas detectors. However, there are cases where the plume volume obtained from CFD simulation is too small, resulting in a high quantity of detectors. Those scenarios present a high cost of implementation, which makes the project inviable. Cases like this are very challenging. Hence, we proposed a novel solution using the TNO Multi-Energy method in conjunction with optimisation procedure and CFD simulations. The TNO Multi-Energy method is used to dimension the smallest plume that causes a significant explosion damage. These results are used to determine the mesh optimisation ensuring a 100% coverage of the area. Transient CFD simulations were used to verify the performance of these methodology and good results are found.

## 1. INTRODUCTION

Toxic and flammable gases can lead to severe consequences if accidental releases take place. In the Oil & Gas (O&G) industry a large variety of toxic and flammable gases are present, such as hydrogen sulphide ($H_2S$), carbon monoxide (CO) and methane ($CH_4$). In the food and beverage industry, the utilisation of ammonia as one of the main refrigerants is also a matter of concern. In the steel sector, the generation of CO throughout the reduction process also calls attention of the process safety department in many organisation around the globe.

Gas leaks can lead to major damage if the accidental clouds are not detected within a short period of time. Ramírez-Camacho et al. [1] discussed the consequences due to O&G pipeline accidental releases. They verified that fire followed by explosion are ordinary events in these cases, which can cause significant economic, environmental, and in worst case human losses. Biezma et al. [2] analysed the most fatal O&G pipelines accidents through history. In their review paper, many accidents caused by natural gas leakage are discussed and the main causes are addressed. One example is the accident in Texas (USA) in March 1937 that killed 309 people, of which 294 were high school students. Liu et al. [3] present a study of the human consequences due to exposure to air pollution near a steel plant and verify that people who live less than 5 km away from a steel plant have an increased pulse rate. It suggests that the air quality in a residential area near a

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steel plant may influence cardiovascular physiology. Those papers present evidence of the gas leakage consequences in minor and major proportions.

On the other end, accidents can be prevented by early detection of gas releases. Currently, gas detectors are the most common device applied when early detection is concerned. To this end, it is fair to anticipate that engineers are looking for the optimal location as well as the minimum number of devices required to protect an industrial area.

To address the optimisation of gas detectores, some methodologies have been put forward. In order to avoid accidents with inflammable gases, the HSE(1993) suggests placing a detector every 5 metres with alarm levels set to 20% and 60% of LEL (Lower Explosion Limit). This methodology is based on the experimental results from Hjertager et al. [4]. Kelsey et al. [5] investigated the 5 metres grid spacing employing simulations of offshore high-pressure gas releases. It has been found in their investigation that the time to detect the gas release was considerably long when small cloud volumes were calculated. The same conclusion could be drawn when the dynamics of the cloud volume was slow when compared with the time scale of the transport of the flammable cloud. Moreover, in many cases the gas cloud was not detected at all.

The authors advocated the importance of gas dispersion simulation to adequately quantify and place the detectors. CFD (Computational Fluid Dynamics) simulations are one of the most used and validated approaches to understand gas dispersion [6], [7], and [8]. Once the gas dispersion is performed, an optimisation technique can be applied to determine the best location and minimum number of gas detectors. Vianna [9] put forward a new model based on the set covering problem and computational fluid dynamics to calculate the minimum number of gas detectors and to determine the best location that ensures 100% coverage of the area.

However, there are some cases where the CFD simulations result in small plume sizes. In these cases, the optimisation will result in a large number of detectors, which can imply high costs and increase the spurious failure rate. In this paper, we investigate a new approach based on the TNO Multi-Energy Method, mathematical programming and computational fluid dynamics to optimise the number of gas detectors when small cloud volumes are calculated. The Multi-Energy method uses typical explosion loads Baraldi et al. [10] to determine the minimum cloud volume that can lead to such level of overpressure. The optimisation is performed based the minimum cloud volume and the gas detection is verified using computational fluid dynamics. A case study is introduced and transient CFD simulations shows that the proposed approach led to good results.

## 2. DESCRIPTION

Figure 1 presents the methodology proposed to determine the number and position of gas detectors. The following subsections deep the discussion of the methodology.

