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OPTIMI – A Novel 3D Computational Tool for Gas Detector Optimisation

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Abstract

An efficient approach to optimise the number and location of gas detectors plays a role of paramount importance when gas leak identification at early stage is required. The novel approach relies on the set covering problem (SCP). The optimisation problem is combined to Computational Fluid Dynamics (CFD) and the discrete optimisation problem is solved using Balas algorithm. Every computational cell is regarded as a node of the graph where the links are the common boards shared by the neighbouring cells. The branch and bound routine searches for all solutions identifying the optimal configuration and number of detectors that guarantee full covering of the industrial area considered in the analysis. The graph is read into the code via its adjacency matrix. The characteristic length that determines the size of the computational cell is obtained from the set of CFD simulations considering atmospheric data and features of the geometry. The geometrical model is imported and combined with the results from the optimisation procedure which can be visualised in a 3D post processing stage. This important step of the analysis favours the sanity test normally conducted once the final gas detectors location is established. Any undesirable location (difficult access for maintenance for instance) can be identified prior to installing the detectors saving time, human and financial resources. Optimi is suitable for onshore and offshore facilities, gas storage, warehouses and gas suppliers.

Introduction

Gas releases are always a matter of concern in the chemical industry as well as in any field that deals with gas storage. In recent years, accidents as the gas explosion in Buncefield storage facility and the BP (British Petroleum) exploration offshore platform in Gulf of Mexico are examples of the outcomes of gas or vapour releases. It is therefore crucial to identify gas releases as early as possible in order to avoid or minimise the effects caused by flammable or toxic gas release. Large releases are more promptly identified than small leaks. Therefore, early identification of small releases is an important aspect when performing gas detector analysis.

One of the first attempts to model the placement of gas detectors combining mathematical programming and computational fluid dynamics considered a 2D investigation area and the set covering problem (SCP) as suggested by Vianna and Ferreira [1]. The CFD simulations were performed using FLACS and the optimisation problem resolved with the first version of Optimi, an “in house” code. Results were validated using CPLEX. The work conducted by Vianna and Ferreira, however, only considered the two dimensional domain in the optimisation, although the gas dispersion simulations were conducted using computational fluid dynamics FLACS tool. More recently, Megg et al. [2] combined stochastic formulation with FLACS simulations in order to calculate hundreds of gas dispersion scenarios which were used in the optimisation approach to minimize the time to detection. The modelling suggested by Megg et al. relies on the number of dispersion scenarios and it does require a significant number of simulations in order to have a candidate for placement of the gas detector. Benavides – Serrano et al [3] investigated previously developed gas detector placement approaches and they suggest the incorporation of additional costs in the risk function. For all approaches investigated the dependency on the number of gas dispersion scenario can significantly increase the cost of the analysis. The random approach (RA), however, does not necessarily require any gas dispersion simulation. Megg et al [4] also combined the conditional risk value with the stochastic formulation of the optimisation problem.

We believe that the reduction of the number of gas dispersion simulations necessary for placement of gas detectors is an important parameter in the optimisation analysis. The combination of the calculated results with tri-dimensional geometrical models is also important in order to anticipate any undesirable location that can make maintenance a more difficult task. Another important aspect of the optimisation analysis is the coverage of the area. To address these problems, we propose the modelling of the gas detector location and minimisation of the number of devices based on the set covering problem (SCP). The objective function of the model comprises the sub areas to receive a detector while the constraint set ensures 100% coverage of the area based on CFD results. The number of CFD simulation is based on the combination of leak direction and wind directions which lead to a gas cloud within the interrogation area. The interrogation area can be understood as the area where the gas detectors are likely to be placed. However, in the current work these areas are treated as volumes. Typical small leak rates are considered on the grounds that if the area is protected from small releases it will certainly be protect from large releases.

