A Gas Detector Optimization Tool Coupled with CFD Simulations in Risk Analysis Area for Industrial Applications

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INTRODUCTION

Gas releases are always a matter of concern in the chemical industry as well as in any field that deals with gas storage; they can be toxic, inflammable or both. As an example of this, we can cite two major accidents in the recent years: gas explosion in Buncefield and the BP (British Petroleum) exploration platform in Gulf of Mexico [1-3]. Therefore, it becomes crucial the identification of these releases (big or small) in early stage as soon as possible in order to minimize or even avoid the effects caused by them and so that saving lives, preserving the environment and also the progress and good maintenance of the industry.

Decades ago, the gas detector location was made only based on experience and on an empirical manner [1]. Nowadays with the arise of computational modeling and advances, Computational Fluid Dynamics (CFD) technique plays a major role in this scenario helping engineers to better calculate the gas dispersion, the cloud it forms and so that where are the point that needs detectors. Although it describes well the gas cloud distribution and size, it still requires the field experience and personal decisions of the technical team (engineers and technical). Therefore, there are no guarantee of the number and position of theses detectors to give a hundred percent of coverage for a process plant, area. Too many installed detector are also not good, once it can be a waste of money invested in buying them and the detector can alarm even in the absence of gases.

Having said that, this work evaluated detectors already installed and the possible implementation of new ones as well as the reallocation of the existing detectors, i.e, the optimization of gas detector in two industry facilities that uses Ammonia as refrigerator fluid, using an optimization tool – OPTIMI [1, 3]. - coupled with CFD simulations.

METHODOLOGY

Two different industrial facilities that uses Ammonia as refrigerator fluid were chosen. Ammonia is toxic and flammable [4] and both facilities already had some detectors. However, it was necessary the evaluation of the current detectors position and the installation and position of new ones and for this some CFD simulations were done as well as OPTIMI ones.

The general methodology is described in Figure 1. From the geometry CAD and HAZOP analysis, we define the leak points and models the conditions for CFD simulations. After that, the cloud gas results generated by CFD are taken into account in OPTMI tool. A sanity test is made and if the results are not feasible, we should repeat this loop until we get feasible results.

OPTIMI is a Fortran code developed to solve the set covering problem (SCP). The code for gas detector optimization analysis uses Balas algorithm and CFD. This tool employs an objective function that aims calculating the minimum number of gas detectors along with a set of constraints, which ensures that each gas leak will be detected, by at least one gas detector. In other words, this mathematical modeling guarantees 100% coverage, according to the nature of the optimization problem solved by OPTMI. The great advantage of this tool is that it uses the 3D geometry model with gas cloud obtained by CFD gas dispersion analysis. As an output, it presents the coordinates x, y and z for each gas detector, as well as its spatial location in the 3D model of the geometry considered in the study, facilitating the sanity test, commonly performed after the optimization study.

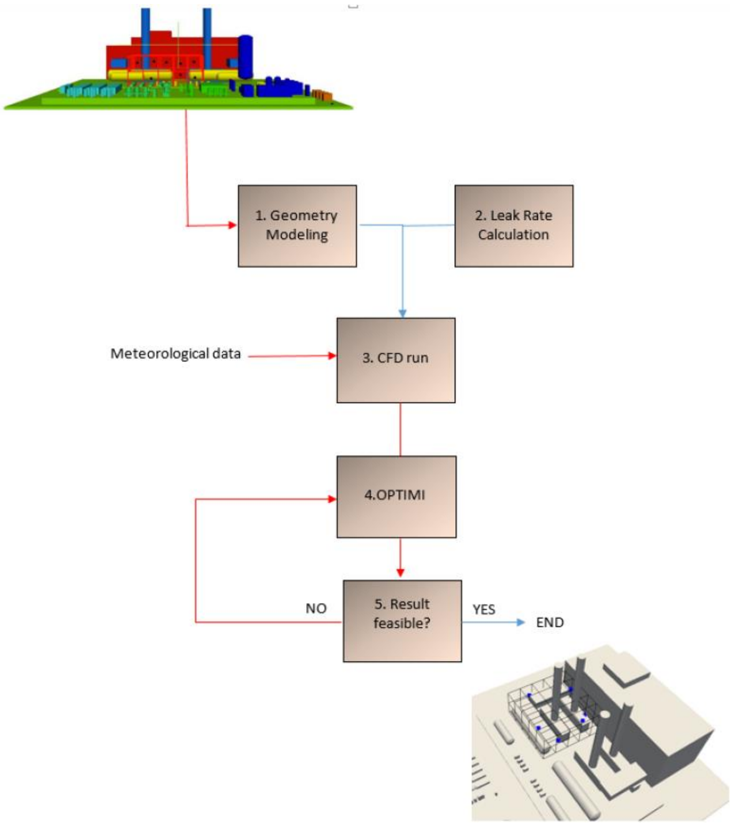


Figure 1 – Methodology for determining gas detectors localization using Computational Fluid Dynamics combined with optimization program, OPTIMI [3].