### 2.1.Define Overpressure

The first step in the procedure is to determine the acceptable overpressure in case of accidental explosions. Typical overpressure tables (Baraldi et al. [10]) can be used to relate the blast overpressure with possible consequences or damage to humans, structures, and equipment (Table 1). In the current analysis we considered the results reported in the work performed by Jeffries et al. [11] and also the AICHE Guidelines [12]. In order to exemplify how the selection of the overpressure is considered in the analysis, take for example damage to the eardrum. In this case, overpressure higher than 13.8kPa should be avoided. As a consequence, cloud volumes associated with this selected overpressure are used in the optimisation calculation.

In the next section we detail how the cloud volume is calculated.

## 2.2.Calculate Gas Plume Size

The volume of the gas cloud is calculated using the TNO Multi-Energy method [13]. The method starts with the calculation of the scaled distance (R) using Eq. (1), where x is the distance from the explosion and $P_0$ is the environmental pressure.

$$R = \frac{x}{\left(\frac{E}{P_0}\right)^{\frac{1}{3}}} \tag{1}$$

$E$ is the blast energy, which is calculated by Eq. 2. $E_c$ is the combustion energy. In this work we adopted 3.5 MJ/m³ . $V_{flam}$ is the volume of the gas plume.

$$E = E_c V_{flam} \tag{2}$$

Once the overpressure is selected, we backtracked the calculations using equations (3), (1) and (2), in this particular order, to calculate the cloud volume associated with the selected overpressure.

The scaled peak side-on overpressure ($P_s^{'}$) is used to calculate the peak overpressure ($P_s$) in accordance with the following non-dimensional formulation

$$P_s = P_s^{'} P_0 \tag{3}$$

## 2.3.OPTIMI

Optimi is a Fortran code developed to solve 0-1 integer problems. It relies on Balas algorithm and the graph generator algorithm [9]. It calculates the minimal number of detectors to ensure 100% coverage of the area. The problem is formulated in accordance with the Set Covering Problem as shown below:

$$MinZ = \sum_{j=1}^{n} c_j x_j \tag{4}$$

subject to:

$$\sum_{j=1}^{n} a_{i,j}x_i \geq 1\,, i = 1, \cdots, m \qquad (5)$$

$$x_j = 0,1, \qquad j = 1, \cdots, n \qquad (6)$$

Equation (4) is the objective function where c is the cost vector and $x_j$ is the decision variable. Equation (5) is the set of inequalities that ensure the full coverage of the area. In the formulation, $a_{i,j}$ is the element subset of the adjacency matrix of the graph that represents the area to be covered.

The final set comprises xj values. If x is assigned 0 it means that no detector shall be installed in that particular location. On the other hand, if x is assigned 1 the gas detector must be installed in the respective location. Therefore, the set of Xs in the problem defined the areas that are candidates to receive a gas detector.

### 2.4. Quantity and Position of Gas Detectors

The number and position of gas detectors are calculated based on the optimisation method presented by Vianna [9]. The value of m and n is estimated based on the size of the optimisation mesh, which is calculated by Eq. 7.

$$L = \sqrt[3]{Min(V_{flam})} \qquad (7)$$

L is the characteristic length of the mesh. Considering the total volume of the area, L is used to calculate the number of elements in the X set that comprises the candidate to receive a gas detector based on the optimal solution calculated using equation (4), (5) and (6).

