Comparative study on toxic gas infiltration in a non-process area using CFD and multi-zone models

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Although the majority of incidents involving toxic gas release in process industries occurs outdoors, nearby buildings and indoor environments are also at high risk. Particularly, non-process areas such as administration buildings and central utility plants are often the least protected, even though they are in the vicinity of potential sources. Ingress of contaminants depends on various factors such as meteorology, building ventilation, building envelope, among others. In literature, indoor exposure modelling techniques range from simple statistical regression and mass balance approaches to more complex models such as multi-zone and computational fluid dynamics (CFD) (Milner et al. 2011). Therefore, to study toxic gas infiltration, a proper selection of models is required. Despite the significant risk posed by such events in process facilities, there is still a lack of data and comparative studies concerning the appropriate models and mitigation methods.

This paper investigates a realistic pipeline leak in a natural gas facility and the subsequent H_2S exposure of the nearby administration building. A comparative study is performed by utilizing a dispersion model (SLAB), a multi-zone model (CONTAM) and a CFD model (Quick Urban and Industrial Complex – QUIC). The influence of ventilation network, nature of openings, wind speed, direction and pressure on toxic gas ingress is examined. Furthermore, we also study the sensitivity of wind pressure calculation on the toxic gas infiltration rate by using American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) handbook and CFD modelling. Indoor toxic levels are attained using multiple combinations of the above mentioned models. Results on indoor toxic levels indicated high sensitivity to wind characteristics which led to varying risks and conclusions. A detailed description of studied scenarios and findings is also presented.

Keywords: Ingress, toxic gas, indoor airflow modelling, infiltration, Multi-zone, CFD

Introduction

Nearly 40% of the world's gas reserves contain high levels of CO_2 and H_2S (Total E&P 2007). Middle East and Central Asia happen to hold the highest reserve of sour gas fields (Total E&P 2007). As of January 2014, Qatar has Middle East's largest and world's third largest proved reserves of natural gas of which majority are sour (*Qatar* 2014). According to the Environmental Protection Agency (EPA), natural gas is called "sour" gas if it contains H_2S in amounts greater than 5.7 milligrams per normal cubic meters (0.25 grains per 100 standard cubic feet) (*Natural Gas Processing* 1995). This makes sour gas extremely poisonous to living beings in relatively low concentrations (Skrtic 2006). Depending on the concentration of H_2S in the air, the effects on human can vary greatly. At concentrations below 100 ppm H_2S cause no long term health impacts but a single breathe of H_2S gas at concentrations above 1000 ppm will result in fatal effects (Chambers and Johnson 2009). Outdoor contamination of air can occur due to various reasons; accidents which involve transportation of liquid agents or a sudden emission in an industrial plant. Such events can produce large scale airborne toxic release which can severely affects nearby communities (Chan et al. 2004). The EPA has stated that accidental release of hydrogen sulphide has not only impacted workers at oil and gas extraction sites but also the public, as such releases can last for an indefinite period (Driver and Freedman 1993).

The 1982 Lodge Pole incident in Alberta, Canada is perhaps the most significant and well documented hydrogen sulphide release incident that may be found in literature (Danielsson et al. 2009). The sour gas with 28% hydrogen sulphide flowed out at an estimated rate of 150 million cubic feet per day. The rotten egg odour of hydrogen sulphide could be smelled as far as 1500 Km (FireFly 2015). In recent times, between 1992 and 2011, three major hydrogen sulphide leakage accidents occurred in China according to the literature (Jianwen, Da, and Wenxing 2011). These release accidents resulted in a cumulative death toll of 249 people. Around 2166 people were hospitalized due to H_2S poisoning and a total of 75000 people had to be evacuated due to the release.

In process industries the majority of accidents involving toxic gas release take place outdoors. However, several non-process areas like administration buildings which are in the vicinity of the release are often least protected. As a result, such buildings and its indoor environments are exposed to high risk of toxic gas infiltration. Contaminated outdoor air can penetrate into the building through cracks, openings and the ventilation network. This phenomenon of air infiltration into buildings is defined as ingress. Ingress of contaminated air into a building is a complex phenomenon. It is not only dependent on driving factors such as air conditioning (HVAC), buoyancy, and atmospheric wind but also on the leakage characteristics of the building envelope. Building leakage is also related to the indoor human activity as well as the turbulent and variable nature of wind. All these various aspects can conclude in uncertainties when trying to quantify these factors (Kandola 1994). Therefore, it is necessary to choose an appropriate tool to study toxic gas ingress. Indoor exposure modelling techniques that range from simple statistical regression and

mass balance approaches to more complex multi-zone and computational fluid dynamics can be found in literature (Milner et al. 2011).

Although toxic gas release in process facilities poses significant risk of exposure due to infiltration, there is lack of data and comparative studies concerning the appropriate models and mitigation methods. Danielsson et al. (2009) also conducted an extensive preliminary data analysis on accidents involving H_2S in industries. They found that there is a lack of adequate knowledge for the occurrence of hydrogen sulphide release and its potential consequences of exposure. This has resulted in inadequate preparedness to deal with the release of toxic gas. Therefore, it is of utmost importance to understand and quantify the dynamics involved with the ingress of outdoor contaminants into building indoors. This paper provides a detailed description of the underlying forces that affect toxic ingress into a building. The study is expedited considering a realistic pipeline leak in a natural gas facility and the subsequent H_2S exposure of the nearby administration building.

Description of accident scenario

The selected scenario is based on actual date from a natural gas facility, but the exact location and detailed description of the facility is not important therefore not disclosed here. A two storey administration building is located 1 km away from a natural gas feed pipeline of 38 inch diameter. High pressure sour natural gas of around 0.77% (mass) H_2S impurity is assumed to be released due to a full bore rupture in the direction of the building. The temperature and pressure inside the pipe are assumed to be maintained at 27^0C and 83 barg, respectively. The duration of the leak is considered to be 1 hour. Studying the toxic gas ingress, various building components were considered, such as windows, door and the main ventilation network connected only to the external air supply.

Methodology

Consequences analysis of a hazardous release i.e. H_2S can be performed using available meteorological data and dispersion models. However, this does not represent the actual exposure levels experienced by people inside a building (Milner et al. 2011). Alternatively, information regarding the dispersion and indoor airflow patterns can also be collected a priori using experimental techniques such as the tracer gas method (Chen and Wen 2010). These techniques are quite costly and require a lot of physical effort, thus prohibited for most facilities. In such cases, multiple air quality models can be coupled and utilized to study ingress of toxic gas from outdoor environments. Indoor air quality models can be classified into statistical, mass balance (multi-zone), and computational fluid dynamics (CFD) ones. This study focus on multi-zone and CFD models for investigating the ingress of H_2S into non process buildings. A brief comparison on the advantages and drawbacks of multi-zone and CFD model was performed by Wang et al. (2010). In order to overcome the shortcomings of each model, this study adopted a combination of multi-zone and CFD models. The tools utilized for multi-zone and CFD models are CONTAM (Walton and Dols 2013) and Quick Urban Dispersion Model (QUIC) (Nelson and Brown 2013), respectively. In addition to these tools, a fast empirical model called SLAB dispersion model (Ermak 1990) is also used to model the outdoor dispersion of the H_2S release caused by the pipeline leak.