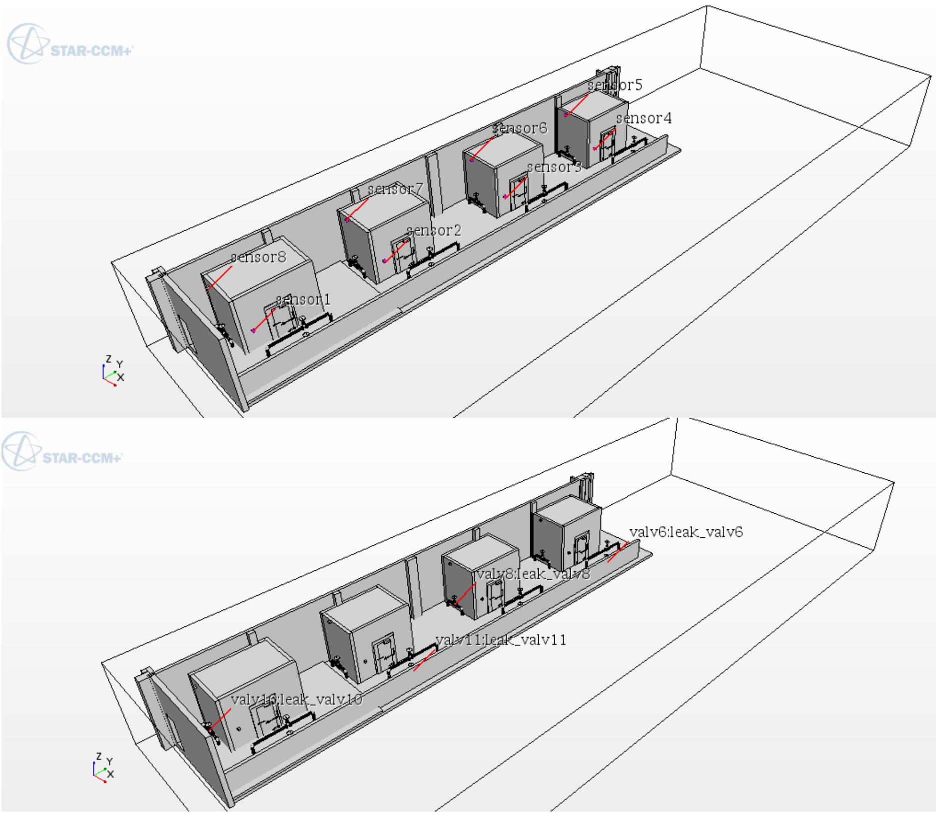
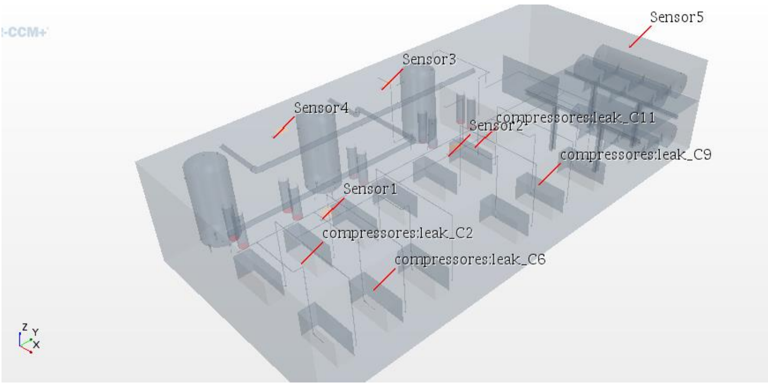


Figure 2 – Palletizing Room showing the current gas detectors (sensor) and the leak points.



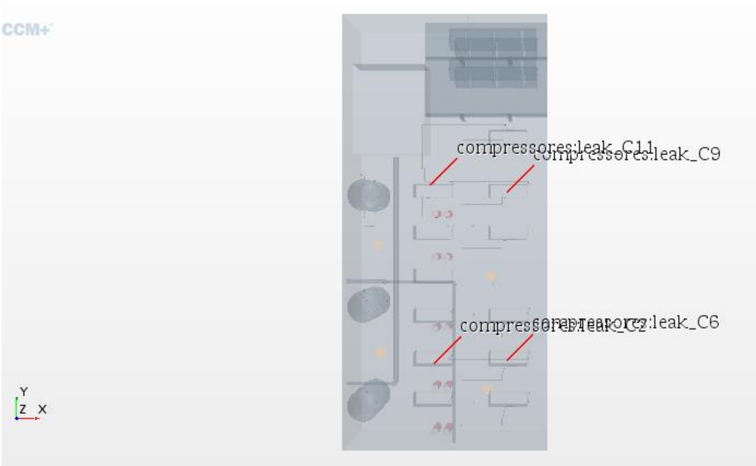


Figure 3 – Refrigeration Room showing the current gas detectors (sensor) and the leak points.

The geometry of the two facilities, Palletizing area and Refrigeration Room, contain the current sensors and the leak points and are illustrated in Figure 2 and Figure 3. For the first case, we chose two flanges valves near the housing and two near the corridor as the leak points. For the latter, we divided the area in four parts due to its length and complexity (it storages Ammonia in 12 compressors, critical area) and chose four different leaks in a manner so that we have a scenario which covers a big Ammonia cloud for the CFD analysis. In both cases, the leak has a 2 mm diameter.

However, in general, for this dispersion study, a continuous leakage of ammonia (gas) through a hole (which could be a crack, for example) was considered in the pipes, flanges and connections and in the valves through which the fluid flows. The type of jet chosen was the axisymmetric one because it is the most used in leakage risk analysis in chemical plants [5, 6]. Based on this, its output condition (pressure, temperature and velocity) and, therefore, the characterization of the type of flow (sonic or subsonic) was calculated from the thermodynamic gas expansion correlations, which include the stagnation condition within the reservoir (tubes, valves, for example). It should be noted that a millimeter hole size and lower pressure ammonia lines were chosen because it would characterize the worst case, that is, less amount of ammonia leaked that would have to be detected in any way

All CFD simulations were held in StarCCM+ software using 10 core (two processor Xeon E5 2670 with 128GB RAM). They were considered 3D ,turbulent, multicomponent (Ammonia +air), monophasic and steady. The governing equations are:

Continuity Equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \qquad (1)$$

Momentum Equation:

$$\frac{\partial(\rho u)}{\partial t}+\nabla\cdot(\rho uu)=\nabla\cdot(\mu\nabla u)-\nabla p+\nabla B+\nabla V \qquad (2)$$

In which, μ is the viscosity, p is the pressure, B gravity force term and V computes the viscous terms.

Chemical Species Equation

$$\frac{\partial(\rho y_i)}{\partial t}+\nabla\cdot(\rho u y_i)=\nabla\cdot(\Gamma_i\nabla y_i)+R_i \qquad (3)$$

In which yi is the mass fraction of the chemical specie i and Ri is the generation or consumption of the chemical species.

Energy Equation

$$\frac{\partial(\rho h)}{\partial t}+\nabla\cdot(\rho u h)=\nabla\cdot(k\nabla T)+S_h \qquad (4)$$

In which h is the specific enthalpy, k is the thermal conductivity, T is the temperature and S_h is the volumetric rate of generated heat. The first term represents the heat transfer by conduction within the fluid.