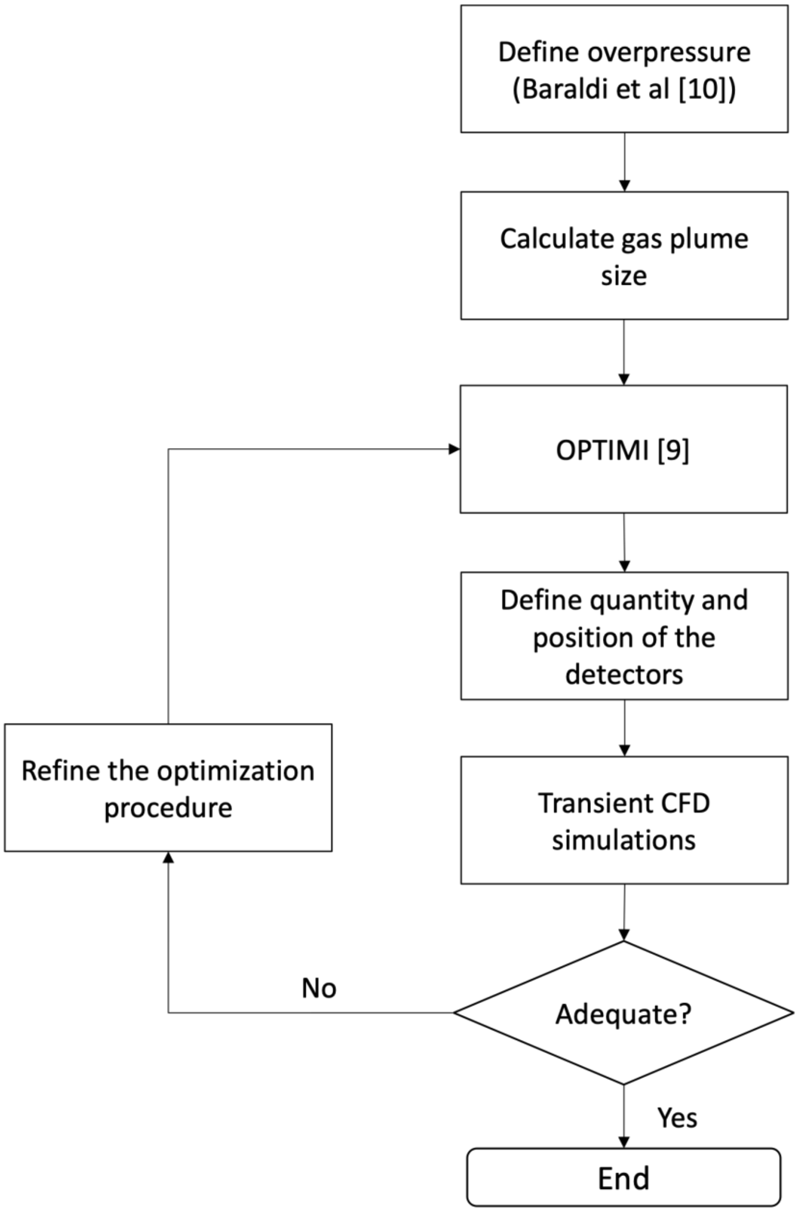



**Fig.1** – Calculation procedure proposed for gas detector optimisation in the framework of small flammable clouds.

**Table.1** – Damage to humans, structures, and equipment due to overpressure (Adapted from Baraldi et al. [10]).

| Overpressure (kPa) | Description of Damage |
|---|---|
| **Direct Effects on People (Jeffries *et al.*, 1997)** | |
| **13.8** | Threshold for eardrum rupture |
| **34.5 to 48.3** | 50% probability of eardrum rupture |
| **68.9 to 103.4** | 90% probability of eardrum rupture |
| **82.7 to 103.4** | Threshold for lung hemorrhage |
| **137.9 to 172.4** | 50% probability of fatality from lung hemorrhage |
| **206.8 to 241.3** | 90% probability of fatality from lung hemorrhage |
| **48.3** | Threshold of internal injuries by blast |
| **482.6 to 1379** | Immediate blast fatalities |
| **Indirect Effects on People (Jeffries *et al.*, 1997)** | |
| **10.3 to 20.0** | People knocked down by pressure wave |
| **13.8** | Possible fatality by being projected against obstacles |
| **55.2 to 110.3** | People standing up will be thrown a distance |
| **6.9 to 13.8** | Threshold of skin lacerations by missiles |
| **27.6 to 34.5** | 50% probability of fatality from missile wounds |
| **48.3 to 68.9** | 100% probability of fatality from missile wounds |
| **Effects on Structures and Equipment (Guidelines, 1998)** | |
| **1** | Threshold for glass breakage |
| **15 to 20** | Collapse of unreinforced concrete or cinderblock walls |
| **20 to 30** | Collapse of industrial steel frame structure |
| **35 to 40** | Displacement of pipe bridge, breakage of piping |
| **70** | Total destruction of buildings; heavy machinery damage |
| **50 to 100** | Displacement of cylindrical storage tank, failure of pipes |