Description of models

CONTAM

Multi-zone models represent a building as a network of well mixed zones. Temperature, humidity, mass flow and contaminant concentration are spatially uniform within each zones (Chen and Wen 2010). CONTAM is a multi-zone indoor air quality ventilation analysis model. It helps to determine airflows, including infiltration, exfiltration, and room-to-room airflows in building systems driven by mechanical means. The model also takes into account wind pressures acting on the exterior of the building, and buoyancy effects induced by the indoor and outdoor air temperature difference (Wang, Dols, and Chen 2010). Airflow analysis is one of the main features of CONTAM. It is based on the algorithm developed in AIRNET (Walton 1989), an airflow network simulation program developed by National Institute of Standard and Technology (NIST). The algorithm solves air flow rate from one zone to another as a function of pressure drop along the flow path. Infiltration, which is the result of air flowing through flow paths or airflow element is assumed to be governed by Bernoulli's equation:

$$\Delta P = \left(P_1 + \frac{\rho V_1^2}{2} \right) - \left(P_2 + \frac{\rho V_2^2}{2} \right) + \rho g (z_1 - z_2) \tag{1}$$

where:

ΔP is the total pressure drop between points 1 and 2
P_1 and P_2 are the entry and exit static pressures
V_1 and V_2 are the entry and exit velocities
ρ is the air density
g   is the acceleration of gravity
z_1 and z_2 are the entry and exit elevations

CONTAM provides various airflow elements that describe the flow through an airflow path and the pressure drop across the path. Flow elements include cracks and openings (e.g. doorways) which allow two way flows and components such as fans which force a flow (Walton and Dols 2013). In this project, airflow elements follow the empirical relationship between flow and pressure difference across a crack or opening in the building envelope. This is given by the following equation:

$$Q = C \left(\Delta P \right)^n \tag{2}$$

where:

Q   is the volumetric flow rate
ΔP is the pressure drop across the opening
C   is the flow coefficient
n   is the flow exponents. Measurements usually indicate a flow exponent of 0.6 to 0.7 for typical infiltration openings.

QUIC

QUIC is a dispersion modelling system which can compute transport and dispersion of different types of airborne contaminants within tens of seconds of minutes taking into account the effects of buildings in an approximate way. This model is applied in scenarios where dispersion of airborne concentrations requires to be computed quickly. It comprises of a QUIC-CFD algorithm equipped with a simple one-equation turbulence model to solve 3-D Navier-Stokes equations for incompressible flow using a projection method (Gowardhan et al. 2011). The simple zero-equation model is based on Prandtl's mixing length theory (Prandtl 1925; Argyropoulos & Markatos 2015). This makes it faster than traditional CFD codes to provide more realistic results than non-building aware dispersion models. It is also composed of a wind model called QUIC-URB which uses an empirical-diagnostic approach to compute a mass consistent 3-D wind field around the buildings. QUIC also includes a Lagrangian dispersion model called QUIC-PLUME which utilizes mean wind field data from QUIC-URB and turbulent winds computed internally using the Langevin random walk equations (Nelson and Brown 2013).

The 3-D Reynolds Averaged Navier Stokes (RANS) equations are solved explicitly in time until a steady state is reached using a projection method. A staggered mesh was selected for the discretisation of Navier-Stokes equations by means of the Finite Volume Method (FVM). In order to compute the motion of incompressible air without body forces in a non-rotating coordinate system, the following set of equations are used:

Continuity equation:

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{3}$$

Momentum equations:

$$\frac{\partial \overline{u}_i}{\partial t} = -\frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} - \frac{1}{\rho_i} \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[v \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \right] - \frac{\partial \overline{u}_i' \overline{u}_j'}{\partial x_j} \tag{4}$$

where $\overline{u}_i$ is the mean velocity in the $i\,th$ direction ($i = 1, 2$ and 3), $\overline{u}_i'$ is the turbulence fluctuating velocity, $\overline{p}$ is the pressure, ρ is the average density, $\overline{u}_i' \overline{u}_j'$ is the turbulence Reynolds stresses, and v is the kinematic viscosity of the fluid. The Reynold stresses are modelled using eddy viscosity which is evaluated using a zero-equation algebraic turbulence model based on Prandtl's mixing length theory (Prandtl, 1925).

QUIC-CFD model utilizes a 3D matrix of zeroes and ones (zero for solid and one for fluid cells) to define buildings on a simple uniform structured grid. This process is done by converting Environmental Systems Research Institute (ESRI) shape files to the required format. Compared to the high fidelity CFD models which require a high quality grid that are often time consuming, QUIC-CFD generates grids in seconds.

SLAB

The SLAB model simulates atmospheric dispersion of denser-than-air releases. It handles release scenarios including ground level and elevated jets, liquid pool evaporation, and instantaneous volume sources. Atmospheric dispersion is calculated by solving the one-dimensional equations of momentum, conservation of mass, species, and energy. The conservation equations are spatially averaged in this model. However, SLAB does not calculate the source release rates.

In this study, a steady state plume is simulated to provide the concentration variation of H_2S with respect to time. In this mode, SLAB averages the conservation equations over the crosswind plane of the plume leaving the downwind distance as the single independent variable. The time averaged volume concentration is expressed as:

$$C(x, y, z, t) = CC(x).[\text{erf}(xa) - \text{erf}(xb)].[\text{erf}(ya) - \text{erf}(yb)].[\exp(-za^2) + \exp(-zb^2)] \tag{5}$$

where:

$$xa = (x - xc + bx) / (\sqrt{2}.betax) \tag{6}$$

$$xb = (x - xc - bx) / (\sqrt{2}.betax) \tag{7}$$

$$ya = (y + b) / (\sqrt{2}.betac) \tag{8}$$

$$yb = (y - b) / (\sqrt{2}.betac) \tag{9}$$

$$za = (z - zc) / (\sqrt{2}.sig) \tag{10}$$

$$zb = (z + zc) / (\sqrt{2}.sig) \tag{11}$$

where:

CC(x), b(x), betac(x), zc(x), and sig(x) are all functions of downwind distance (*x*), while xc(*t*), bx, and betax are all functions of time (*t*).

Method of solution

A realistic administration building is modelled using the multi-zone model CONTAM. The building is exposed to an outdoor toxic cloud of H_2S modelled using SLAB dispersion model. SLAB takes into account turbulent mixing with vertical and horizontal entrainment velocities which are influenced by meteorological parameters (Barrett 2009). The model provides information on the time taken for the plume to reach building, the maximum concentration that building is exposed to as well as the duration of the exposure. The output from SLAB is then imported into CONTAM via ambient contaminant (CTM) file.

