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18<sup>th</sup> Annual International Symposium  
October 27-29, 2015 • College Station, Texas

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## **A CFD-based Approach for Gas Detectors Allocation**

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### **Abstract**

Accidental gas releases are detected by allocating sensors in optimal places to prevent escalation of the incident. Gas release effects are typically assessed based on calculating the dispersion from releasing points. In this work, a CFD-based approach is proposed to estimate gas dispersion and then to obtain optimal gas sensors allocation. The Ansys-Fluent commercial package is used to estimate concentrations in the open air by solving the governing equations of continuity, momentum, and energy combined with the realizable  $\kappa$ - $\epsilon$  model for turbulence viscosity effects and species convection-diffusion. CFD dynamic simulations are carried out for potential gas leaks, assuming worst-case scenarios with F-stability and 2 m/s wind speed during a 4min releasing period and considering 8 wind directions. The result is a scenario-based methodology to allocate gas sensors supported on fluid dynamics models. The three x-y-z geographical coordinates for the sensor allocation are included in this analysis. To highlight the methodology, a case study considers releases from a large container surrounded by different types of geometric units including sections with high obstacles, low obstacles, and no obstacles. A non-redundant set of perfect sensors are firstly allocated to cover 100% detection for all simulations releases. The benefits of redundant detection via a MooN voting arranging scheme is also discussed. Numerical results demonstrate the capabilities of CFD simulations for this application and highlight the dispersion effects through obstacles with different sizes.

## 1. Introduction

Accidental gas releases have caused several accidents all over the world. Hence detection of toxic and flammable gas has become a subject of growing importance in industrial environments. In spite of several measures to minimize the possibility of leaks, releases keep appearing in the industry causing severe damages. There is a rather limited defense against flammable or toxic gas leaking and developing into severe consequences without an effective gas detection. Appropriate allocation of detectors could reduce the injury risk, environmental damage and, lately, financial loss to be held in a tolerable level. The need of having gas detectors has been widely accepted in the industry; remaining questions concern about the amount of them and their allocation in the plant. Thus two overall strategies have been often applied: spacing criteria that became convenient for design and number of detectors that impacts cost reporting.

Most releases into atmosphere tend to be time-varying but most dispersion models are limited to continuous or just instantaneous releases. It has been also indicated that leak rates below 0.1kg/s do not typically reach dangerous cloud sizes (Davis, 2015). Relevant aspects of atmospheric turbulence have been detected and various dispersion models outlined with simple corrections for obstructions and topography effects to make calculations more realistic (Deaves, 1992). Pasquill has defined a range of stability categories from A to F to characterize the tendency of vertically displaced parcels of air to move within the atmosphere (Pasquill, 1962). A particular methodology for risk assessment for high pressure CO<sub>2</sub> pipelines using Phast has been presented recently (McGillivray *et al.*, 2014). Another interesting work has indicated the existence of a range of holes sizes where releases may produce worst consequences (Sanguino and Hissong, 2013).

For hazardous releases, consequences depends very much on the extent of the dispersion in the surroundings. When gas is released into any open area, it gets dispersed due to the action of its own momentum and buoyancy, being affected by environmental conditions and degree of congestion (Galeev *et al.*, 2013). Typical releases come from flanges, junctions, etc. and, among consequences, they can generate explosions, jet-fires, or pool fires. The stochastic behavior of the gas dispersion has been successfully modelled via computational fluid dynamics simulation (CFD). Earlier studies had focus on simulating dispersions inside buildings (Gilham *et al.*, 1997; Gilham *et al.*, 2000) but CFD models have been also validated with open-air experimental data (Sklavounos and Rigas, 2004; Habib *et al.*, 2014). Assuming turbulent and non-isothermal flow, preliminary CFD simulations have been carried out based on the  $\kappa$ - $\epsilon$  method to estimate dense gas concentration in buildings (Deaves *et al.*, 2000; Gilham *et al.*, 2000). These model were also validated based on experimental results from simple geometries such as the Silsoe room (Gilham *et al.*, 1997). A parametric sensitivity analysis has been carried out using Phast to understand the influence of user-adjustable input parameters on model outputs while estimating dispersion of nitric oxide, ammonia and chlorine (Pandya *et al.*, 2012).

Allocating sensors based on CFD tends to reduce blind sensing spots due to high concentrations in unexpected regions. API has suggested allocation of sensors depending on the kind of gas for detection. For instance, detection instruments for combustible gas should be able to detect at least two gas concentrations to activate alarms at no greater than 25 and 60 percent of the lower explosive limit (API, 2007). In particular, placement of hydrogen sulfide detectors is a particular subject analyzed in this regulation due to its properties of both toxicity and flammability. It involves consideration of many variables such as concentration of toxic gas in process streams,

specific gravity of the gas mixture, process pressure, atmospheric conditions, ventilation, equipment location, type of decking (solid or grated), and direction of prevailing winds. A detailed design analysis that might include dispersion modeling should be performed to determine the need for and placement of detector systems. The industry has also adopted new systematic methods for detectors placement as suggested in ISA TR84.00.07 (Baybutt, 2012; Marszal, 2015). There exist several sensor types (Center for Chemical Process, 2009); the current most sensitive and reliable technology uses infrared spectroscopy for either point or line-of-sight detection. Senscient produces laser gas detectors with cost around \$15,000-\$20,000 usd/set depending on the gas to be detected (ammonia, carbon dioxide, hydrogen chloride, hydrogen fluoride, hydrogen sulphide, methane or ethylene), in the order of 11-12 ppm as far as 200m (Hudson, 2014). One set covers 5-60 m and a typical plant may need 7-8 sets.

A five-step procedure based on risk estimations has been suggested for finding gas detector spacing where CFD is mainly used to predict consequences such as overpressure values (DeFriend *et al.*, 2008). While modelling optimal detection time in the placement of gas detectors using FLACS, Legg *et al.* (2012) found that a computational bottleneck may appear in the CFD simulations. Their work has been extended to analyze the possibility that a detector may produce false negative alarms or might not be able to perform its intended function due to unavailability (Benavides-Serrano *et al.*, 2013). A parallel research was carried out to include uncertainty analysis based on conditional-value-at-risk (Legg *et al.*, 2013). A meta-modelling strategy has been suggested to reduce the number of CFD simulations by selecting a reduced set but sufficient to rebuild an approximated model based on Gaussian regression models (Wang *et al.*, 2014). Some existing approaches for gas detector allocation have been compared recently in Benavides-Serrano *et al.* (2015). A heuristic approach based on maximizing floor coverage has been used to allocate flame detectors (Mariotti *et al.*, 2014). This assessment indicates that 90% target coverage is set for alarm on a 1ooN voting logic whereas 75% target coverage is obtained for fire detection on a 2ooN voting logic. More recently, four existing approaches for gas detector placement were studied: the Random Approach, the Volumetric Approach, the minimization of the distance between the detectors and the leak sources, and a greedy scenario coverage approach (Benavides-Serrano *et al.*, 2015).