The turbulent model chosen was κ-ω SST [7] because it is more robust and suitable for gas dispersion applications in complex geometries [6 - 10].

RESULTS

Palletizing Room

The Palletizing Room has dimensions of 7.1 m x 33.9 m and height of 5.2m, approximately. It has four Ammonia detectors (10, 100 or 200 ppm) installed and future installation of 10,000 ppm new one. Figure X shows a schematic representation of the Upper Floor Palletization. Note the existence of ammonia ducts containing 12 valves. The detectors are arranged in the intermediate region of the wall for the valves located near the eaves, and in the upper region of the wall just above some valves, where in this region the detectors are located within each niche (closed rooms containing cooling). Such a configuration in the region is intended to cover the areas around the valves, which is where there is a greater probability of leakage.

The Palletizing room is semi-open, consisting of pipe assemblies and 12 valves through which ammonia flows. It currently has four sensors scattered near the niches and four boxes installed in the ceiling and containing the electronics of the sensors installed inside the niches (considered as Sensors 1 to 8 of Figure 2). As the environment is semi-open, we had to consider a farfield to perform the simulation, that is, to consider a semi-confined space with ammonia leakage through one of the flanges connected to the valve.

The computational mesh had 5,012,502 of elements of the polyhedral type, considering 2 layers of prism near the walls to capture the physics of the boundary layer. It was adequately refined to obtain an accurate solution compatible with the simulated case.

The polyhedral mesh was chosen because it is relatively easy and efficient to construct, provides a balanced solution for complex mesh generation problems and is suitable for internal flow.

Fluids were considered as ideal gases and their main properties are presented in Table 1. The initial and boundary conditions are presented in Table 2 and Table 3, respectively.

Table 1–Fluid Properties.

Fluid Property	Ammonia	Air
Viscosity [Pa.s]	1.0342E-5	1.85508E-5
Molar Mass [kg/kmol]	17.0306	28.9664

Table 2– Initial Condition – Palletizing Room.

Initial Condition	Value
Mass Fraction NH3	0.0
Mass Fraction Air	1.0
Room Temperature	29.7º C

Table 3– Jet Leak Boundary Condition – Palletizing Room.

NH3 Reservoir (pipe) Variable - Value	Applied Condition to the leak hole Variable - Value
T: -3ºC	T: 234.50 K
P: 3bar	P: 1.63 bar
Γ (cp/cv): 1.304	Q: 0.0015 m^3/s

Four different simulations were performed with a leakage point each (4 leaks in the total), and in this section the ammonia plumes of each of these cases are presented, as well as the amount of ammonia detected by the sensors.

In addition, the dispersion study of this room takes into account the overlap of the clouds formed by ammonia, that is, a global mean final result was obtained for dispersed quantity evaluation and how much the current sensors were able to detect.

Table 4 shows the directions of the leak points:

Table 4– Leak points and its directions - Palletizing Room.

Leak Points	Direction
Leak_valv6	- y
Leak_valv8	+z
Leak_valv10	-x
Leak_valv11	+y

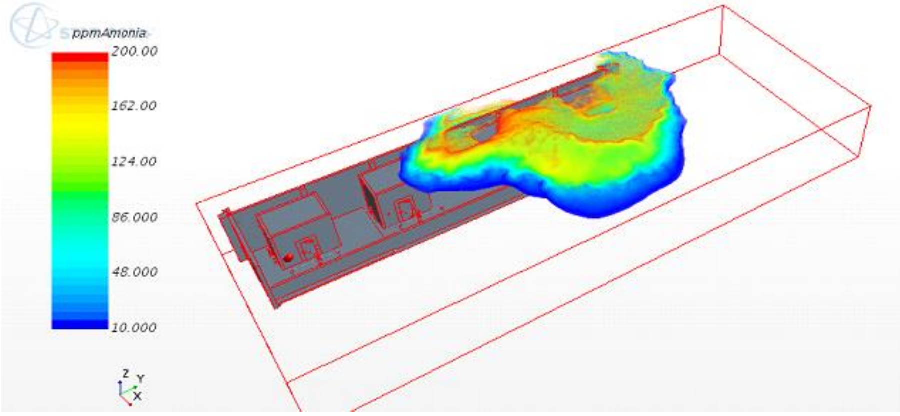


Figure 4 – Gas cloud for the leakage leak_valv6. Ammonia concentration ranges between 10 and 200 ppm.

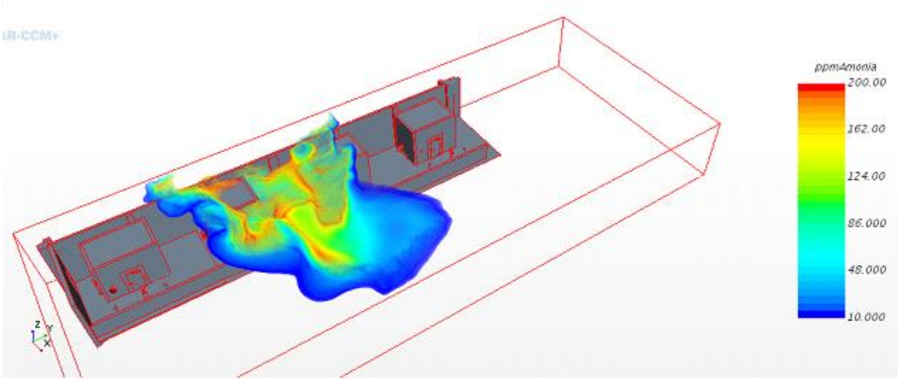


Figure 5 – Gas cloud for the leakage leak_valv8. Ammonia concentration ranges between 10 and 200 ppm.