The rest of this paper is organized as follows. In the next section the set covering problem is briefly introduced. The mathematical formulation of the problem applied to gas detector is introduced and algorithm approach to resolve the optimisation problem is presented as it is coded in Optimi. The section following the formulation discusses the results for a simple example of the set covering problem as well as for a complex p-median problem. The results calculated by Optimi are compared with CPLEX in order to validate the model implemented. The formulation is then applied to a real engineering case where a process area of 625 m^2 is considered. The optimisation of the number of gas detectors and its respective location is discussed. The results are presented qualitatively via graphical outcomes of the code and in quantitative manner providing details of the gas detector location based on geometrical coordinates. In the last section, we finally draw our conclusions.

The set covering problem

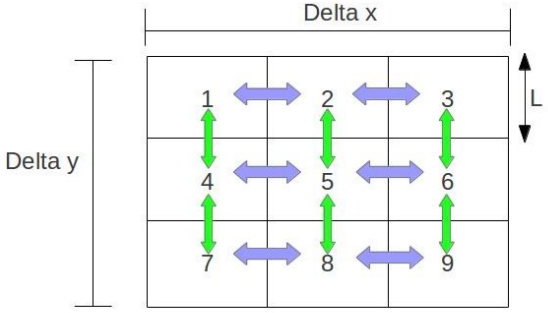
The set covering problem (SCP) was selected as the preferable class model for the optimisation of gas detectors. The selection is based on the set of constrains which ensure 100% coverage of the area to be protected. The principle behind the modelling is to find the minimum set of nodes of a graph that reaches all the remaining nodes that are not in the minimum set.

The problem can also be understood as the minimum number of locations that control/dominate the whole extension area under analysis. The idea discussed above was applied an industrial area. The approach consists in dividing the interrogation area (area to be protected) into sub-areas as shown in Figure 1. The entire area is divided into 9 smaller areas, named subareas. In doing so, each subarea is a candidate to receive a gas detector.

The first part of the analysis relies on input from Computational Fluid Dynamics (CFD) gas dispersion to calculate the characteristic length. The characteristic length is used alongside the x length (*Delta x*) and y length (*Delta Y*) of the interrogation area to calculate the number of subareas in the problem. The same approach is used when the three dimensional case is considered. In the latter case an extra length (*Delta Z*) is considered. The coverage constraint is graphically represented by the arrows in Figure 1. Should a gas detector be placed in the subarea *5*, the methodology ensures that the neighbours subareas (*2,4,6 and 8*) are protected by subarea *5*, in accordance with the dominance criterion. In summary, if a gas detector is placed within subarea *5*, there is no need to place a detector in the neighbour subareas as they will be protected by subarea *5*.

The concept is easily extended to 3D case. In this case, the subarea will also protect the subarea immediately above and below it as illustrated in Figure 2.

Figure 1 (lower view) shows the adjacency matrix of the graph that represents the area from Figure 1 (upper view) to be protected. The colouring scheme helps on the understanding of the dominance.



	1	2	3	4	5	6	7	8	9
1	1	1	0	1	0	0	0	0	0
2	1	1	1	0	1	0	0	0	0
3	0	1	1	0	0	1	0	0	0
4	1	0	0	1	1	0	1	0	0
5	0	1	0	1	1	1	0	1	0
6	0	0	1	0	1	1	0	0	1
7	0	0	0	1	0	0	1	1	0
8	0	0	0	0	1	0	1	1	1
9	0	0	0	0	0	1	0	1	1

Figure 1: Graph dominance in the *x-y* plane. The coloured arrows indicate the dominance. Upper view shows the plane distribution and the lower view shows the adjacency matrix that is read by Optimi. It contains the set of information that ensures the coverage of the interrogation area.