The implementation of MooN voting arrangement means that only upon activation of any M or more sensors in a monitor area will end up in the activation of the specified safety action. It has been indicated that the 1ooN voting arrangements covers 100% of possible scenarios whereas 88% of possible hazard scenarios are covered for the 2ooN; however, these percentages may change due to obstructions (ISA-TR84.00.07, 2010). It is worth mentioning that different voting arrangements are also used to reduce the probability of nuisance or false trips (Torres-Echeverría *et al.*, 2011; Torres-Echeverría *et al.*, 2012; Innal *et al.*, 2015). The risk control represents also a compromise between the safety of the monitored system relating to the SIS safety integrity and its production availability due to false trips relating to the SIS operational integrity (Innal *et al.*, 2015).

The likelihood and severity of consequences due to a leakage could certainly be reduced via prevention with good design practices. However, there is always the possibility of releasing gas and sensors will always be allocated to decrease severity such as the potential escalation of the releasing incident. In previous works, CFD has been used even when either a large number of potential detection points or a target degree of scenario coverage to achieve has been initially

established. Assuming that gas detectors are able to detect flammable gas in the air at concentrations well below the lower flammable limit (LFL), this work presents a scenario-oriented and CFD-based methodology to allocate an appropriate number of sensors. It firstly produces data from CFD for the dispersed gas and then suggest sensor allocation in the process plant. The approach groups wind directions into 8 sectors assuming calm wind conditions and worst-case flowrate releases.

## 2. Approach for sensors allocation

The proposed methodology focusses on allocating sensors to detect gas concentration to prevent fires or explosions before the gas migrates from releasing points to other areas of the plant where this hazard might not normally be expected. The overall idea is that CFD simulations provides excellent estimates for risk concentrations due to gas releases. However, it is important to consider that gas detection per se do not result in risk reduction. A prompt detection will help to reduce consequence effects by applying planned safety actions. The main steps for the sensors allocation procedure are shown in Fig. 1. Explanation of each step is given next.

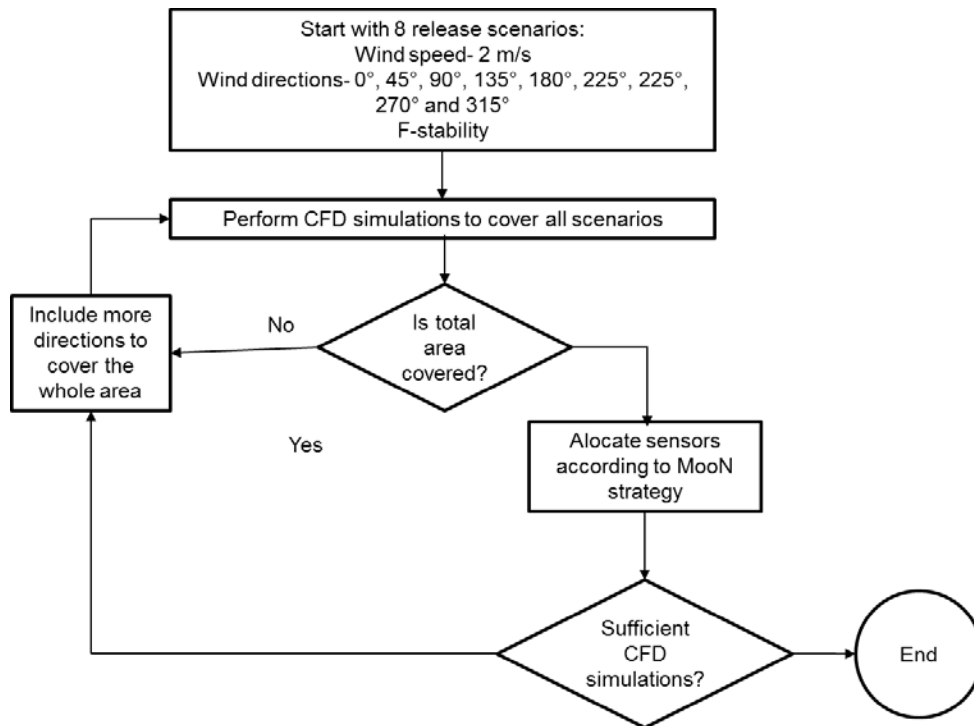


Fig. 1: The overall strategy.

### Step 1: Establishing releasing scenarios

Since detection is the essential component of any mitigation measure, the proposed approach starts by establishing all releasing-threat scenarios. A survey of possible leakage points can be produced using typical HAZOP (hazard and operability) and PHA (preliminary hazard) analysis. However, the possibility of leaks should be reduced as far as practical but further risk analysis

could be contemplated to selectively identify potential releasing scenarios. During process design, safety engineers should ensure that the suggested inherent safety techniques have been reviewed and appropriate safety design standards have been applied to reduce the likelihood of leakage. Risk assessment procedures should also be carried out to take appropriate design measures to ensure that risk remains under tolerable level criteria. The risk evaluation would identify toxic, fire and explosion possibilities under different operation modes and environmental conditions. It will then demand layouts with appropriate safeguards and barriers through identifying potential consequences. Even in cases where appropriate standards are followed, it is suggested to estimate the probability of leakage and verify if the values are inferior to threshold references. In this way, the amount of scenarios with credible probability of leakage could be substantially reduced. Thus the starting step in this methodology consists on allocating the set of points, in pipes or units, where releases could produce threats. Once the whole set of releasing points are defined, next steps in this procedure will be applied in each releasing point.

The use of CFD is suggested to get good dispersion estimations though a large amount of time could be consumed, not only in incorporating the physical description but also in performing calculations. Scenarios for each releasing point are defined according to the following guidelines: Since gas dispersion strongly depends on atmospheric conditions such as wind speed and wind direction, the whole  $360^\circ$  are divided in 8 equally distributed directions to end up in analyzing, for instance, the following wind directions:  $0^\circ$ ,  $45^\circ$ ,  $90^\circ$ ,  $135^\circ$ ,  $180^\circ$ ,  $225^\circ$ ,  $270^\circ$ , and  $315^\circ$ . Wind speed is considered always as wind in calm, 2m/s, as suggested for the worst-case scenario (Crowl and Louvar, 2011). The F-stability level, also suggested for the worst-case scenario, fulfill the requirements for environmental conditions. Thus a rather reduced number of CFD simulations, 8, is initially suggested for the sensors allocation procedure.