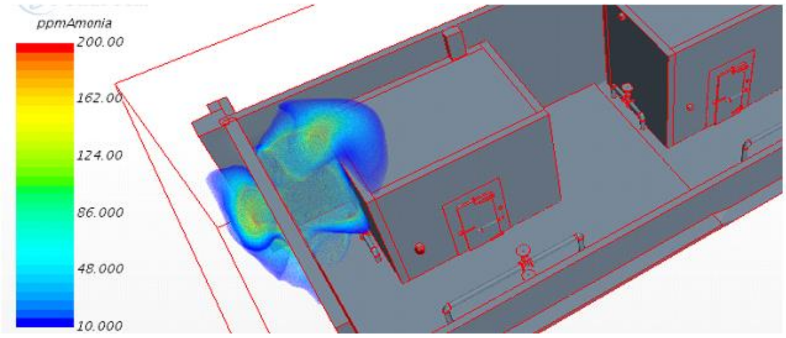


Figure 6 – Gas cloud for the leakage leak_valv10. Ammonia concentration ranges between 10 and 200 ppm.

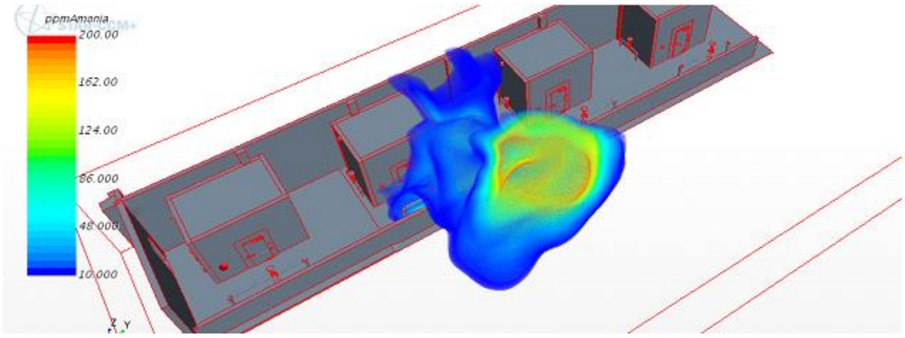


Figure 7 – Gas cloud for the leakage leak_valv11. Ammonia concentration ranges between 10 and 200 ppm.

By the analysis of all the Figure 4, Figure 5, Figure 6 and Figure 7 presented, it can be seen that the clouds have a similar behavior, independently of their location in the room. That is, this behavior can be replicated to leak points on the flanges of the other valves that were not simulated. Such behavior is the tendency to rise (go to the ceiling) and to go out of the aisle (Figure 4 to Figure 7). The most peculiar leakage in this sense is leak_valv10 (Figure 6), as it hits the wall, goes to the ceiling and spreads sideways through the opening in front of it. This happens because it is the only one that contains three walls in its surroundings.

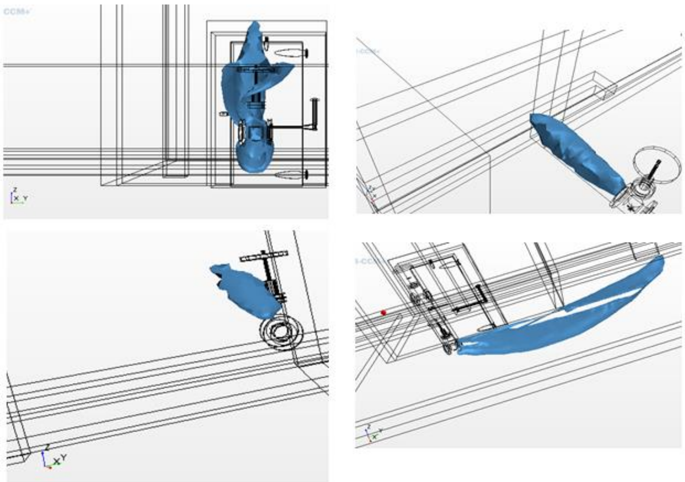


Figure 8 – Iso-Countor of Ammonia cloud for a 10,000 ppm concentration the leakage of the four leak points, leak_valv6, leak_valv10, leak_valv8 e leak_valv11, respectively.

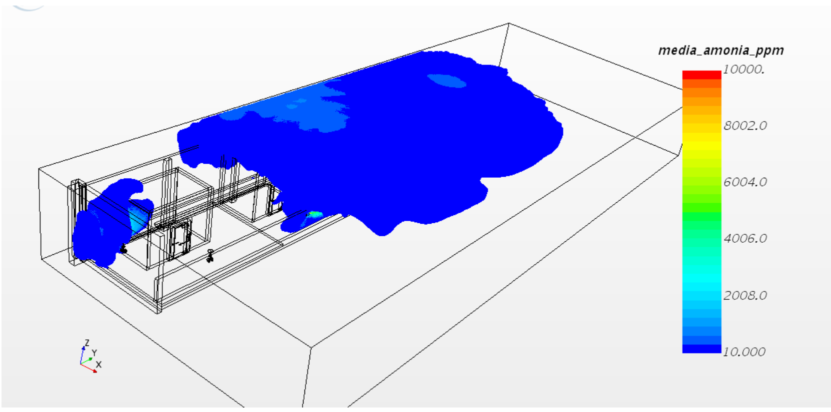
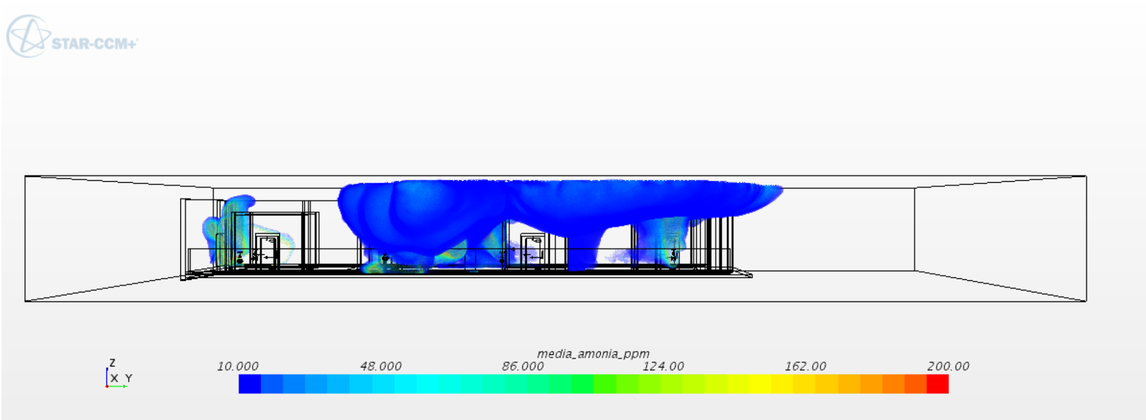
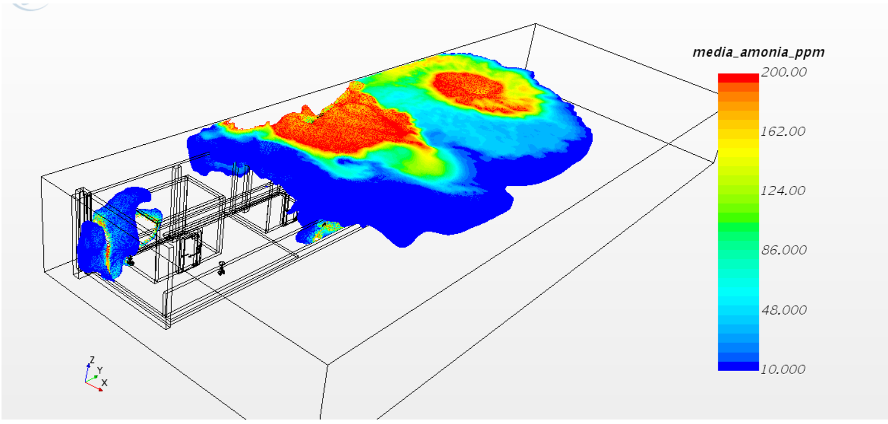