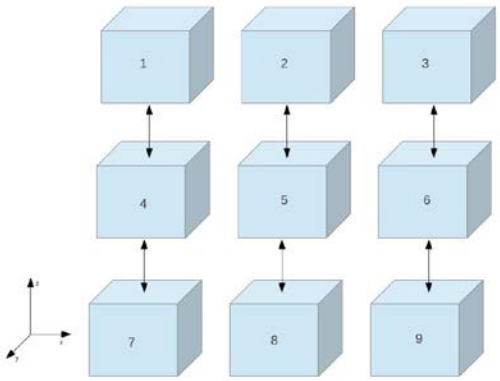


Figure 2: Graph dominance in the *z* orientation. The arrows indicate the dominance. In the suggested approach it means that a detector placed in cell 4 protects cell 1 and 7. The same idea is valid for cells 5 and 6.

The mathematical formulation

The mathematical model of the set covering problem comprises the objective function (*Z)* that must be minimised and the set of constraints which ensures the area coverage.

The inequalities in the set of constraints represent the connection links in the graph of the area where the gas detectors are likely to be placed. At least one detector will protect the area. The {*0,1*} set means that if a particular x_j is *1* it belongs to the final solution set, otherwise x_j is *0.*

Minimize

$$\boldsymbol{Z = \sum_{j=1}^{n} c_j x_j}$$

Subject to:

$$\sum_{j=1}^{n} a_{ij} \geq 1 \quad 1, \dots, m$$

$$x_j = \{0,1\}$$

The key aspect of the model is the size of the subarea, namely the characteristic CFD length scale *L*. It is straightforward to see that as the size of the subarea goes to zero the number

of the nodes of the graph goes to infinity.

The subarea size is defined based on gas dispersion modelling. Ideally a set of CFD cases for small leak rates is performed for each investigation area. The simulation must take into account the meteorological conditions, chemical process operational parameters of the plant and the effects of the geometry. For each leak location 8 wind speeds must be considered together with 6 leak directions, leading to a minimum of 48 CFD simulations. There are however, particular situations where the number of CFD calculations can be reduced. It will depend on the location of the leak in the process area. The characteristic CFD length scale can be calculated based on the expression below;

$$L = \sqrt[3]{Min\left(V_{j,\%LEL}, 0\right)} \quad j = 1, \dots, n$$

where $V_{j,\ \%LEL}$ is the volume of the cloud at a particular percentage of LEL (Lower Explosive Limit) and n is the number of gas dispersion simulation. Based on the cloud volume, the characteristic length is used to calculate the number of candidate subareas to receive a gas detector.

The code implementation has followed the standard form of the binary linear programming for zero-one problems defined as follows;

$$Min\ Z = \sum_{j=1}^{n} c_j x_j$$

Subject to:

$$\sum_{j=1}^{n} a_{i,j} \leq b_j \qquad j = 1, \dots, m$$

$$x_j = 0,1, \quad j = 1, \dots, n$$

The vector c has been assumed to be nonnegative and the search algorithm has been applied to enumerate all 2^n possible zero-one vector x. Following the classical search tree approach, the nodes of the three correspond to a zero-one candidate solution for the vector x. The nodes which are connected by the branch of the three have been set to one or zero or free. A new node has been defined by fixing the value of the variable to one (moving forward in the three) and a node has been revisited if the variable is set to zero (moving backward).