In CONTAM, inter room airflows are driven by wind pressures acting on the exterior of the building. In order to account for the fluctuating meteorological conditions acting on the building exterior, CONTAM enables the option of entering variable wind pressure data. Wind tunnel studies and on-site measurements are known to be the most reliable methods of obtaining variable wind pressure data (Persily and Ivy 2001). These approaches are often time consuming and can be very expensive. Swami & Chandra (1988) developed a correlation that describes wind pressure coefficients as a function of wind direction for low rise buildings. This can be found in American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) handbook. These correlations are incorporated into CONTAM libraries to account for the variable wind pressure data while describing airflow paths. However, the well mixed assumption of CONTAM is not valid in realistic scenarios where air properties are highly non-uniform. Also, the available correlations in the CONTAM library are building specific and only give averaged wind pressure coefficients over a building façade. In such situations, CFD is an appropriate tool to model the wind pressure acting on the buildings (Wang, Dols, and Chen 2010). QUIC, a building aware CFD tool, can take into account the building shape and orientation while calculating the wind pressure coefficients on the airflow paths. A path location data (PLD) file created by CONTAM is imported to QUIC to capture the exact location of the airflow paths. QUIC then calculates the wind pressure coefficients acting on each opening and generates a Wind Pressure and Contaminant (WPC) file. The WPC file can be imported back to CONTAM in order to provide a more realistic variable pressure data for modelling the ingress of H_2S inside the building. The influence of ventilation network and nature of openings on ingress of H_2S are also considered.

In order to achieve the objectives of this study the following steps were followed:

1. Design specific scenarios concerning accidental release and building.

2. Simulation of accidental release using SLAB.

3. Estimate building's pressure field in CONTAM based on ASHRAE formulations as well as QUIC.

4. Simulation of the building ingress using CONTAM assembling input from either of the above sources (release and building pressure field).

5. Results analysis for each scenario and models inter comparison.

A detailed description of the results is provided in the section below.

Results and discussion

Accidental release

The external environment of the building was exposed to H_2S toxic cloud from a pipeline leak as described above in the accident scenario. The accidental release was modelled using SLAB. Figure 1 shows the centreline concentration profile of the toxic plume resulting from the full bore rupture. It can be seen that the H_2S concentration in the vicinity of the leak is around 9700 ppm and gradually decreased to less than 1000 ppm at a distance of 1200 m from the release source. Figure 2 depicts the contours of the plume 40 m away from the release. The centre of the plume appears a maximum concentration of 6000 ppm, as it is closer to the source. Conversely, the front end of the plume is slightly over 1000 ppm. This is due to the fact that as the plume moves further towards the building, the concentration decreases due to dilution with ambient air and lofting. From Figure 1, it is observed that the extent of dilution is found to have subsided once the plume is around 600 m away from the source of the release. The building located 1 km away from the source of the release was exposed to a maximum concentration of 660 ppm for a period of 10 minutes. The duration of the plume to reach the building was found to be 100 s, according to the SLAB calculations. This duration is considered as the time taken for the plume to hit the first wall of the building. In order to provide adequate spatial and temporal coverage of the dispersion domain, the maximum downwind distance was adjusted for the completion of SLAB calculation.

Building geometry

Figure 3 exhibits the geometry of the domain used in the multi-zone model CONTAM to study the effect of meteorological condition, variable wind pressure and ventilation network on the toxic gas infiltration. Each room is considered as a zone in CONTAM and each zone is assumed to be well mixed. The well mixed assumption also extends to properties such as temperature, pressure and contaminant concentration. In order to compute building ingress, wind pressure acting on the windows utilized the ASHRAE formulation for low rise rectangular buildings (Persily and Ivy 2001). The building is composed of 94 rooms including a corridor. The corridor area (yellow colour) of the building covers the maximum area (876 m^2) of the building. It is also connected to all the rooms exposed to the outdoor environment making it the most vulnerable area in the building. Hence, this area is preferred over other rooms for analysis. For comparison, another room (blue colour) in the middle section of the building is considered. The room was selected based on its size (144m^2) and the fact that it is exposed to the ambient atmosphere and at the same time connected to multiple rooms in the vicinity. To consider a worst case scenario, all doors inside the building are assumed to be completely open at all times. The exposed windows are considered to have a leakage area of 1.73 cm^2/m (Persily and Grot. 1986).
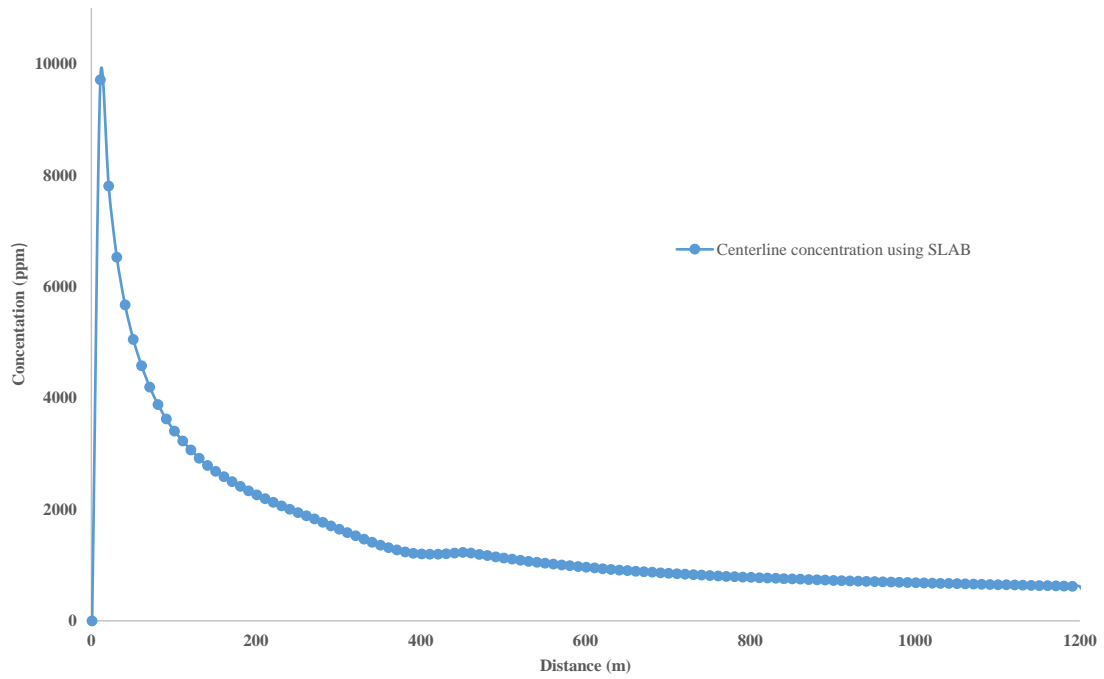
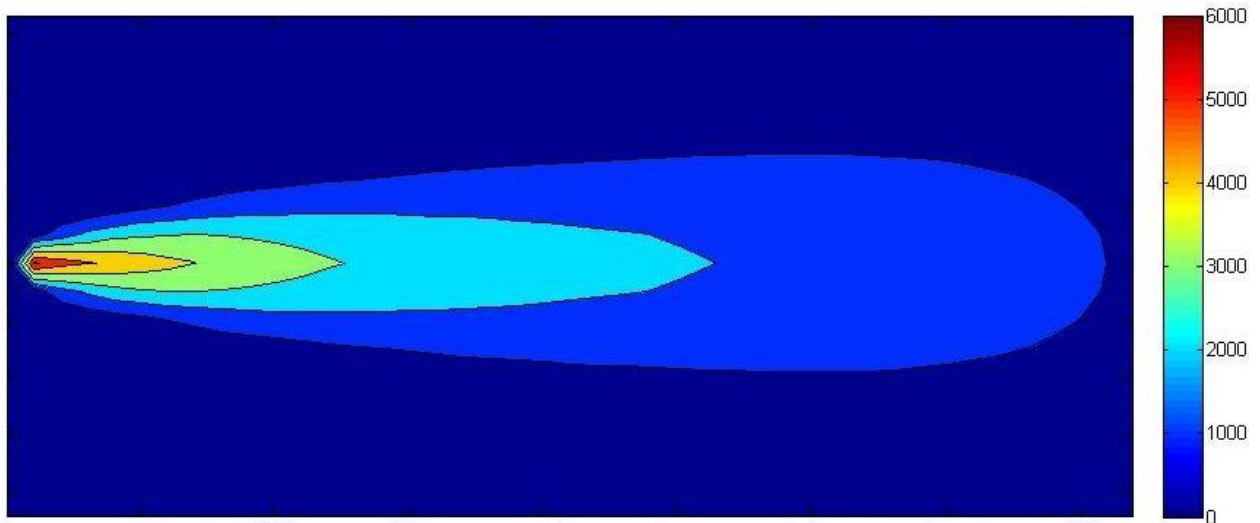*Figure 1: Maximum concentration (centerline) of the H_2S plume.*