## Step 2: Modelling threats: CFD simulations

Threats are typically modelled according to their nature. For instance, a hole in a tank might be modelled as a series of instantaneous releases at decreasing masses or by using an instantaneous release. The need of dynamic models has been discussed in (Witlox *et al.*, 2015) since all releases proceed as a time-varying release with changes in surrounding concentrations. Dynamic CFD simulations are suggested here to estimate concentration levels in each relevant part of the plant under the assumption of continuous release.

An advantage of most CFD codes is that even complex geometries can be incorporated for the simulations, removing the typical “well-mixed” assumption in their calculations. Once the whole physical system has been incorporated into the CFD package, the required number of CFD simulations is performed to estimate concentrations due to the gas dispersion for each releasing point. It has been reported in databases that leaks are critical or hazardous when the detected concentration, a few feet from the leak, is greater than around 25% of the LFL (DeFriend *et al.*, 2008). API (2007) has suggested using 20% as the lower concentration to be detected to prevent threats of fire and explosion. Thus we take as a reference the 20% of the LFL within 3m distance from the releasing point.

Time is probably the most important variable to define sensors allocation (Obenschain *et al.*, 2004). A direct relationship exists among the number of sensors and coverage area for a given detection time: increasing the number of sensors gets lower detection times for a given process plant. In the worst-case scenario, it has been suggested to consider a 10min period for releasing

the entire contents of a vessel or piping system (Crowl and Louvar, 2011). It means that the detection time should be lower than 10min. Hence 4min is suggested here for the dynamic simulation.

Thus CFD dynamic simulations are carried out during 4min with all process units or obstacles affecting the dispersion 2m far from the analyzed releasing point included in the physical description. In particular, the ANSYS-Fluent package is used to perform CFD simulations in this work. Every process unit, pipe or relevant obstruction for the gas dispersion is then incorporated in this computer program using the environment included in the package though other compatible codes could be used for this purpose. Points having concentrations of at least 20% of the LFL, or any other suggested value, should be graphically displayed for further analysis of the sensor allocation. Experimental LFL values for several compounds have been already published in several papers, e.g. Le *et al.* (2013).

Step 3: Is total area covered?

After performing all CFD simulations, 8 proposed here for the first iteration, the percent of covered area should be identified. All clouds indicating concentrations of at least 20% of LF could then be constructed for each release scenario. Allocating a circle with a radius of 2m centered in the releasing point will have one of the following results: 1) all clouds remain inside the 2m-circle meaning that no sensor is required at all since the release is not sufficient to achieve high risk; 2) the 2m circle centered in the releasing point is fully covered by the clouds and the procedure should continue with the following step to allocate sensors; and 3) some areas are not covered by the clouds in which case more CFD simulations should be carried out. Additional CFD simulations should consider wind directing towards uncovered areas. Fig. 2(a) shows a pictorial description of the three types of results.

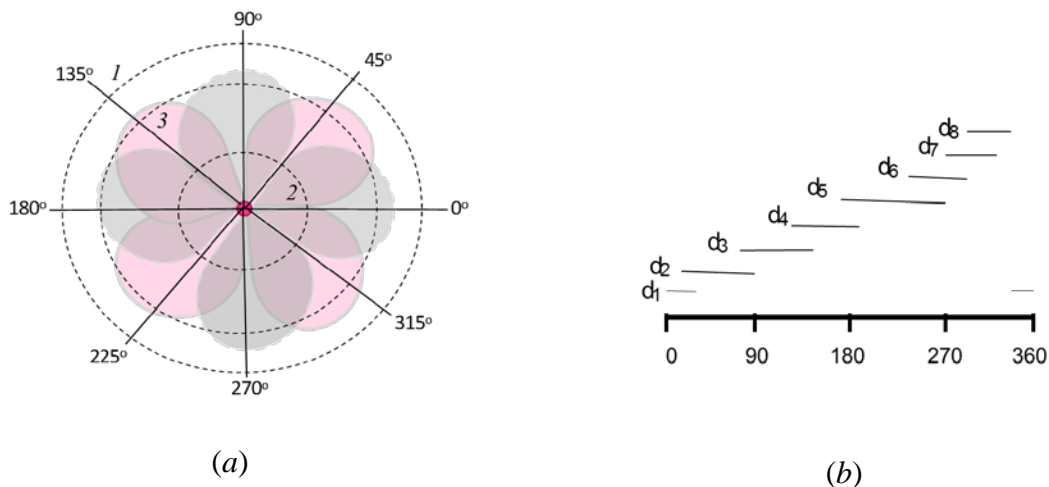


Fig. 2: Results of CFD simulations: a) Contour for gas dispersion in 8 d-directions; b) covered angular map sectors at 2m separation distance.

#### Step 4: Allocating sensors

The main purpose of the optimal location of sensors is to protect population and assets against exposure and effects due to the released substances. This work focus on fire and explosion but the approach can easily be adapted for toxic releases. The objective is to maximize the detection coverage in the geographic area using CFD simulations. Optimal allocation scheme normally depends on the type of sensor and several stopping criteria have been used to declare success of the allocation (Lee and Kulesz, 2008). Gas sensors or detectors are devices detecting concentrations of flammable or toxic products and they can be either fixed or portable and either point or open-path. The open-path detectors works by emitting an infrared light which presents distortions in the receiver when crossing a gas cloud. They could cover big distances, up to 150 meters, but there should be no physical obstructions in between the emitter and receiver neither be subject to vibrations. Alarms could then be activated to notify people about formation of a flammable or toxic atmosphere. The methodology developed here is restricted to using fixed-point sensors so that the purpose is to maximize coverage of a geographic or geometric area though considering three dimensions, the plain and height. The insight gained information from CFD simulations contains spatial variations used here to identify a number of spatial regions where sensors should be allocated. The three coordinates could be detected during the CFD simulation.

A typical criterion to allocate sensors had been based on detecting areas with concentrations above 2% volume or 20% LFL regardless of prevailing wind direction (ISA-TR84.00.07, 2010; Marszal, 2015). From a CFD simulation, an angular interval can be extracted to indicate the section where a sensor could detect the release 2m far from the emission. A lines graph can be extracted to indicate all angular sector affected for each simulated releasing scenario. Figure 2(b) shows an example for 8 CFD simulations averaged in the corresponding 8 directions 0°, 45°, 90°, etc. It is clear that allocating one sensor for each simulated scenario will cover the indicated area. However, it should also be noticed that sensors could be allocated in such a way that they could detect more than one scenario. A simple procedure can be used to allocate the minimum number of sensors: start by allocating a sensor detecting the biggest number of scenarios and remove these scenarios; then repeat the procedure until all scenarios have been detected. In this way, some scenarios might be detected with more than one sensor but the whole set will not be redundant. Some irregularities could be produced when surrounding obstacles produce different sizes in the horizontal lines shown in Figure 2(b). Knowledge of this non-uniformity concentration in the open area is then particularly crucial for appropriate sensors allocation.