### 2.5.Transient CFD Simulation

Based on the results obtained from the optimisation procedure. Transient CFD simulations of the gas dispersion are set up. The positioning of the probes are in accordance with the optimal solution provided by Optimi optimisation tool. In each problem, the gas concentration dynamics is recorded. The findings are used to verify whether the optimal location of gas detectors is able identify the accidental gas release.

The optimal number and location of the gas detectors is considered adequate if at least one detector can detect the gas leak. Otherwise, the refinement of the optimisation mesh is performed and the procedure is repeated as shown in Figure 1.

## 3. DISCUSSION

A chemical process plant presented in Fig. 2 is used to verify the methodology introduced in this paper. As shown in Fig. 2, the storage area of the plant is the focus of analysis. For the CFD simulation, a computational domain three times the size of the plant was adopted. The main dimension of the domain is 350 m x 188 m x 30 m.

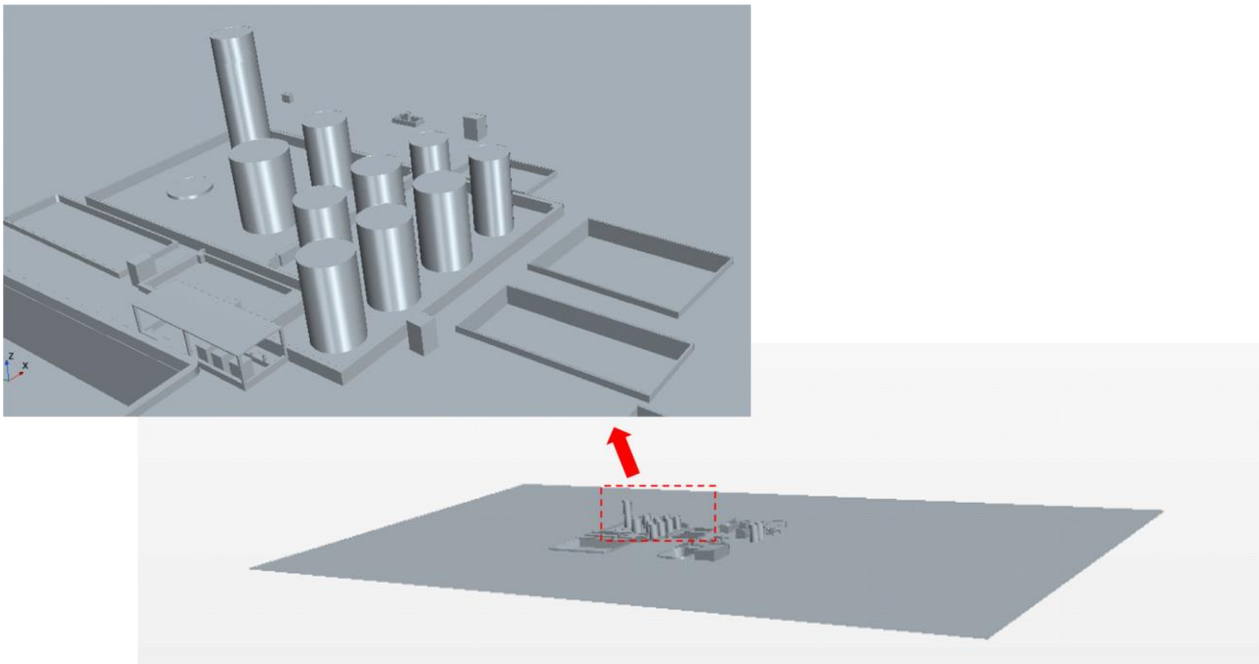


**Fig.2** – Geometry of the chemical process plant studied in the paper.

Figure 3 presents the mesh used in CFD simulation. Approximate 4 million polyhedric elements were used to discretise the computational domain with prismatic elements near the wall. The mesh was refined in the main area of the plant

The definitions of the wind and leak directions are presented in Fig. 4. Figure 5 shows the natural gas plume for 60% of the LEL (Lower Explosion Limit) concentration. In this case, 60% of the LEL was considered due to the low calorific potential of the natural gas present in the chemical plant. This figure shows four different cases changing the leak and wind direction. In all cases, a small plume volume is observed.