Figure 9 – Ammonia Cloud obtained by overlap of the results of the 4 leaks with a concentration range varying from 10 to 1,000 ppm



(a)



(b)

Figure 10 – Front (a) and isometric (b) views of the plume resulting from the overlap of the results of the 4 leaks with a concentration range ranging from 10 to 200 ppm of ammonia

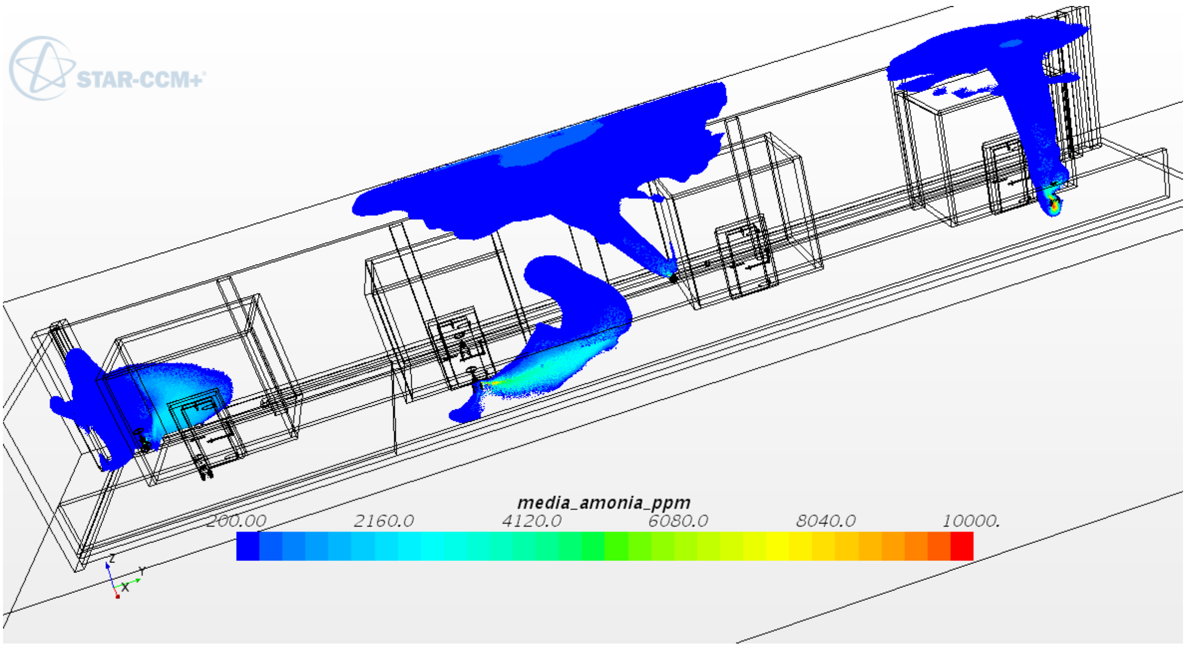


Figure 11 – Isometric views of the plume resulting from the overlap of the results of the 4 leaks with a concentration range ranging from 200 to 10,000 ppm of ammonia

When analyzing the result of the overlapping of the clouds of the 4 simulated leaks (Figure 9, Figure 10 and Figure 11), the behavior described above is confirmed, and it is observed that the environmental ammonia plume is concentrated in the ceiling in case of leakage. The Table 5 and Table 6 show the detected values of ammonia concentration in ppm for the individual cases and for the case of the average of these. Since the GD25, GD27, GD329 and GD31 detectors are located inside the niche, only with their electronics on the outside, it is necessary to reposition the other detectors (GD24, GD26, GD28 and GD30) to a height roof to ensure coverage of the

Table 5–Ammonia concentrations (in ppm) detected by the sensors for the 4 cases of simulated leakage – Palletizing Room

Sensor	Leak_valv6	Leak_valv8	Leak_valv10	Leak_valv11
Sensor 1 – GD24	5.77e-15	8.53e-17	1.127592e-08	6.70e-08
Sensor 2 – GD 26	1.27e-14	3.17e-13	2.470140e+02	6.83e-11
Sensor 3 – GD28	2.19e-06	1.35e+00	2.028949e-13	1.12e+01
Sensor 4 – GD30	1.50e-06	2.72e+01	2.291189e-13	9.14e-03
Sensor 5 – GD31	2.34e-01	4.94e+00	1.276399e-17	1.98e-03
Sensor 6 – GD29	5.36e+00	1.04e+02	2.415130e-17	4.96e+00
Sensor 7 – GD27	5.87e+00	2.79e-02	3.515360e-20	2.47e-13
Sensor 8 – GD25	3.31e+01	2.62e-02	3.760558e-19	2.21e-11

Table 6– Maximum Ammonia concentrations (in ppm) detected by the sensors for the 4 cases of simulated leakage – Palletizing Room.