Lastly, the height of the sensor depends very much on the gas density. For instance, hydrogen clouds are normally farther from the ground level or buildings than in the case of methane clouds because of buoyancy and often higher sonic speed at the release. It in fact tends to decrease the probability of ignition and reduce the flame acceleration due to obstacles in case of ignition (Wilkening and Baraldi, 2007). The same procedure above described is suggested to allocate the height where sensors should be allocated. Side views of the clouds in CFD simulations can easily be used to detect where concentration is at least 20% of the LFL. Fig. 3 shows the result of height vs average angle for the starting 8 simulated scenarios. When a sensor is expected to sense two directions cannot detect one of them due to the height then two sensor must be allocated.

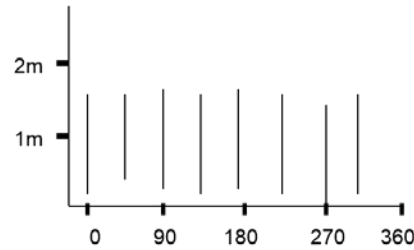


Fig. 3: Vertical coverage area

Sensors are assumed at this stage to be perfect detectors, i.e. any amount of material passing through them will always indicate when the set point is achieved. Redundancy becomes a requirement when considering that detectors might be unable to perform their intended function, i.e. sensors can fail and become inoperative until replaced or repaired. Allocation of sensors is thus carried out in two stages. In the first stage, the minimum number of sensors is determined to produce a non-redundant set and, in a second stage, redundancy is used to protect the system.

A question merging concerning a redundancy analysis is related to a MooN architecture competing with marginal utility. A MooN scheme is used to avoid spurious operations: 1oo1 architecture consists of a single channel, where any dangerous failure leads to a failure of the safety function when a demand arises; 1oo2 architecture consists of two channels connected in parallel so that either channel can process the safety function (Guo and Yang, 2007; Lu and Jiang, 2007). The interest in using certified safety instrumented systems (SIS) has considerably increased in recent years. A typical MooN architecture is assumed to configure each of SIS parts where M out of N channels must work for the safety function to be successfully fulfilled (Innal *et al.*, 2015). In allocating sensors, redundancy is introduced when more than one sensor is required to activate the alarm when values above the set point are detected.

Step 5: More CFD simulations?

CFD is used to determine a minimum number of sensors for any desired architecture. A non-redundant set is the one detecting all dangerous abnormal releases without using more than one sensor, 1ooN voting architecture. A redundant system means that each scenario should be detected by more than just one sensor. Then it must be verified that the expected criteria, one or more sensors detecting each release scenario, can be satisfied. When more CFD simulations are required to achieve the goal then more release scenarios are defined; otherwise, the final allocation is done.

### 3. The CFD model

Computational fluid dynamics is a branch of scientific computing and mathematics that has undergone large growth in last decade. It produces numerical solution to a system of partial differential equations describing fluid flow. According to Rizzi and Engquist (1987), the works by L.F. Richardson marks the beginning of the CFD era with his work in 1917, compiled in his book “Weather prediction by numerical process” in 1922. The discovery of the basic equations is attributed to the works by Euler and Navier and Stokes. Solution to these equations have been coded in several computational commercial codes. In this work, the code ANSYS FLUENT is used to calculate the momentum, heat and mass transfer from the Reynolds averaged Navier-Stokes equations. An interesting comparison of methods to estimate gas dispersion of varying



complexity has been produced in Habib *et al.* (2014). The  $\kappa$ - $\varepsilon$  turbulence model (Launder and Spalding, 1974) is used here to account for the turbulence. It also offers the possibility to easily adapt the turbulence parameters  $\kappa$  and  $\varepsilon$  to measured wind and turbulence profiles. Based in this model, another strategy called the  $\kappa$ - $\varepsilon$  realizable emerged to increase precision in estimating speed fluctuations (Shih *et al.*, 1995). In this model, dissipation rate equation is based on the positivity of normal Reynolds stresses and the Schwarz' inequality for turbulent shear stresses in the dynamic equation of the mean-square vorticity fluctuation at large turbulent Reynolds number. Hence the mathematical model solved in this work corresponds to a dynamic, compressible, homogeneous, non-isothermal, and without generation of momentum or energy system.

Thus the release is simulated as a flow through a small hole between a high-pressure pipeline and the environment in a 3-D scenario. The government equations are continuity, momentum conservation, energy conservation and  $i$ -species conservation, respectively described as follows:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \rho \mathbf{v} \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) = -\nabla \cdot \rho \mathbf{v} \mathbf{v} - \nabla P - \nabla \cdot \boldsymbol{\tau} - \rho \mathbf{g} \quad (2)$$

$$\frac{\partial}{\partial t}(\rho C_p T) = -\nabla \cdot (\rho C_p T \mathbf{v}) - \nabla \cdot \mathbf{q} - \boldsymbol{\tau} : \nabla \mathbf{v} \quad (3)$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{v}) = -\nabla \cdot \mathbf{J}_i \quad (4)$$

where  $\rho$  is the density,  $\mathbf{v}$  is the velocity vector,  $P$  is pressure,  $\boldsymbol{\tau}$  is the stress tensor,  $\mathbf{g}$  is the gravity vector,  $C_p$  is the heat capacity,  $T$  is temperature,  $\mathbf{q}$  is the heat flux vector which involves conduction,  $\mathbf{Y}_i$  is the mass fraction of  $i$ -species,  $\mathbf{J}_i$  is the diffusive mass flux which involves the Fick law.

The  $\kappa$ - $\varepsilon$  realizable model is:

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot \rho \mathbf{v} k = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + \mu_t \left[ \left[ (\nabla \mathbf{v})^T + (\nabla \mathbf{v}) - 2(\nabla \cdot \mathbf{v}) \mathbf{I} / 3 \right] - 2\rho k \mathbf{I} / 3 - \frac{1}{\rho \text{Pr}} \mathbf{g} \cdot \nabla \rho \right] - \rho \varepsilon + \frac{2\rho \varepsilon k}{\gamma RT} \quad (5)$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot \rho \mathbf{v} \varepsilon = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} - C_{1\varepsilon} \frac{\varepsilon \mu_t}{\rho k \text{Pr}} \mathbf{g} \cdot \nabla \rho + \rho C_{1\varepsilon} \left[ (\nabla \mathbf{v})^T + (\nabla \mathbf{v}) - 2(\nabla \cdot \mathbf{v}) \mathbf{I} / 3 \right] - 2\rho k \mathbf{I} / 3 \quad (6)$$

where  $k$  is the kinetic turbulent energy,  $\varepsilon$  is the dissipated energy,  $C_{1\varepsilon}$ ,  $C_2$ ,  $\sigma_k$  y  $\sigma_\varepsilon$  are parameters determined from experiments. Thus, the release is simulated as a flow through a small hole between the high-pressure pipeline and the environment in a 3-D scenario.