Therefore, the proposed procedure was applied considering an overpressure lower than 10.3 kPa. In this case, all the calculations were carried out adopting a level 4 for blast strength. It was based on the geometry and gas properties of the problem. The TNO Multi-Energy method calculation led to a plume volume of approximately 350 $m^3$ required to cause an overpressure of 10.2 kPa at a 2 m distance from the explosion. Then using Eq. 7, it is found a characteristic length L for the optimisation procedure of 7 meters.

Application of the calculated characteristic length L led to the optimisation mesh reported in Fig. 6. The computations result in 4 detectors placed as presented in Fig.6.

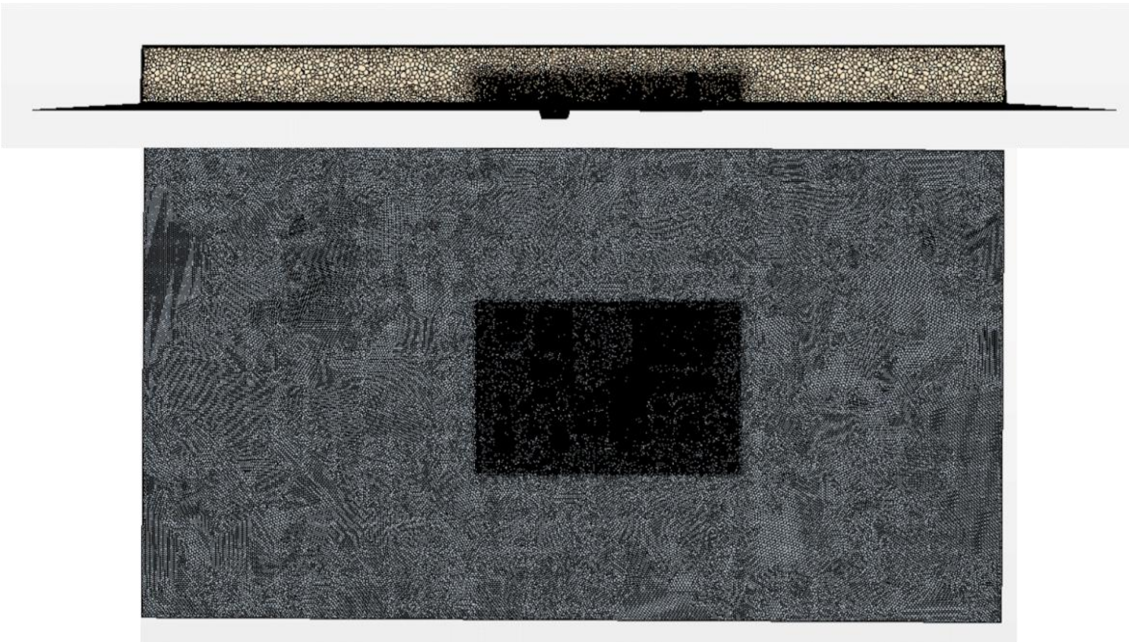


**Fig.3** – CFD computational mesh used in the simulations.

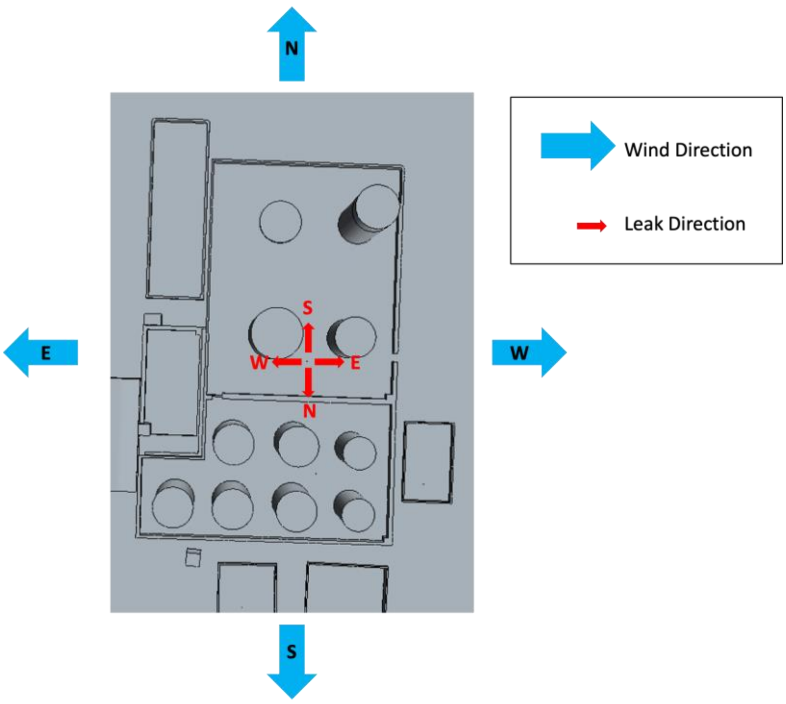
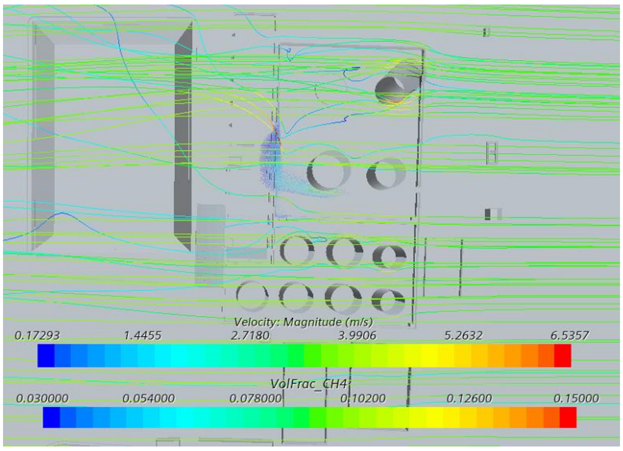
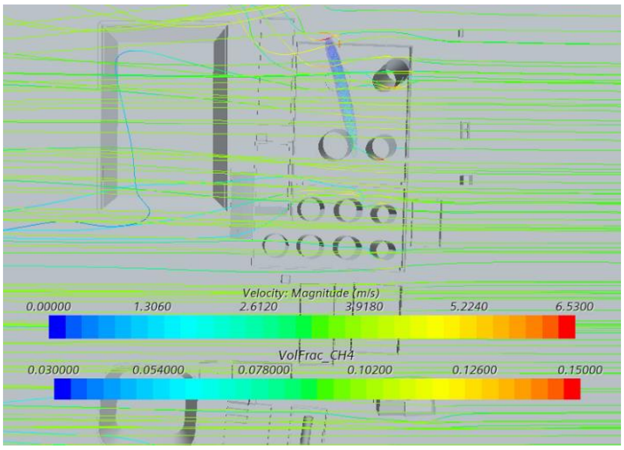



**Fig.4** – Definition of wind and leak direction adopted in the paper.




(a)