Figure 2: Contours of concentration (ppm) 40 m downwind from the source.
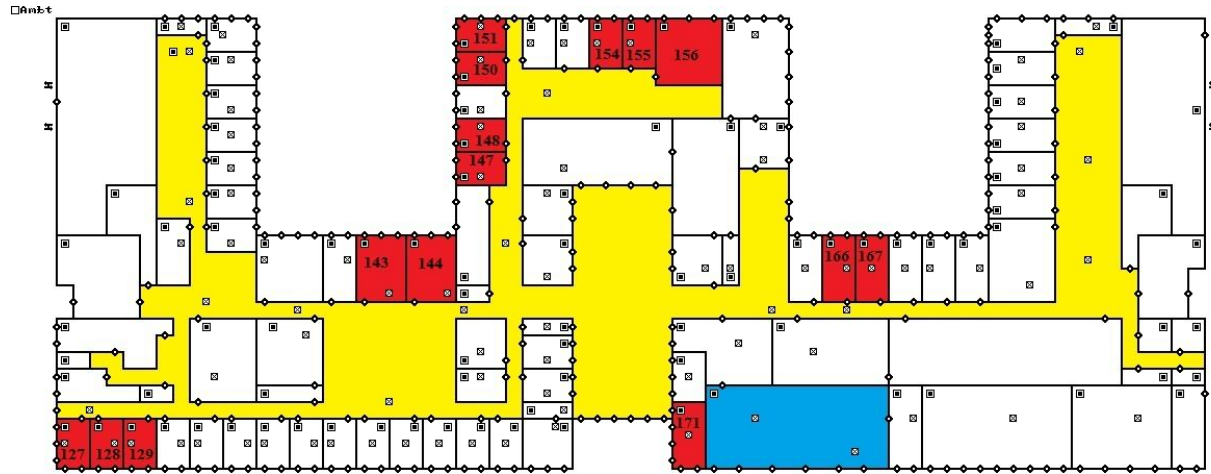
Figure 3: Building floor plan of the first floor drawn using CONTAM.

Effect of meteorological conditions

Meteorological conditions such as wind direction and wind speed were found to be sensitive to the toxic gas ingress rate. Three different wind directions, namely 40^0, 80^0 and 120^0 were considered to cover all sides of the building. Since the stable atmospheric stability (F class) was considered, the wind speed was chosen at 3 m/s. Variation of concentration profile for the yellow and blue area is shown in Figure 4 and Figure 5, respectively. Depending upon the direction of the wind, it is observed that there is a difference in the maximum concentration attained in both areas. The concentration values are only slightly different for the yellow area. This is due to the fact that there will always be diffusion of toxic gas from the surrounding rooms to the yellow area irrespective of the direction of the wind. Conversely for the blue area, Figure 5 exhibits a much higher concentration at 80^0 direction compared to 120^0. In both cases, 80^0 wind direction achieved a higher impact on the concentration profile.

Wind direction is also shown to influence the dispersion of toxic gas inside the room. This is exhibited by comparing the time taken for the concentration in the room to go above and below the Acute Exposure Guideline Levels (AEGL) limit for a particular wind direction. AEGL-3 limit is chosen, as it represents the airborne concertation of a substance above which an individual can experience life threatening effects or death. Since the toxic gas tends to stay inside the room for periods as long as 100 min, the AEGL-3 (60 min) value of 50 ppm for H_2S was considered. It can be observed from Figure 5 that though all wind directions go above the AEGL-3 limit around the same time. However, the 120^0 wind direction tends to take a much longer period below the 50 ppm limit than the 40^0 and 80^0 wind directions, respectively. These results indicate the importance of utilizing realistic meteorological data while studying toxic gas ingress in buildings.