#### 4. Case Study

The case study proposed here is used to highlight the above described methodology. A large spherical tank of 5m diameter containing 1-butene. It is considered that several units exist in south surrounding area whereas an empty field is allocated in the north. Surrounded units are

modelled here as different sizes obstacles. All obstacles are considered of rectangular shape (hexahedra) and dimensions for those in the south-east direction are higher than those in the south-west. Figure 4 gives an upper view of the physical description. The environment is assumed to be according to the worst scenario where wind speed is 1.5 m/s at 300K and F-atmospheric condition. The vertical speed profile is represented with the model:

$$v = v_{ref} \left( \frac{z}{z_{ref}} \right)^p \quad (7)$$

where  $v$  is the speed at  $z$ -high,  $p$  is an atmospheric parameter ( $p = 0.43$ ) and subindex  $ref$  indicates reference parameters  $v_{ref} = 1.5 \text{ m/s}$  y  $z_{ref} = 10 \text{ m}$ .

A rupture is assumed to occur at 0.5m above surface level to release 1-butene (LFL= 1.6% vol) at 1kg/s and 290K. Dimensions for the low obstacles footprints were 5m x 1.7m, and 4.5m high representing 90% of the sphere height. The second group of obstacles contains footprints of 1.8m x 1.7m and 1.6m x 4.6m, all of them 2.5m height that represents 50% of the sphere height. The final grid contains 118,529 hexahedral elements and the grid strategy was proximity and curvature to refine spaces of lower size. The transition of the grid was slow with smootinh level following a growth level of 1.1. Figure 5 shows a radial cut of the grid at 3m above surface.

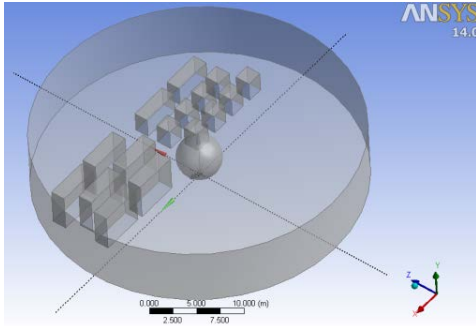


Fig. 4: Geometric system description.

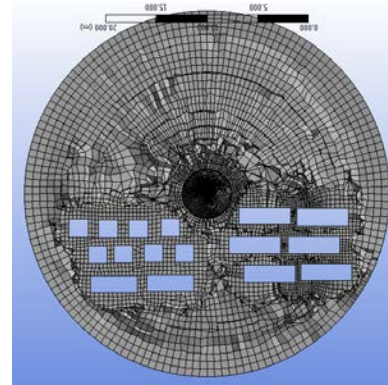


Fig. 5: Grid in a radial cut 3m above surface.

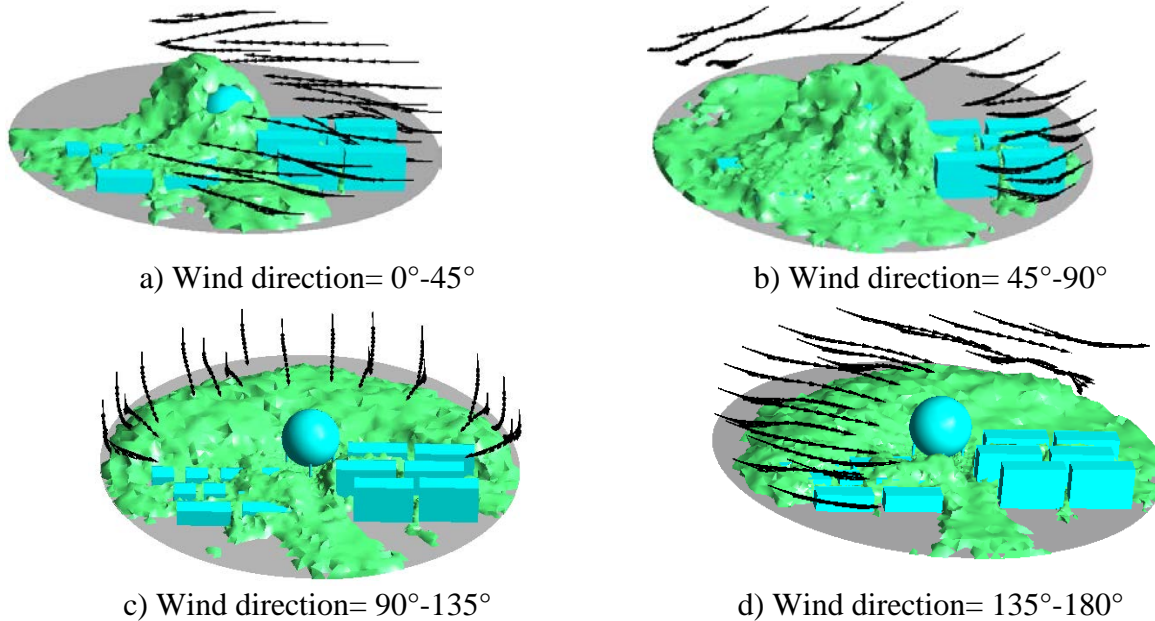
In the case study, 8 wind directions were considered as indicated above. CFD results indicate that directions  $90^\circ$ - $135^\circ$ ,  $135^\circ$ - $180^\circ$  and  $180^\circ$ - $225^\circ$  have shown largest clouds due to the obstructions effect in the opposite wind direction. Directions  $225^\circ$ - $270^\circ$ ,  $270^\circ$ - $315^\circ$  and  $315^\circ$ - $360^\circ$  have shown smaller clouds due to the different type of obstacles in the opposite wind direction. Fig. 6 shows clouds of 60% LFL where lines indicate wind direction, during a 4min release. Fig. 7 shows contours for different mass fractions of isobutene: 0.0184, 0.0157, 0.013, 0.0103, and 0.0077, being the blue one (mass fraction= 0.0077) the one corresponding to the 20%LFL and required in our proposed procedure. These CFD simulations were then used to extract the angular distribution suggested in Fig. 2. From final results shown in Fig. 8a, it can be suggested that a single sensor is sufficient and it should be allocated in between directions  $200^\circ$ - $315^\circ$ . The height is obtained by extracting results as suggested in Fig. 3. These results are given in Fig. 8b where it is observed that the concentration of 20%LFL covers the whole 2m height. It means that sensors inside this interval will be able to detect probable releases from the analyzed

process unit. Thus the single sensor could be allocated at a typical 1.5m height to cover all potential releases. It is worth mentioning that using a single sensor implies a non-redundant system. However, CFD results are sufficient to design a MoonN scheme to produce a more effective redundant scheme.