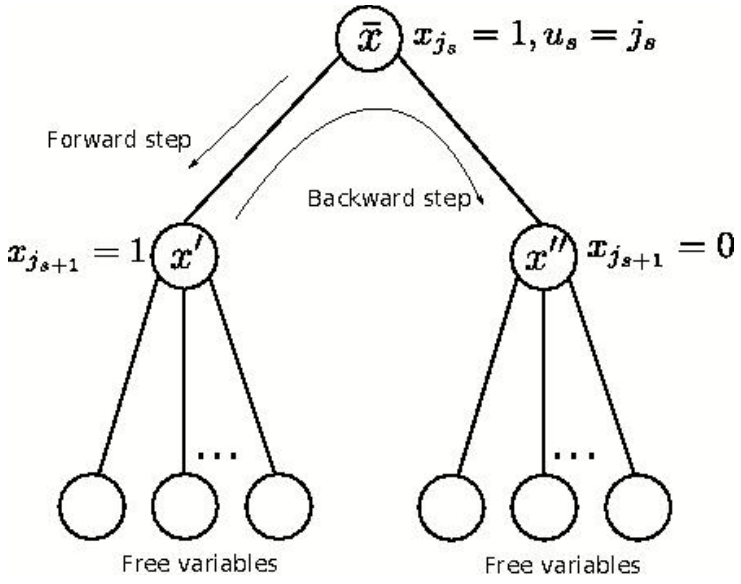


Figure 3: Schematic of the search method for the optimal solution.

In summary the procedure applied here consisted of three main tasks:

- Set the free variable x_{js+1} at value 1
- Solve the sub problem in the remaining free variables
- Set x_{js+1} at value 0 and repeat the process with $x_{js+1} = 0$

In order to keep track of the enumeration process the Balas zero – one additive algorithm was applied. The algorithm was coded in Fortran and it serves as the main routine within Optimi. Detailed description of the steps of the algorithm as it was coded can be found in [5].

Results and discussion

The modelling discussed in the previous sections was applied in three distinct problems. The first problem considered a simple example from the literature. The second problem that was investigated addresses the complex p-median problem. Finally the third problem deals with an engineering application. The optimisation of the number of detectors as well as its location in process area was considered.

The two first problems were used in order to validate the modelling proposed in this work and the implementation of the procedure in the computer code developed.

The set covering problem

The set covering problem considered numerical problem was extracted from Kowalik [5] and the mathematical formulation is presented below;

$$Min\ Z = 10x_1 + 14x_2 + 21x_3 + 42x_4$$

Subject to:

$$-8x_1 - 11x_2 - 9x_3 - 18x_4 \leq -12$$

$$-2x_1 - 2x_2 - 7x_3 - 14x_4 \leq -14$$

$$-9x_1 - 6x_2 - 3x_3 - 6x_4 \leq -10$$

$$x_1, x_2, x_3, x_4 = 0,1$$

The calculation procedure is split into three main parts. The data reading, the implicit enumeration and the post processing of the results. The data reading is performed in accordance with the parameters described in table 1. For the particular problem discussed here the number of variables and the number of constrains is set to *be n = 4, m = 3*, respectively. The constrain matrix *a[1..m, 1..n]*, the right hand side vector *b[1..m]* and the cost vector *c[1..n]* are presented below:

$$a[1..3,1..4] = \begin{bmatrix} -8 & -11 & -9 & -18 \\ -2 & -2 & -7 & -14 \\ -9 & -6 & -3 & -6 \end{bmatrix}$$

$$b[1..3] = [-12 \quad -14 \quad -10]$$

$$c[1..4] = [10 \quad 14 \quad 41 \quad 42]$$

The solution obtained is;

$$X[1..4] = [1 \quad 0 \quad 0 \quad 1]$$

$$Z = 52$$

Table 1 presents the description of all variables used in the problem formulation

Table 1: Variables used in the modelling and their respective description

Input	Description
m	Number of constrains
n	Number of variables
a [1..m,1..n]	Array of constrain matrix
b [1..m]	Array of the right hand side vector
c [1..n]	Array of the cost vector

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The p-median problem

The p-median problem is a location problem with several applications in engineering. The problem is classified as NP-hard what makes the current test case far more complicated than the previous test case considered. It serves as an excellent test for the computer program proposed in this work. The mathematical model of the p-median is presented below. The idea behind the p-median problem is to locate the *p* facilities at a location *J* aiming to minimise the distance between the demanded node *i* and j facility that will attend the demanded node.

$$Min\ Z = \sum_{i \in I} \sum_{j \in J} d_{i,j} x_{i,j}$$

Subject to:

$$\sum_{j \in J} x_{i,j} \geq 1\ , i \in I$$

$$x_{i,j} - y_i \leq 0, i \in I, j \in J$$

$$\sum_{j \in J} y_i = p$$

$$x_{i,j} \in \{0,1\},\ \ i \in I, j\ \in J$$

$$y_j \in\ \{0,1\}, j \in J$$

Table 2 below presents the description of all variables used in the p-median problem modelling.