Sensor	Maximum Ammonia Concentration in ppm
Sensor 1 – GD24	6.70e-08
Sensor 2 – GD 26	2.47e+02
Sensor 3 – GD28	1.12e+01
Sensor 4 – GD30	2.72e+01
Sensor 5 – GD31	4.94e+00
Sensor 6 – GD29	1.04e+02
Sensor 7 – GD27	5.87e+00
Sensor 8 – GD25	3.31e+01

Refrigeration Room

The Cooling Room is a complex room and the one that has the most storage and ammonia passes and therefore is a very critical area. It has 12 compressors and three different ammonia piping lines, plus 6 insufflators and 4 exhaust fans. Currently, it has 5 ammonia sensors installed

Figure 3 shows the simulated geometry with the positions of the sensors and the location of the leak points. It should be emphasized that the compressors were replaced by rectangular boxes of equivalent size, since it is not necessary to detail these equipments in the CFD simulation. On the contrary, they would only leave the larger computational mesh and raise the computational cost unnecessarily because it would not change the problem's physics at all.

The computational mesh had 6.824.474 of elements of the polyhedral type, considering 2 layers of prism near the walls to capture the physics of the boundary layer. It was adequately refined to obtain an accurate solution compatible with the simulated case.

Fluids were considered ideal gases and their main properties are presented in Table 1. The initial and boundary conditions are presented in Table 7, Table 8 and Table 9 , respectively.

Table 7–Initial Condition – Refrigeration Room.

Initial Condition	Value
Mass Fraction NH3	0.0
Mass Fraction Air	1.0
Room Temperature	33º C

Table 8–Jet Leak Boundary Condition - Refrigeration Room.

NH3 Reservoir (pipe) Variable - Value	Applied Condition to the leak hole Variable - Value
T: 72.5ºC	T: 300.04 K
P: 2 bar	P: 1.09 bar
Γ (cp/cv): 1.304	Q: 0.0017 m^3/s

Table 9–Boundary Condition - Refrigeration Room

Air Insuflator Variable - Value	Exhaust Fan Variable - Value
T: 25ºC	T: 26.8ºC
U: 6.0m/s	P: -70 Pa
Mass Fraction (Air): 1.0	

Due to the size and complexity of the room, it was chosen to divide it into 4 parts with a leakage point in each one, being these different and scattered per room in order to cover a greater possible area. The dispersion study of this room takes into account an overlap of the clouds formed by Ammonia, that is, an average final result was obtained for the evaluation of the dispersed quantity and how much are (current) sensors capable of detecting

Table 10– Gas cloud volume for the 4 cases of simulated leakage – Refrigeration Room

Id	Leak - direction	Vol (m^3) 10 ppm	Vol (m^3) 100 ppm	Vol (m^3) 200 ppm	Vol (m^3) 10,000 ppm
Leak C2	-y	13.7394	10.3202	6.2546	0.0041
Leak C6	+z	35.3095	11.1981	3.9822	0.0105
Leak C9	+z	228.4718	76.4325	49.6434	0.0107
Leak C11	+y	24.6283	20.4231	9.3087	0.0170

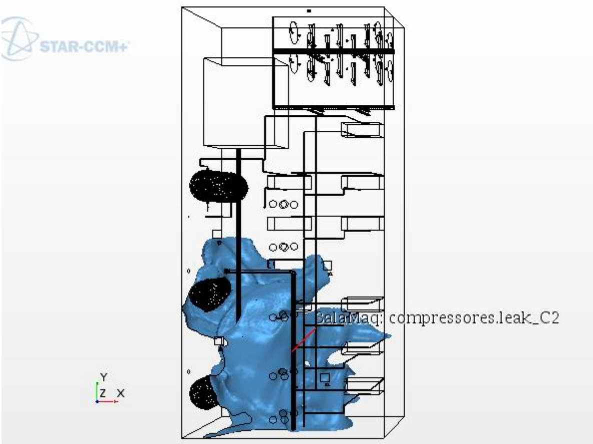


Figure 12 – Iso-Countor of Ammonia cloud of 10 ppm concentration for the leakage leakC2

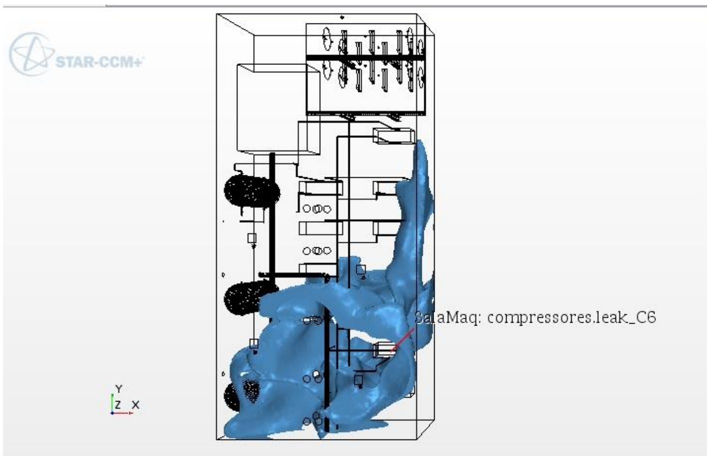


Figure 13 – Iso-Countor of Ammonia cloud of 10 ppm concentration for the leakage leakC6