## 5. Conclusions

A CFD-based methodology to allocate sensors has been presented in this work. The proposed methodology places sensors based on a sufficient number of CFD simulations. A minimum of 8 simulations is suggested but the final number will depend on covering all 360° directions. Worst-case scenarios are also assumed for meteorological conditions but, if preferred, these conditions could be adapted with historical conditions. Sensors are then placed to detect the releases whenever they might occur, thereby protecting potentially affected population. Following suggested standards, a release should be detected to prevent concentrations above 20%LFL at 2m distance from potential release points. It is also suggested to perform a MoonN scheme analysis to prevent false trips.

**Acknowledgements:** The authors would like to acknowledge the support provided by CONACyT-Mexico and the Mary Kay O'Connor Process Safety Center in the Texas A&M University.



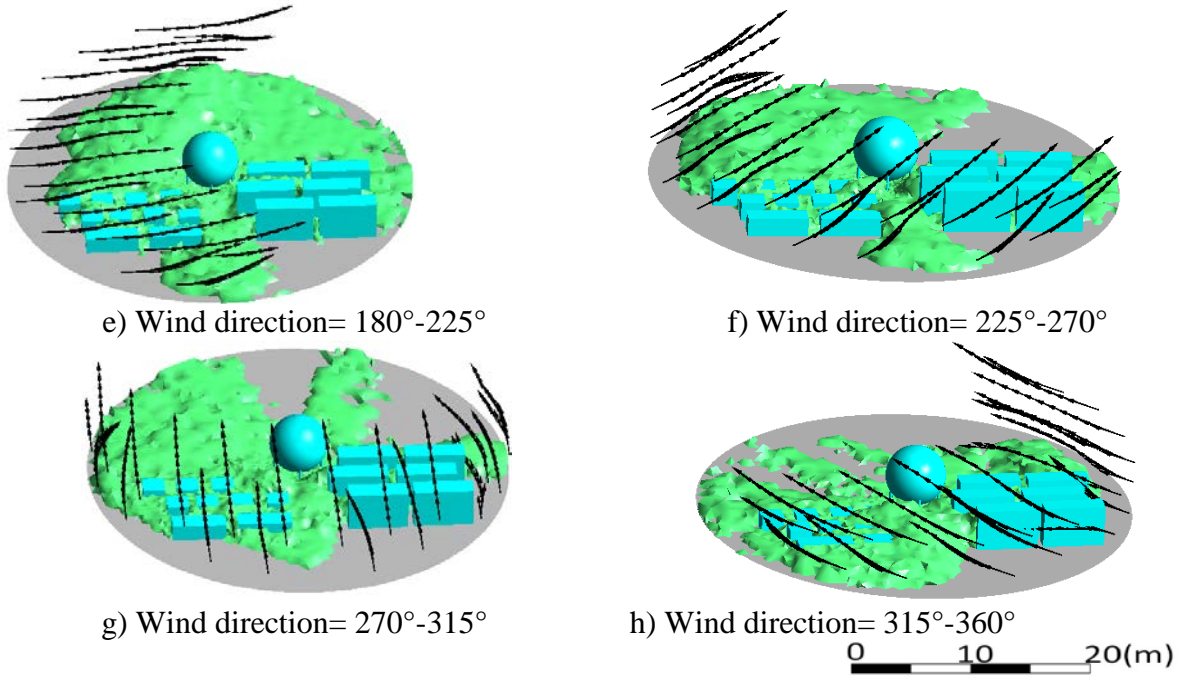
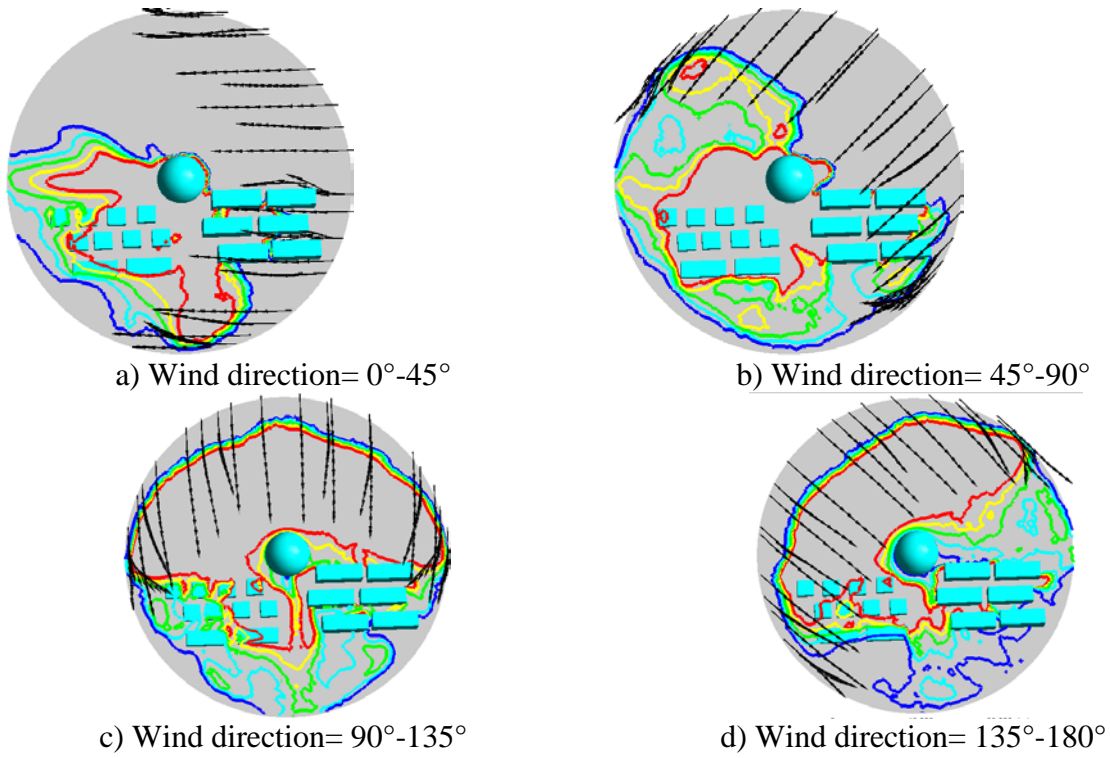