Effect of HVAC

Mechanical ventilation systems such as HVAC form an integral part of a building. It is also crucial to understand the influence of HVAC on the ingress of toxic gas into the building when designing mitigation methods in the event of a toxic gas leak. The infiltration of toxic gas in the yellow area is examined in the presence and absence of a HVAC system as described in Figure 6. The infiltrated toxic gas remains inside the building for more than 2 hours. However, the presence of a HVAC system tends to spread the toxic gas inside the building at a much faster rate compared to the case where HVAC is absent. The maximum concentration attained was 50% higher for the HVAC system. The air intake unit is placed at an elevated height of 7.9 m outside the building. The HVAC system is also interconnected with the entire building and the outdoor atmosphere through the air intake unit. This results in a higher concentration of toxic gas inside the building compared to the absence of HVAC system.
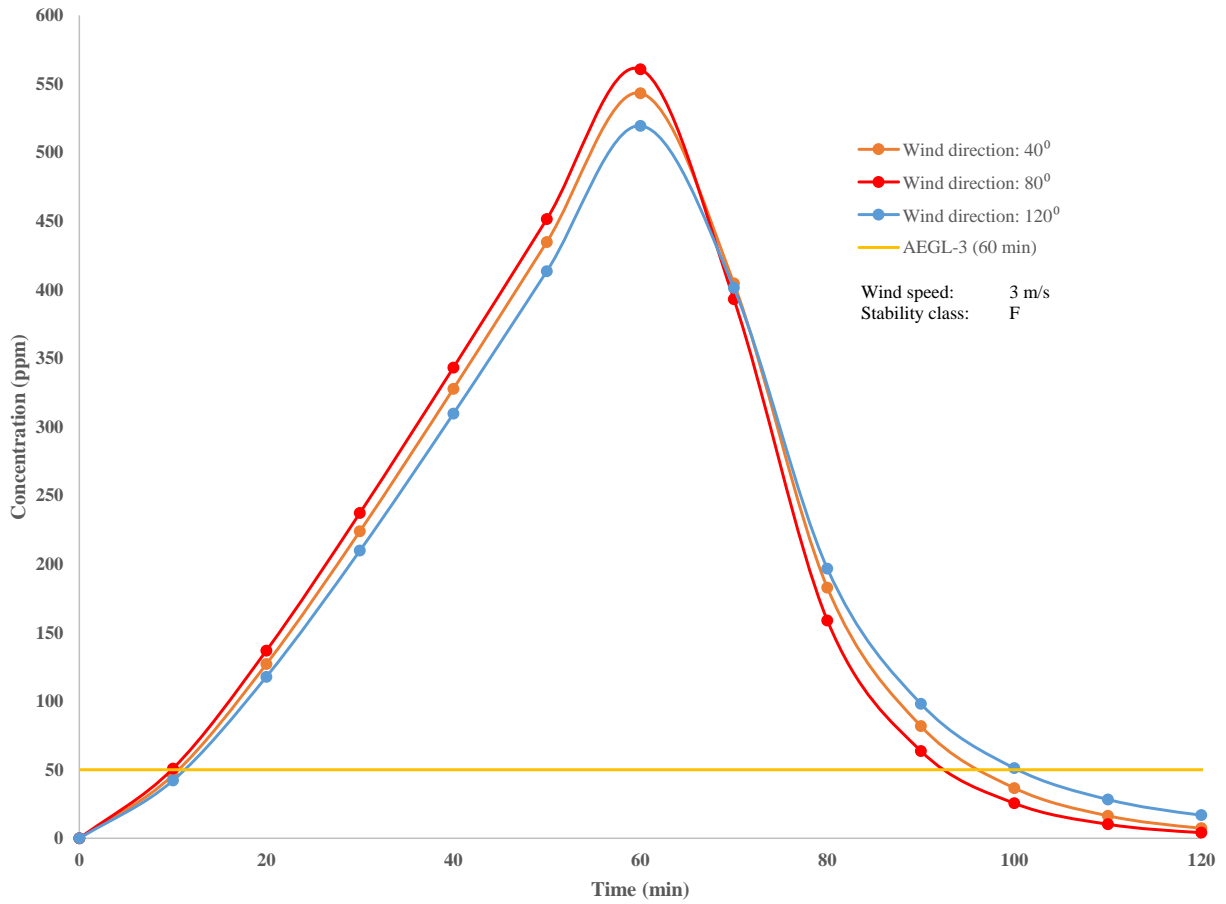
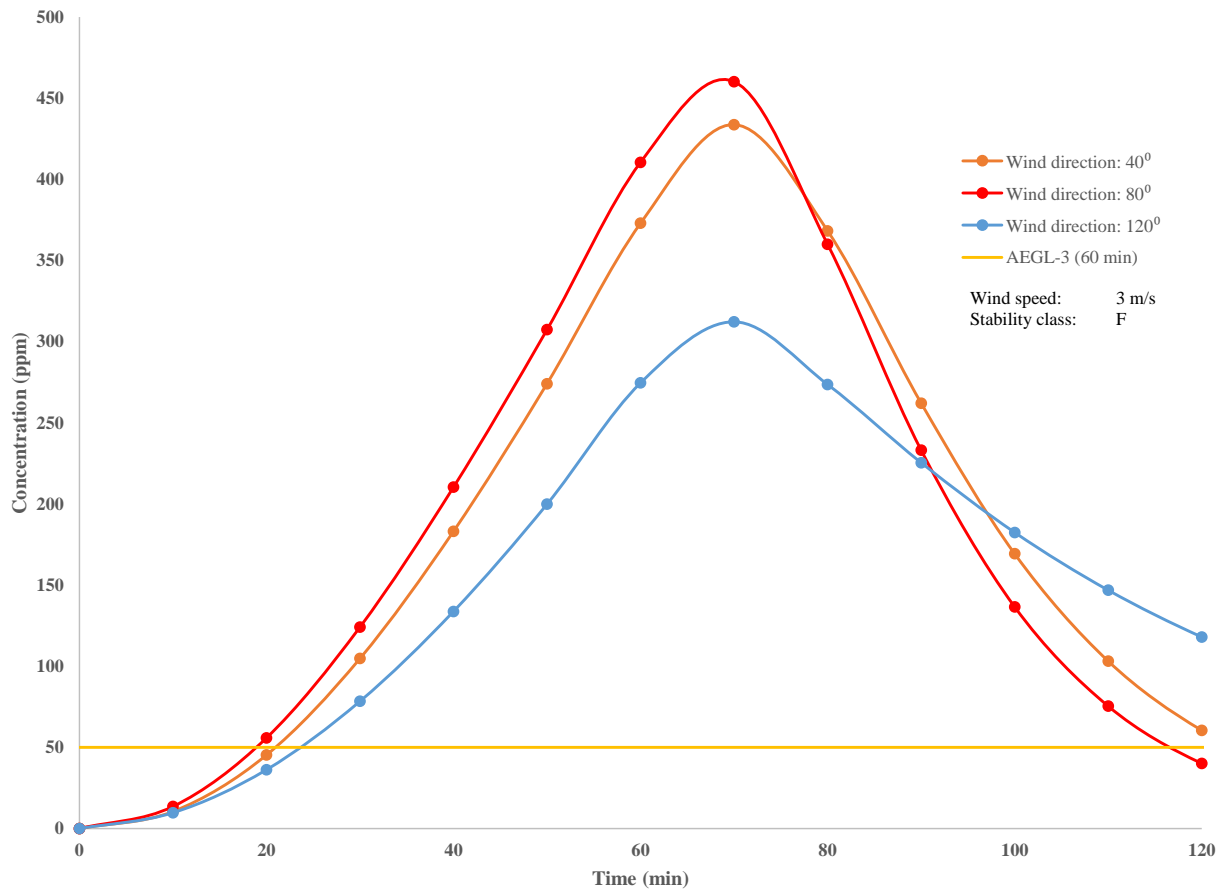Figure 4: Effect of meteorological conditions on toxic gas ingress for the yellow area.