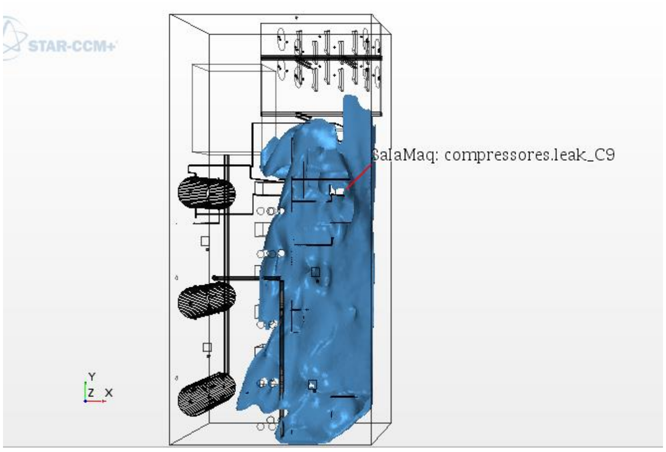


Figure 14 – Iso-Countor of Ammonia cloud of 10 ppm concentration for the leakage leakC9

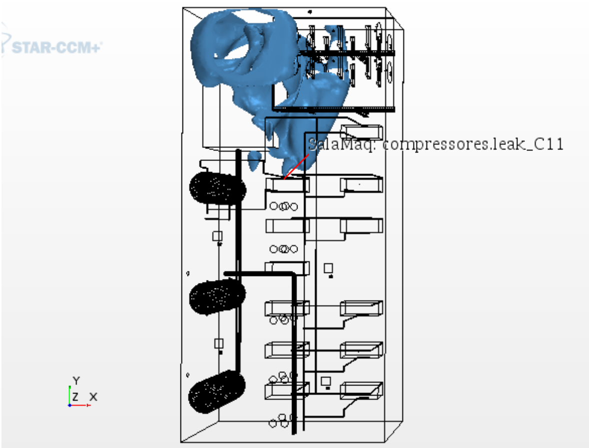
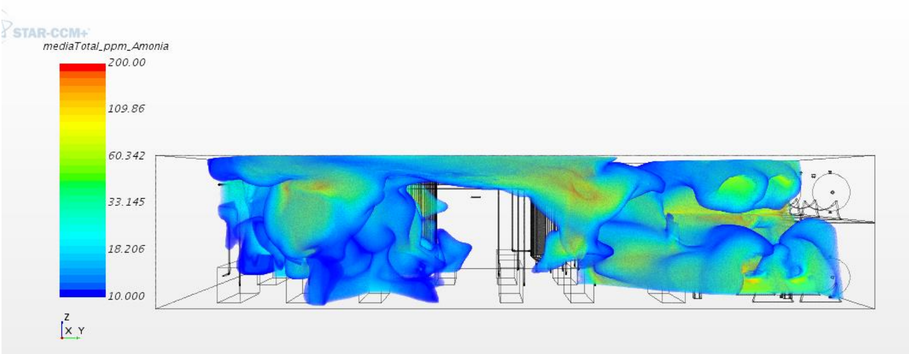


Figure 15 – Iso-Countor of Ammonia cloud of 10 ppm concentration for the leakage leakC11



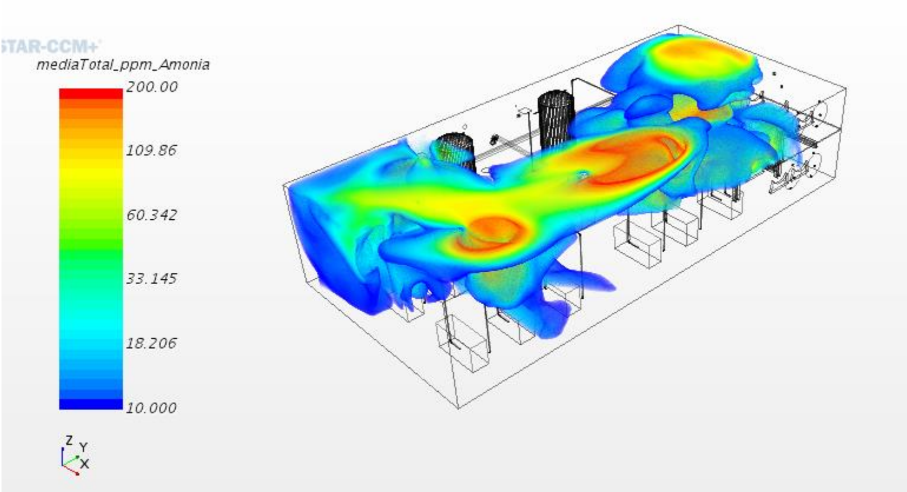


Figure 16 – Isometric views of the plume resulting from the overlap of the results of the 4 leaks with a concentration range ranging from 10 to 200 ppm of ammonia

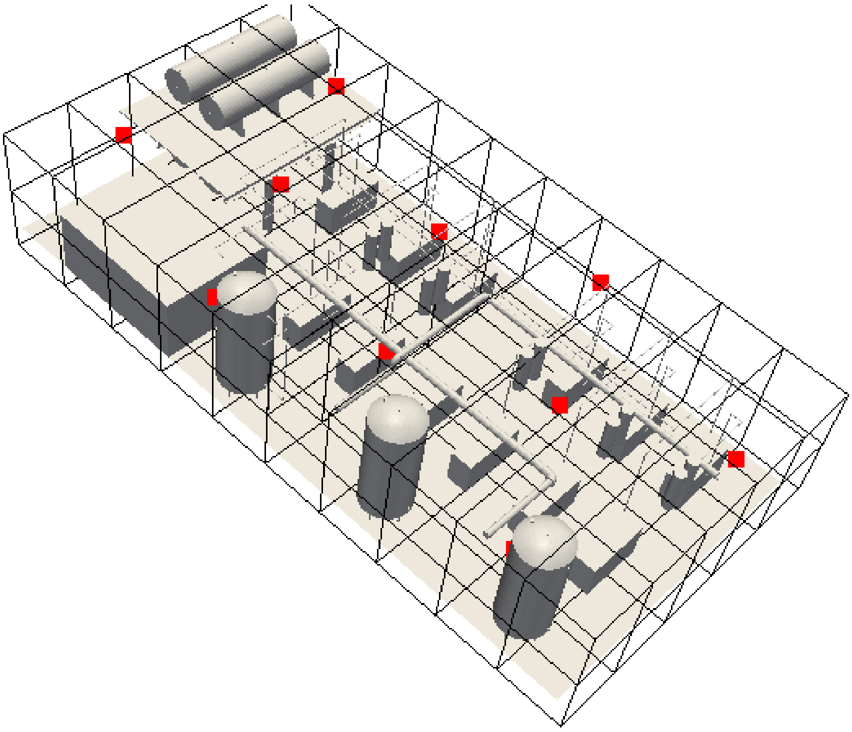


Figure 17 – Detectors localization obtained after OPTIMI post-processing. Isometric view of the Refrigeration Room.