The p-median problem discussed above was also resolved using CPLEX. The results obtained via CPLEX were compared with the findings form Optimi in order to verify the performance of the code. The total number of facilities selected was 10 with the distances between demanded nodes and sites presented below in matrix $d_{i,j}$.

Table 2: Problem variables for the zero-one p-median optimisation problem

Input	Description
d	Distance between the demand node i and site j
i	Number of demand nodes
j	Number of sites
p	Number of facilities
x	Decision variable for the demand node served by facility j
y	Decision variable for the facility location

$$d[i,j] = \begin{bmatrix} 0 & 3 & 10 & 14 & 13 & 18 & 15 & 15 & 13 & 6 \\ 3 & 0 & 7 & 11 & 10 & 15 & 12 & 17 & 15 & 8 \\ 10 & 7 & 0 & 4 & 6 & 11 & 8 & 16 & 22 & 15 \\ 14 & 11 & 4 & 0 & 4 & 9 & 6 & 14 & 22 & 15 \\ 13 & 10 & 6 & 4 & 0 & 5 & 2 & 10 & 18 & 11 \\ 18 & 15 & 11 & 9 & 5 & 0 & 3 & 11 & 23 & 16 \\ 15 & 12 & 8 & 6 & 2 & 3 & 0 & 8 & 20 & 13 \\ 15 & 17 & 16 & 14 & 10 & 11 & 8 & 0 & 16 & 9 \\ 13 & 15 & 22 & 22 & 18 & 23 & 20 & 16 & 0 & 7 \\ 6 & 8 & 15 & 15 & 11 & 16 & 13 & 9 & 7 & 0 \end{bmatrix}$$

Table 3 below presents the results obtained for the problem considered above. Analysis of the results shows that the same solution has been obtained independent of the computer program used in the calculation. Table 4 below shows the time required to compute the results using Optimi and using CPLEX. Analysis of table 4 shows a significant difference in the time required to calculate the results. However, it is important to bear in mind that the time required by Optimi to provide the solution is well within the acceptable time scale in engineering problem modelling.

Table 3: Results calculated applying Optimi and CPLEX for the p-median problem considering 10 facilities and the distances between the demand nodes and the sites as presented in matrix $d_{i,j}$

# Facilities	1	2	3	4	5	6	7	8	9	10
Optimi	79	47	35	26	18	12	8	5	2	0
CPLEX	79	47	35	26	18	12	8	5	2	0

Table 4: Time required by Optimi and CPLEX to compute the p-median problem with 10 facilities

# Facilities	Optimi Time (cs)	CPLEX Time (cs)
1	6500	7
2	25700	5
3	25500	7
4	11600	7
5	3300	5
6	30000	5
7	16000	3
8	6500	5
9	6000	3
10	0.2	0.02

The Set Covering Problem (SCP) applied to gas detector analysis.

The process area considered in the analysis is 122 m long and 104 m wide. The administration building is 38.5 m high. The leak is placed in the middle of the area between the administration building and adjacent process area close to the limit of the process plant.

A set of 40 gas dispersion simulations was performed for this particular leak location. The CFD analysis considered 8 wind directions and 5 leak directions. Releases pointing upwards were not considered in the analysis as they do not contribute for the gas cloud in the process area.

Figure 4 shows the 3D process plant considered in the analysis. It is also shown in figure 4 the wind directions used in the calculation and the leak location. Analysis of figure 4 also shows the details of the leak hole considered *(x+,x-,y+,y- and z-)* during the gas dispersion.