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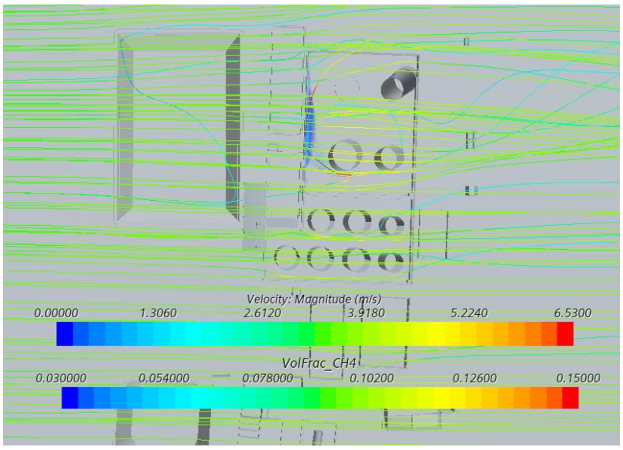
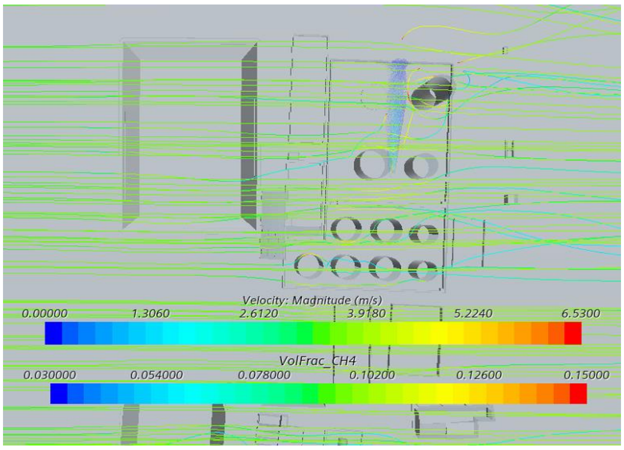



(c)




(d)

**Fig.5** – Natural gas plume size for 60% LEL concentration obtained by CFD simulation for different leak and wind direction: (a) Leak in W-direction and wind from E; (b) Leak in S-direction and wind from E; (c) Leak in W direction and wind from W; (d) Leak in S-direction and wind from W.

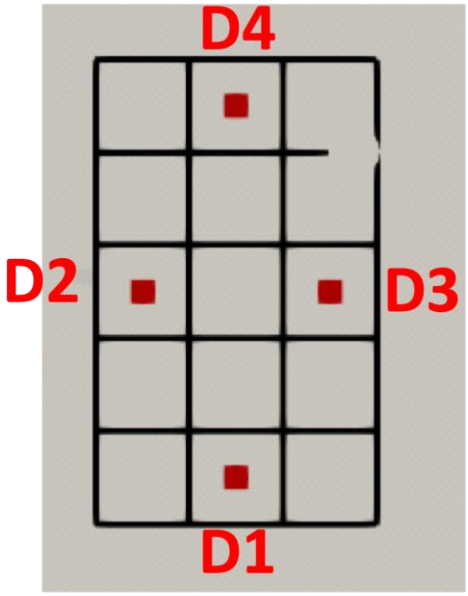



**Fig.6** – CH4 detector placement obtained from OPTIMI.

Transient CFD simulation is carried out considering a gas leakage in the S-direction and wind from E-direction. The leakage occurs in the middle of the area as shown in Fig. 7. The plume is for natural gas volume fractions varying from 0.01 to 0.15, which represent 20% of LEL (Lower Explosion Limit) and UEL (Upper Explosion Limit). Figure 8 presents the measurement recorded in 4 gas detectors as shown in Fig. 7 (red dots). Analysis of Fig. 8 shows that the D4 detector promptly captures the gas plume.