Figure 5: Effect of meteorological conditions on toxic gas ingress for the blue area.
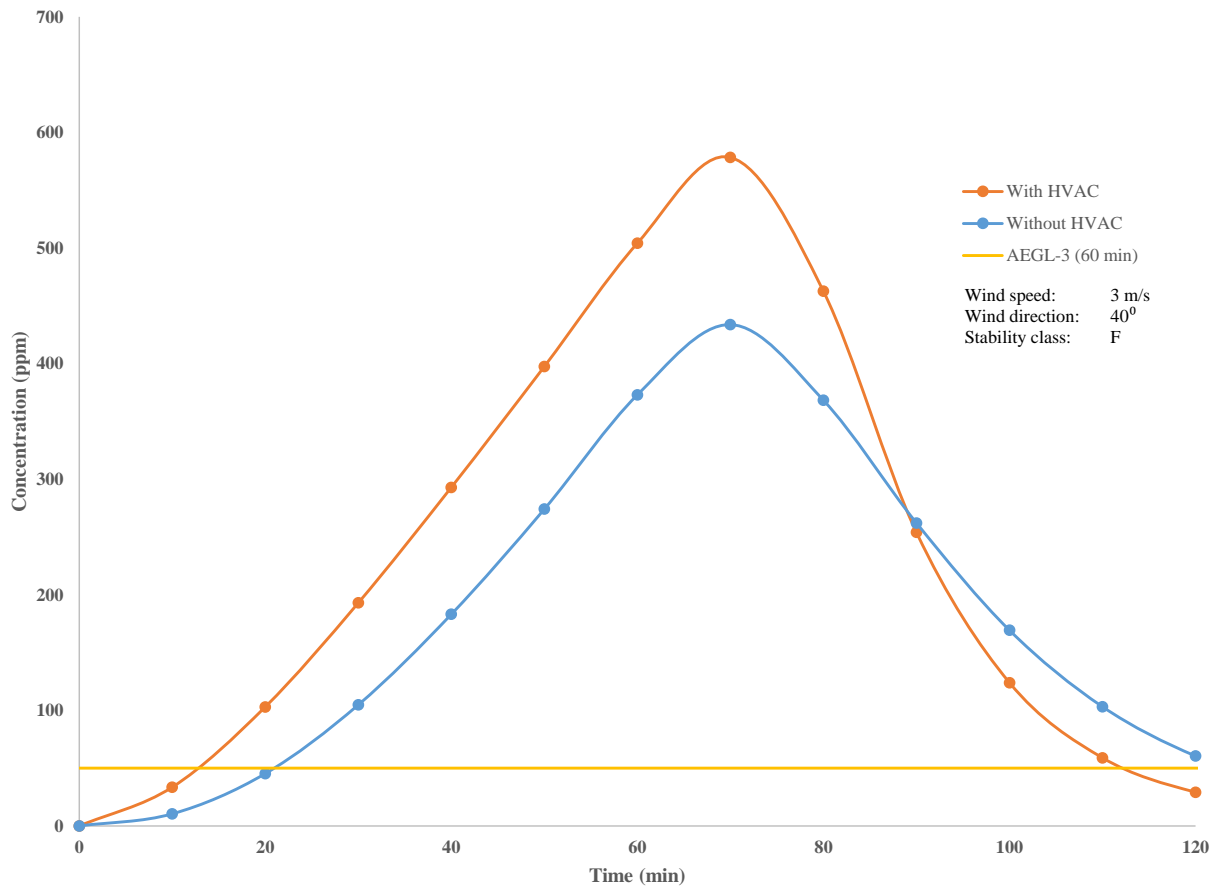
Figure 6: Effect of HVAC on toxic gas ingress for corridor (yellow) area.

Effect of wind pressure

All buildings operate with their internal atmospheres in some sort of dynamic equilibrium with the outside atmosphere (Hall and Spanton 2013). Wind pressure acting on the exterior of the building influences the infiltration of the air from the outdoor environment to the indoor environment. In this study, ASHRAE correlation for low rise rectangular buildings was considered in the CONTAM model to calculate the variable wind pressure acting on the exterior facade of the building. However, more accurate variable wind pressure data were obtained using the QUIC-CFD model. QUIC takes into account the building geometry while calculating the wind pressure acting on the building openings. The data obtained from QUIC were imported into the CONTAM model as a WPC file to study the airflow rates within the building.

Figure 7 exhibits the airflow rate prediction between the yellow and red zones (see Figure 3) by both models. It is observed that QUIC predicts an airflow in all the rooms surrounding the yellow area whereas CONTAM (ASHRAE correlation) fails to predict in most of the rooms. Subsequently, this will be reflected in the contaminant concentration data obtained for a particular zone. In zones where airflow rates are not predicted, the toxic gas may tend to remain at high levels as there is no mixing with the air from the surrounding zones. Failure of airflow rates prediction by the CONTAM model can be attributed to the fact that the ASHRAE correlation used in the model caters only to low rise buildings. However, in our case there is a two level building.