The simulations were conducted using ANSYS-CFX. The gas dispersion was modelled using the Reynolds Averaged Navier – Stokes and the turbulence problem was closed using the standard k-ε model. Leak rates of 5kg/s were considered. The average wind speed adopted was 6.0 m/s. The log-law wind profile was modelled in accordance with the Moni-Obukhov similarity theory.

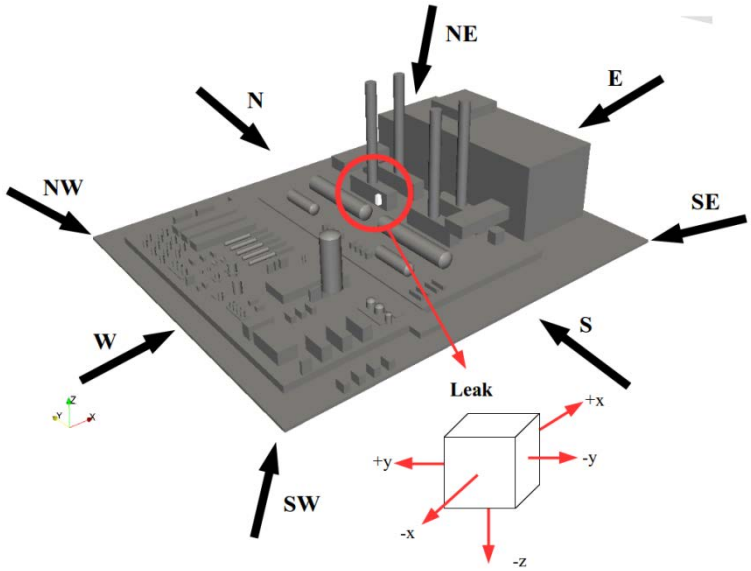


Figure 4: 3D geometrical model of the chemical process area. The leak location is enclosed by the red circle. The leak directions considered in the analysis are presented in detail. The eight wind directions are represented by the black arrows indicating the orientation and direction of wind profile used in the CFD simulations.

Table 5 shows the 40 CFD results obtained by the combination of leak direction and wind direction. The smallest cloud volume calculated was 20.59 m^3. The largest cloud volume was 35.20 m^3. Both cloud volumes were calculated within the flammable limit.