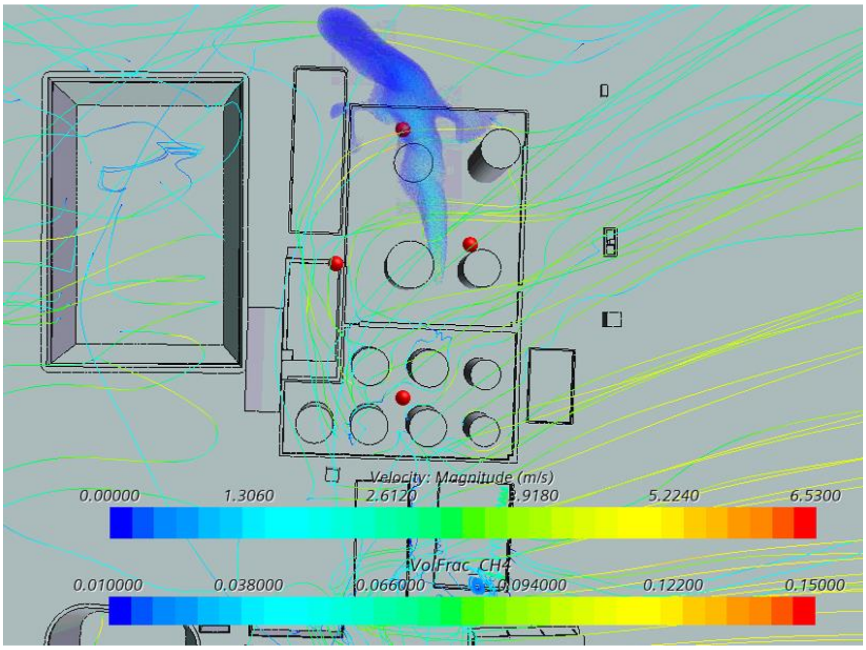



**Fig.7** – Transient CFD simulation result.

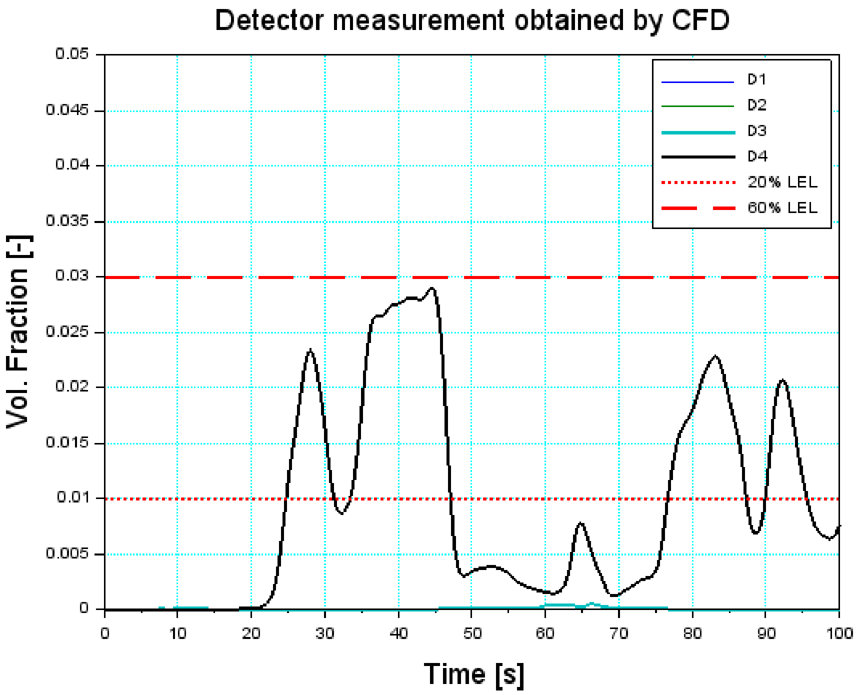



**Fig.8** – Measurements obtained by 4 detectors in the transient CFD simulation.

## 4. CONCLUSION

This paper presented a new procedure based on the TNO Multi-Energy Method to calculate the number of detectors when gas cloud volumes are small. The approached combined the Multi-Energy explosion model, mathematical programming and computational fluid dynamics. It has been found that the cloud generated by the accidental gas leak was detected by the optimal distribution of gas detectors for the test case considered. Moreover, the gas leak was detected within 5 seconds of the initialisation of the release. The analysis considered as threshold 10.3kPa to calculate the cloud volume. At the moment, the performance of the procedure for different values of threshold remains open. Additionally, the new findings can be compared with the traditional approach in order to verify the reduction of the number of gas detectors. It is also not clear, whether the novel approach introduced here will work satisfactory for different substances. Bearing in mind that ammonia and hydrogen, for example, behave quite different from natural gas it is worth investigating the effect of buoyancy on the dispersion of the gas plume.

## 5. ACKNOWLEDGEMENT

The authors would like to thanks to National Agency of Petroleum, Natural Gas and Biofuels (ANP), Shell and Petrobras for the financial support to conduct this research.

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