Figure 8 compares the amount of H_2S gas dispersed in the yellow area based on the method of wind pressure calculation. The calculation of wind pressures using QUIC predicted a higher maximum concentration (393 ppm) in the yellow area compared to the ASHRAE method (330 ppm). Though QUIC computed higher concentration in the initial stages of infiltration, ASHRAE prediction showed that H_2S tend to stay for a longer period of time in the area. At 100 min, the concentration was found to be 43 ppm using QUIC whereas ASHRAE prediction showed a value of 60 ppm which is above the AEGL-3 (60 min) limit of 50 ppm. This is associated to the airflow dynamics which is affected by a difference in wind pressure considered. Information such as the maximum concentration attained and time taken for the toxic gas to reach safe levels can be crucial to emergency response planning.
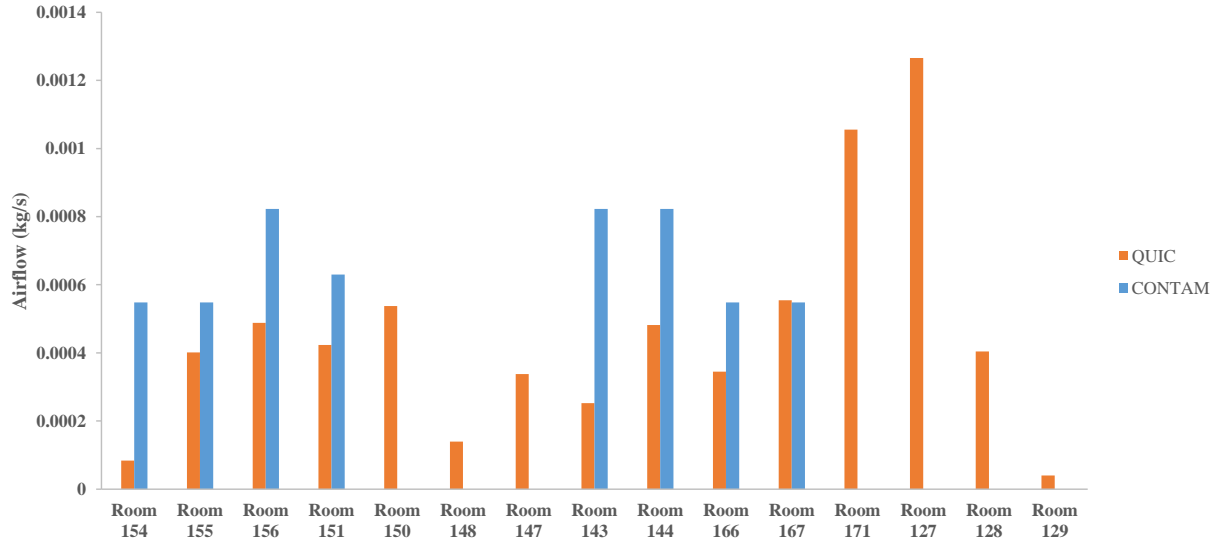
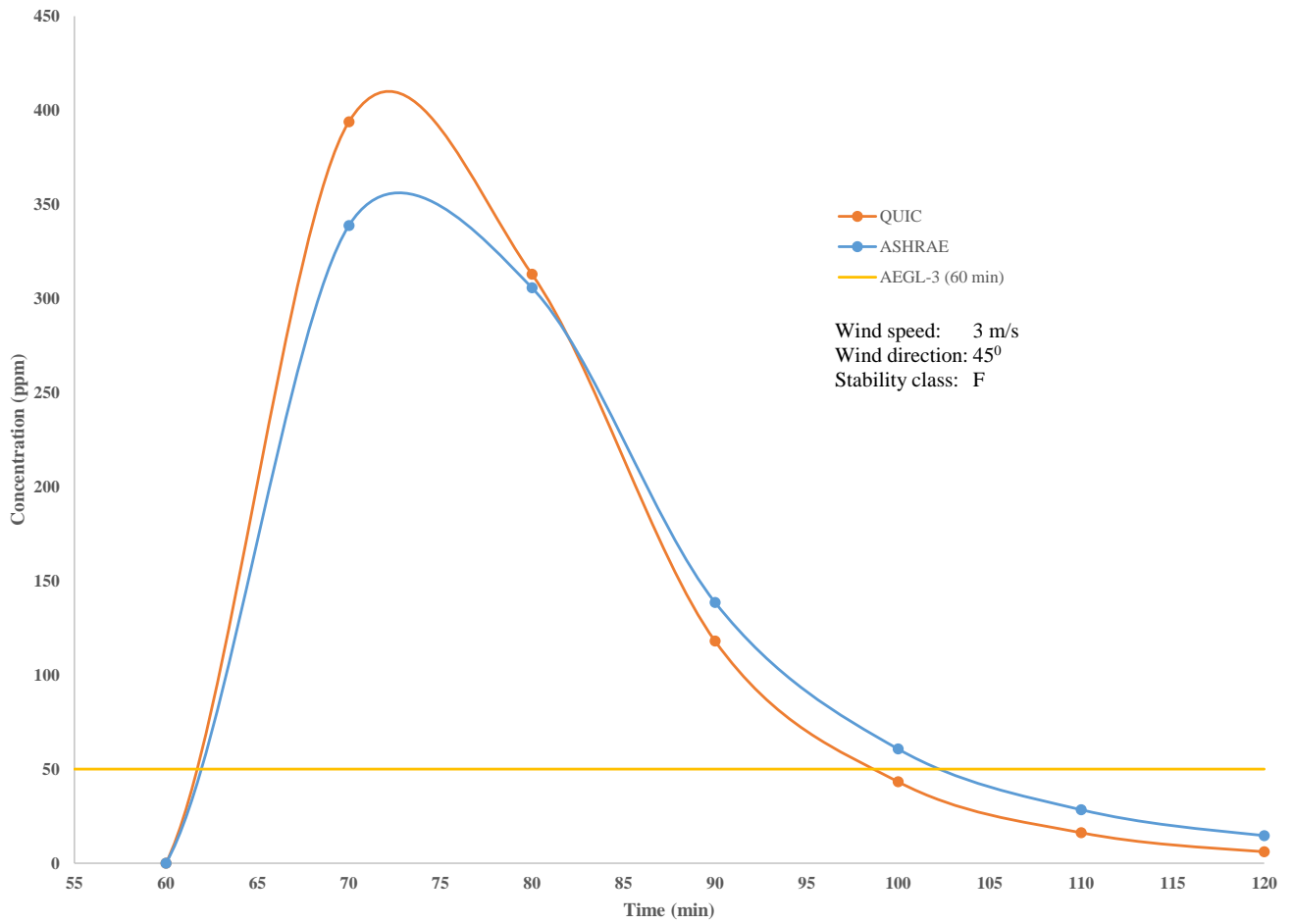*Figure 7: Comparison of the rate of airflows between the yellow and red areas using QUIC and CONTAM.*

Figure 8: Effect of wind pressure calculation method on toxic gas ingress for the corridor (yellow) area.

Conclusion

Conventionally, assessment of exposure to air pollution has been done using data from a fixed network of ambient air quality monitoring stations (Milner et al. 2011). But this does not represent the actual pollution levels experienced by people inside the building. In such situations, models prove to be an effective way to examine a potential outcome of a catastrophic event. However, various parameters influence the ingress of toxic gas into a building. A two level administration building was chosen to study and analyse various factors affecting the ingress of contaminants. The ingress was modelled using a combination of multi-zone model (CONTAM) and a CFD model (QUIC). Dispersion of the H_2S cloud resulted from a full bore pipeline rupture was modelled using the heavy gas dispersion model (SLAB). The influence of meteorological properties, leakage characteristics of the building and ventilation system on the toxic gas ingress was investigated. The sensitivity of wind pressure calculation method on the amount of toxic gas ingress was also examined.

The corridor (yellow colour) was realized to be the most susceptible area in the building. This can be attributed to the fact that this area is connected to all the rooms in the building which are exposed to the outdoor environment. In all cases concentration inside the building was found to be above the AEGL safe limits for periods as long as 2 hours. Ingress of toxic gas is sensitive to meteorological conditions and by the presence of mechanical ventilation. The main entrance doors which are completely open (worst case scenario) are most exposed at 80^0 wind direction. As a result, the building was found to be most vulnerable for 80^0 wind direction. Findings revealed that ingress of toxic gas behaves differently in the presence of a ventilation system. Consideration of the ventilation system resulted in a 50% increase in the maximum concentration attained in the corridor area. It was also observed that the infiltrated toxic gas dispersed inside the building much faster when the HVAC system was taken into account.