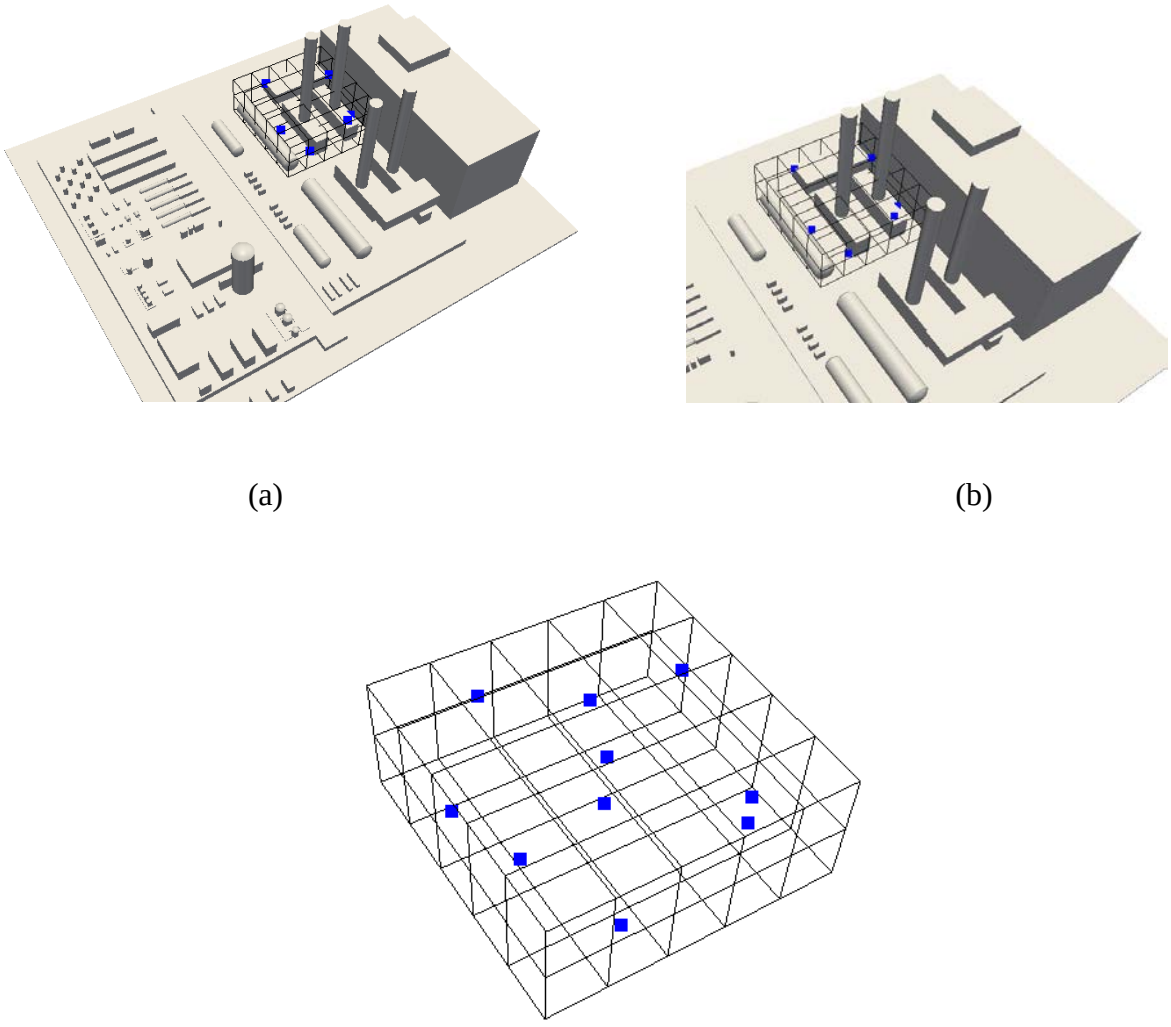
Based on the findings from the CFD analysis, the characteristic length scale selected was 6 m. The process area selected for the placement of gas detectors is 25 metres wide by 25 metres long by 12 metres high. The volume was divided in 50 sub-volumes which were candidates to receive a gas detector. The division is made in accordance with the dominance criterion that is behind the modelling of the set covering problem.

For the area considered in the analysis 10 gas detectors were calculated to cover 100% of the area. Figure 5 shows the results obtained by the proposed model. Figure 5 (a) shows the entire process area as well as the area considered for the placement of the gas detectors. The wire framed box, in black, delimitates the investigation area. The blue dots in figure 5 (a) e (b) show the location of the gas detectors. Figure 5 (c) shows the investigation area (wired frame box) and the blue dots are the suggested distribution of gas detectors based on the set covering problem.

Table 6 shows the *x,y,z* coordinates of the gas detectors based on the origin of the original 3D geometry used in the CFD simulations.

Table 5: CFD dispersion cases used as input in Optimi to calculate the optimal number of gas detector
and the respective optimal location. An overall of 40 cases were considered for the selected leak location. The leak direction is shown in terms of geometrical coordinates. Cloud volumes within the flammable region are also presented in the two last columns of the table.