Fig. 6: 1-isobutene clouds with 60% LFL iso-volume in all wind directions



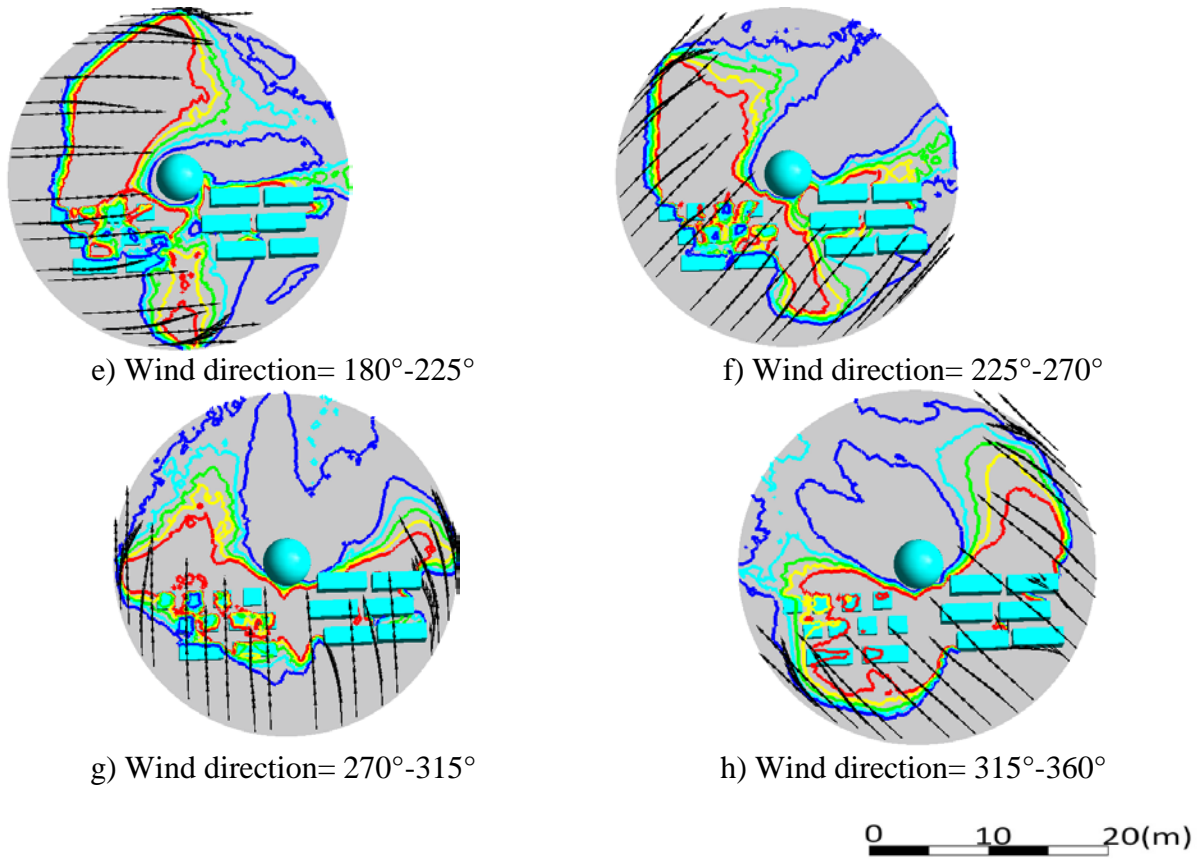


Fig. 7: 1-isobutene mass fraction contours in all wind directions: — 0.0184, — 0.0157, — 0.013, — 0.0103, and — 0.0077.

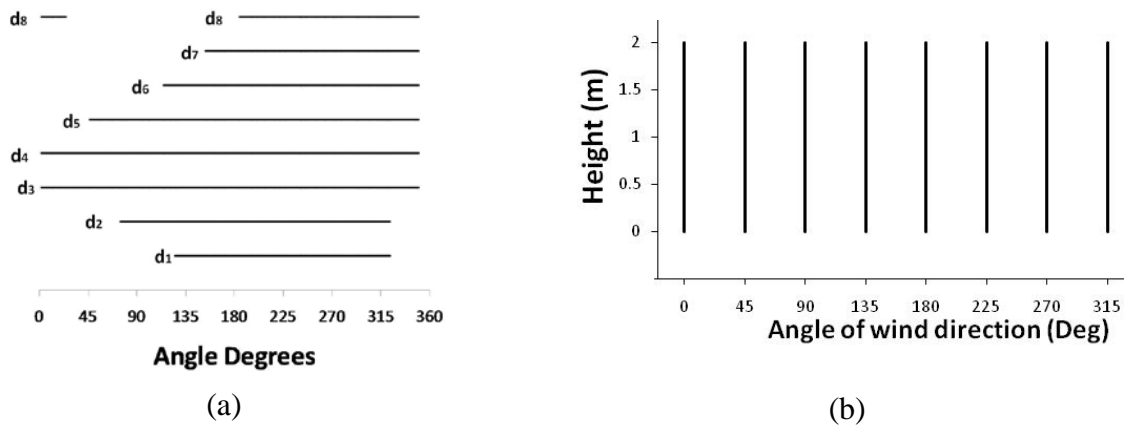


Fig. 8. Results for a) covered angular map in all wind directions, and b) vertical coverage.