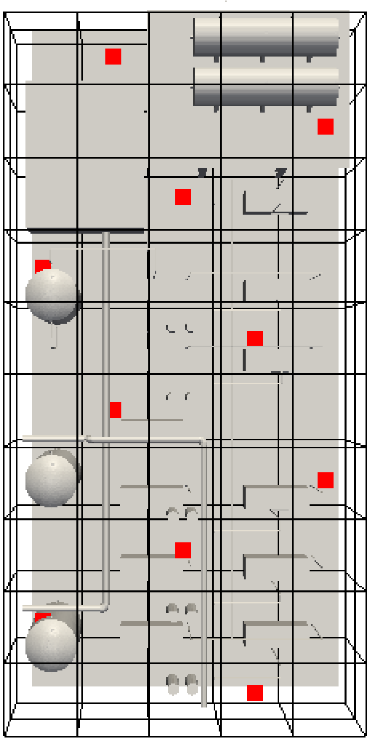


Figure 18 – Detectors localization obtained after OPTIMI post-processing. Top view of Refrigeration Room.

Table 11 – Coordinates of the location of the suggested detectors. A variation of 1.5 meters in each measurement is acceptable. The source is located in the lower left corner of Figure 18.

Detector	Coordinate X (m)	Coordinate Y (m)	Coordinate Z (m)
1	10.5	1.5	4.5
2	7.5	7.5	4.5
3	13.5	10.5	4.5
4	4.5	13.5	4.5
5	10.5	16.5	4.5
6	7.5	22.5	4.5
7	13.5	25.5	4.5
8	4.5	28.5	4.5

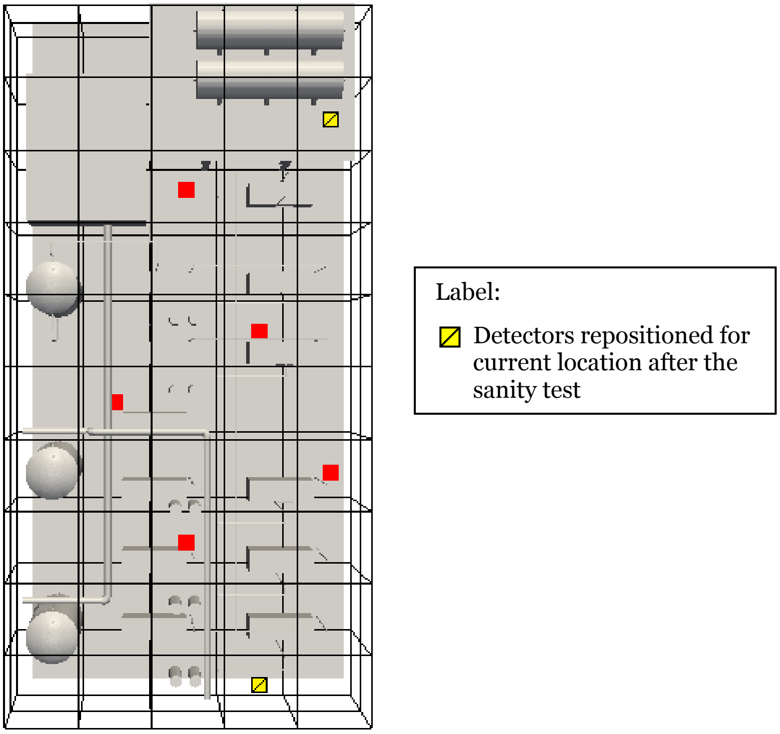


Figure 19 – Detectors localization obtained after the sanity test. Top view of Refrigeration Room.

Analogously to the other results, the simulations of the dispersion study of the Refrigeration Room presented an upward behavior and were dispersed by a good part of the Room. An optimization study was carried out in order to guarantee the coverage of the entire studied area. Optimi software was used, which suggested the use of 17 point detectors.

Taking into account the upward behavior of the plume, a post-optimization was performed which indicated the need for 10 detectors installed in the upper region of the Room (Figure 17 and Figure 18).

After a thorough study with the team of operators and engineers who are involved in the operation of the refrigeration system and are familiar with the room as well as the preventive maintenance process. ("Sanity test"), considering the probable points of leaks and the feasibility of the installation of detectors, the need for 7 detectors were evaluated (Figure 19).

CONCLUSIONS

CFD simulations were conducted for Ammonia dispersion for two industry facilities coupled with OPTIMI tool for evaluation of current and new gas detectors position. But the final decision of the quantity and location of the detectors it is strongly suggested to perform after a "sanity test " with the technical staff of the process plant and the outcomes were:

• Upper floor palletization: after analysis of CFD results and "sanity test" with industry technical staff, it is recommended to reposition 4 detectors (GD24, GD26, GD28 and GD30) to a height close to the ceiling in order to guarantee the coverage of the area.

• Refrigeration room: after the post-optimization and "sanity test" with industry technical staff, it is recommended to add 2 gas sensors to guarantee the area coverage.

Therefore, the obtained results showed to be of great importance in terms of covering 100% of the studied areas allowing the industry to minimize hazardous and risks that Ammonia could cause, once it is an inflammable and high toxic gas and accidents involving this fluid is very common. Besides this, interesting results were found concerning economic savings, once some detectors installed could be reallocated and new ones were not necessary to be bought or installed. Therefore, besides safety concerns there is also the economic savings that can be improved using CFD coupled with OPTMI tool.

Acknowledgement

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