			LFL=0.03 UFL=0.15	LFL=0.05 UFL=0.15
Simulation Number	Wind direction	Leak direction	Volume (m^3)	Volume (m^3)
1	E	_z	66.60	30.24
2	W	_z	57.46	32.62
3	N	_z	46.14	20.70
4	S	_z	35.20	9.37
5	NE	_z	117.74	65.20
6	SE	_z	79.26	52.63
7	NW	_z	46.20	27.52
8	SW	_z	57.97	36.36
9	E	x	93.16	38.43
10	W	x	49.75	23.35
11	N	x	32.44	19.68
12	S	x	42.36	21.47
13	NE	x	70.05	48.18
14	SE	x	97.97	54.71
15	NW	x	35.62	20.93
16	SW	x	46.66	28.19
17	E	_x	50.71	27.05
18	W	_x	20.59	13.93
19	N	_x	21.14	13.61
20	S	_x	23.25	14.64
21	NE	_x	46.75	32.24
22	SE	_x	45.70	33.16
23	NW	_x	30.08	18.14
24	SW	_x	35.52	21.57
25	E	y	78.77	36.96
26	W	y	43.10	24.12
27	N	y	23.34	14.19
28	S	y	25.75	13.53
29	NE	y	52.61	33.75
30	SE	y	83.12	55.38
31	NW	y	28.22	17.65
32	SW	y	42.27	24.56
33	E	_y	58.63	30.46
34	W	_y	31.27	18.16
35	N	_y	24.28	14.76
36	S	_y	24.95	13.82
37	NE	_y	83.73	59.74
38	SE	_y	64.14	46.77
39	NW	_y	35.32	19.61
40	SW	_y	36.14	20.83



(a) (b)

(c)

Figure 5: Optimi output for the investigation area. (a) Overall view of the process area. The investigation region is shown by the black wired frame box. Blue dots indicate the location of the gas detectors. (b) Detailed view of the process area. (c) The sole investigation region with the placement of the gas detectors indicated by the blue dots.

The graphic visualisation of the results is an important feature of the tool developed in this work. It speeds the process of localisation of the gas detectors during the sanity test avoiding additional sensitivities when placing the devices in the field.

Table 6: Optimal location of gas detectors and the respective computational cell identification

Cell number	x-coordinate (mm)	y-coordinate (mm)	z-coordinate (mm)
2	64,000	53,000	5,500
10	82,000	59,000	5,500
13	70,000	65,000	5,500
16	58,000	71,000	5,500
24	76,000	77,000	5,500
29	76,000	53,000	11,500
31	58,000	59,000	11,500
38	70,000	65,000	11,500
45	82,000	71,000	11,500
47	64,000	77,000	11,500

Conclusions

An integer 0-1 optimisation tool, namely Optimi, was developed for tridimensional optimisation of gas detectors based on CFD data. The methodology is focused on the reduction of the number of gas detectors required to cover 100% of the interrogation area. CFD volume cloud is used as input data to generate the set of constraint. For each leak location is necessary a minimum of 48 CFD cases based on weather condition information and leak direction. This number of CFD simulation is sufficient for the problem modelling due to the characteristics of the set covering problem.

Once the location of the detector is provided, it is possible to calculate the time required for detection. The approach provides graphical results of the optimisation procedure that allows for sanity test prior to installing the devices. This feature saves a lot of time avoiding undesirable situations during the installation.

In the current study, the cost vector c of the objective function was set to one. This means that all sub areas have the same chance of receiving a gas detector. It is possible, however, to attribute a weight for each sub area based on the leak frequency of the process area. This approach would favour specific regions of the interrogation area where the gas leakage is more likely to occur.

It is also possible to address the maximum coverage problem. Assuming that the maximum number of available number of gas detector is known, the procedure developed in the frame work of Optimi is capable of calculating the maximum coverage area.

The methodology discussed in this work can also be combined with a probabilistic gas dispersion analysis based on Monte Carlo simulation. The idea is to reduce the probability of ignition of the gas cloud. The procedure can be repeated until a desirable risk level is reached. Once the risk criterion is match the number of gas detector obtained can be used as an upper bond in the optimisation process of the location of the gas detectors subject to the maximum coverage constraint.

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