## References

- API (2007). API Recommended Practice 14C: Recommended practice for analysis, design, installation, and testing of basic surface safety systems for offshore production platforms, 7th Edition.
- Baybutt, P. (2012). "Using layers of protection analysis to evaluate fire and gas systems." Process Safety Progress **31**(3): 255-260.
- Benavides-Serrano, A. J., S. W. Legg, R. Vázquez-Román, M. S. Mannan and C. D. Laird (2013). "A Stochastic Programming Approach for the Optimal Placement of Gas Detectors: Unavailability and Voting Strategies." Industrial & Engineering Chemistry Research **53**(13): 5355-5365.
- Benavides-Serrano, A. J., M. S. Mannan and C. D. Laird (2015). "A quantitative assessment on the placement practices of gas detectors in the process industries." Journal of Loss Prevention in the Process Industries(In press, <http://dx.doi.org/10.1016/j.jlp.2014.09.010>).
- Center for Chemical Process, S. (2009). Continuous monitoring for hazardous materials release, Center for Chemical Process Safety/AIChE.
- Crowl, D. A. and J. F. Louvar (2011). Chemical process safety : fundamentals with applications, 3rd ed., Prentice-Hall international series.
- Davis, S. (2015). "Using CFD to Analyze Gas Detector Placement in Process Facilities."
- Deaves, D. M. (1992). "Dense gas dispersion modelling." Journal of Loss Prevention in the Process Industries **5**(4): 219-227.
- Deaves, D. M., S. Gilham and H. Spencer (2000). "Mitigation of dense gas releases in buildings: use of simple models." Journal of Hazardous Materials **71**(1–3): 129-157.
- DeFriend, S., M. Dejmek, L. Porter, B. Deshotels and B. Natvig (2008). "A risk-based approach to flammable gas detector spacing." Journal of Hazardous Materials **159**(1): 142-151.
- Galeev, A. D., E. V. Starovoytova and S. I. Ponikarov (2013). "Numerical simulation of the consequences of liquefied ammonia instantaneous release using FLUENT software." Process Safety and Environmental Protection **91**(3): 191-201.
- Gilham, S., D. M. Deaves, R. P. Hoxey, C. R. Boon and A. Mercer (1997). "Gas build-up within a single building volume — comparison of measurements with both CFD and simple zone modelling." Journal of Hazardous Materials **53**(1–3): 93-114.
- Gilham, S., D. M. Deaves and P. Woodburn (2000). "Mitigation of dense gas releases within buildings: validation of CFD modelling." Journal of Hazardous Materials **71**(1–3): 193-218.
- Guo, H. and X. Yang (2007). "A simple reliability block diagram method for safety integrity verification." Reliability Engineering & System Safety **92**(9): 1267-1273.
- Habib, A., B. Schalaus and D. Schmidt (2014). "Comparing tools of varying complexity for calculating the gas dispersion." Process Safety and Environmental Protection **92**(4): 305-310.
- Hudson, L. (2014). Personal communication: Gas detectors produced by Sencient (<http://www.sencient.com>).
- Innal, F., Y. Dutuit and M. Chebila (2015). "Safety and operational integrity evaluation and design optimization of safety instrumented systems." Reliability Engineering & System Safety **134**(0): 32-50.
- ISA-TR84.00.07 (2010). ISA-TR84.00.07 Technical Report-ISA: Guidance on the Evaluation of Fire, Combustible Gas and Toxic Gas System Effectiveness.

- Lauder, B. E. and D. B. Spalding (1974). "The numerical computation of turbulent flows." Computer Methods in Applied Mechanics and Engineering **3**(2): 269-289.
- Le, H., Y. Liu and M. S. Mannan (2013). "Lower Flammability Limits of Hydrogen and Light Hydrocarbons at Subatmospheric Pressures." Industrial & Engineering Chemistry Research **52**(3): 1372-1378.
- Lee, R. W. and J. J. Kulesz (2008). "A risk-based sensor placement methodology." Journal of Hazardous Materials **158**(2-3): 417-429.
- Legg, S. W., A. J. Benavides-Serrano, J. D. Siirola, J. P. Watson, S. G. Davis, A. Bratteteig and C. D. Laird (2012). "A stochastic programming approach for gas detector placement using CFD-based dispersion simulations." Computers & Chemical Engineering **47**(0): 194-201.
- Legg, S. W., C. Wang, A. J. Benavides-Serrano and C. D. Laird (2013). "Optimal gas detector placement under uncertainty considering Conditional-Value-at-Risk." Journal of Loss Prevention in the Process Industries **26**(3): 410-417.
- Lu, L. and J. Jiang (2007). "Analysis of on-line maintenance strategies for -out-of- standby safety systems." Reliability Engineering & System Safety **92**(2): 144-155.
- Marszal, E. M. (2015). Using Computational Fluid Dynamics (CFD) to Place Gas Detection Equipment. 70th Annual Instrumentation and Automation Symposium for the Process Industries. Texas A&M University, College Station, Tx, <http://www.kenexis.com/gas-detection-boiler-rooms/>
- McGillivray, A., J. L. Saw, D. Lisbona, M. Wardman and M. Bilio (2014). "A risk assessment methodology for high pressure CO<sub>2</sub> pipelines using integral consequence modelling." Process Safety and Environmental Protection **92**(1): 17-26.
- Obenschain, K., J. Boris and G. Patnaik (2004). Using CT-Analyst to optimize sensor placement. Proc. SPIE: Chem. Biol. Sens. **5416**: 14-20.
- Pandya, N., N. Gabas and E. Marsden (2012). "Sensitivity analysis of Phast's atmospheric dispersion model for three toxic materials (nitric oxide, ammonia, chlorine)." Journal of Loss Prevention in the Process Industries **25**(1): 20-32.
- Pasquill, F. (1962). Atmospheric diffusion, London (Van Nostrand Co.).
- Rizzi, A. and B. Engquist (1987). "Selected topics in the theory and practice of computational fluid dynamics." Journal of Computational Physics **72**(1): 1-69.
- Sanguino, O. and D. W. Hissong (2013). "Methodology for selecting hole sizes for consequence studies." Journal of Loss Prevention in the Process Industries **26**(3): 483-488.
- Shih, T.-H., W. W. Liou, A. Shabbir, Z. Yang and J. Zhu (1995). "A new k- $\epsilon$  eddy viscosity model for high reynolds number turbulent flows." Computers & Fluids **24**(3): 227-238.
- Sklavounos, S. and F. Rigas (2004). "Validation of turbulence models in heavy gas dispersion over obstacles." Journal of Hazardous Materials **108**(1-2): 9-20.
- Torres-Echeverría, A. C., S. Martorell and H. A. Thompson (2011). "Modeling safety instrumented systems with MooN voting architectures addressing system reconfiguration for testing." Reliability Engineering & System Safety **96**(5): 545-563.
- Torres-Echeverría, A. C., S. Martorell and H. A. Thompson (2012). "Multi-objective optimization of design and testing of safety instrumented systems with MooN voting architectures using a genetic algorithm." Reliability Engineering & System Safety **106**(0): 45-60.

- Wang, K., T. Chen, S. T. Kwa, Y. Ma and R. Lau (2014). "Meta-modelling for fast analysis of CFD-simulated vapour cloud dispersion processes." Computers & Chemical Engineering **69**(0): 89-97.
- Wilkening, H. and D. Baraldi (2007). "CFD modelling of accidental hydrogen release from pipelines." International Journal of Hydrogen Energy **32**(13): 2206-2215.
- Witlox, H. W. M., M. Harper, S. Natarajan and A. Williamson (2015). "Modelling of time-varying dispersion for elevated pressurised releases without rainout." Journal of Loss Prevention in the Process Industries(0).