Finally, the influence of wind pressure and its calculation method on the ingress phenomena was examined by comparing the ASHRAE correlation and QUIC-CFD modelling. A comparison of the airflow rates between the corridor area and the surrounding rooms indicated that wind pressure modelled using QUIC predicted airflows in rooms where the ASHRAE correlation failed to. This behaviour can be explained by the superiority of QUIC to consider the actual geometry of the building in order to model wind pressures. This advantage of QUIC was also evident when the concentration profile for the yellow area was compared for both calculation techniques. In comparison to the ASHRAE method, QUIC displays a higher maximum concentration and a faster decay rate.

In circumstances where there is a lack of ambient air quality data and on site measurements of wind pressure, both of which can be time consuming and expensive to attain, the proposed method can be used to get a preliminary understanding of the present consequences and the required mitigation methods that needs to be designed. The sensitivity analysis on the governing variables of the ingress phenomenon can also provide a basis in order to achieve realistic results.

References

Argyropoulos, C.D., and N.C. Markatos. 2014. "Recent Advances on the Numerical Modelling of Turbulent Flows." *Applied Mathematical Modelling* 39: 693–732. doi:10.1016/j.apm.2014.07.001.

Barrett, AM. 2009. "Mathematical Modeling and Decision Analysis for Terrorism Defense: Assessing Chlorine Truck Attack Consequence and Countermeasure Cost Effectiveness." PhD diss., Carnegie Mellon University, Pittsburgh, Pennsylvania. http://research.create.usc.edu/nonpublished_reports/170/.

Chambers, T., and J.A. Johnson. 2009. *Environmental Mitigation Monitoring: Hydrogen Sulfide (H2S) Gas Dispersion Potentials & Release Scenarios for Pacific OCS Region Oil & Gas Platforms & Pipelines Located in the Santa Barbara Channel and Santa Maria Basin, California.MMS OCS Report 2009-021.*

Chan, W.R., P.N. Price, A.J. Gadgil, W.W. Nazaroff, G. Loosmore, and G. Sugiyama. 2004. "Modeling Shelter-In-Place Including Sorption On Indoor Surfaces." In *84th American Meteorological Society Annual Meeting*. Seattle, WA: American Meteorological Society, Boston, MA.

Chen, Y.L., and J. Wen. 2010. "Comparison of Sensor Systems Designed Using Multizone, Zonal, and CFD Data for Protection of Indoor Environments." *Building and Environment* 45 (4). 1061–71. doi:10.1016/j.buildenv.2009.10.015.

Danielsson, F., R. Fendler, M. Hailwood, and J. Shrives. 2009. *Analysis of H 2 S – Incidents in Geothermal and Other Industries*.

Driver, L., and E. Freedman. 1993. "Report to Congress on Hydrogen Sulfide Air Emissions Associated with the Extraction of Oil and Natural Gas. Final Report." http://www.osti.gov/scitech/biblio/5394599.

Ermak, Donald. 1990. "User's Manual for SLAB: An Atmopheric Dispersion Model For Denser Than Air Releases." http://www3.epa.gov/scram001/models/nonepa/SLAB.PDF.

FireFly. 2015. "About Us - FireFly Critical Well Safety Equipment Ltd." Accessed December 6. http://www.fireflycriticalwellsafety.com/about-us.html.

Gowardhan, A., E.R. Pardyjak, I. Senocak, and M.J. Brown. 2011. "A CFD-Based Wind Solver for an Urban Fast Response Transport and Dispersion Model." *Environmental Fluid Mechanics* 11: 439–64. doi:10.1007/s10652-011-9211-6.

Hall, D J, and A M Spanton. 2013. "Ingress of External Contaminants into Buildings – A Review." In *ADMLC-R7*. UK Atmospheric Dispersion Modelling Liaison Committee.

Jianwen, Z., L. Da, and F. Wenxing. 2011. "Analysis of Chemical Disasters Caused by Release of Hydrogen Sulfide-Bearing Natural Gas." *Procedia Engineering* 26: 1878–90. doi:10.1016/j.proeng.2011.11.2380.

Kandola, B. 1994. "Smoke Hazard Assessment On Offshore Oil And Gas Installations." *Fire Safety Science* 4: 1233–44. doi:10.3801/IAFSS.FSS.4-1233.

Milner, J., S. Vardoulakis, Z. Chalabi, and P. Wilkinson. 2011. "Modelling Inhalation Exposure to Combustion-Related Air Pollutants in Residential Buildings: Application to Health Impact Assessment." *Environment International* 37 (1). 268–79. doi:10.1016/j.envint.2010.08.015.

Natural Gas Processing. 1995. *The Petroleum Industry*. 5th ed. Environmental Protection Agency. http://www.epa.gov/ttn/chief/ap42/ch05/final/c05s03.pdf.

Nelson, Matthew, and Michael Brown. 2013. "The QUIC Start Guide (v 6 . 01)." http://www.lanl.gov/projects/quic/.

Persily, A. K., and R. A. Grot. 1986. "Pressurization Testing of Federal Buildings." In *Measured Air Leakage of Buildings: A Symposium - Issue 904*, edited by H. R. Trechsel and P. L. Lagus., 184–200. Philadelphia, PA, USA: American Society for Testing and Materials.

Persily, A. K., and E. M. Ivy. 2001. *Input Data for Multizone Airflow and IAQ Analysis.*

Prandtl, L. 1925. "Report on Inestigation of Developed Turbulence." *ZAMM* 5: 136–39.

Qatar. 2014. *International Energy Data and Analysis*. U.S. Energy Information Administration. http://www.eia.gov/beta/international/analysis_includes/countries_long/Qatar/qatar.pdf.

Skrtic, Lana. 2006. "Hydrogen Sulfide, Oil and Gas, and People's Health." *Energy*. Msc diss., University of California, Berkeley.

Swami, M. V., and S. Chandra. 1988. "Correlations for Pressure Distributions on Buildings and Calculation of Natural-Ventilation Airflow." In *ASHRAE Transactions*, 94, no. 1:243–66.

Total E&P. 2007. "Sour Gas, A History of Expertise." *Group*, 24.

Walton, G.N. 1989. *AIRNET - A Computer Program for Building Airflow Network Modelling*. *NISTIR*. Gaithersburg, MD.

Walton, G.N., and W.S. Dols. 2013. "CONTAM User Guide and Program Documentation." Gaithersburg, MD. http://www.bfrl.nist.gov/IAQanalysis/CONTAM/userguide.htm.

Wang, Liangzhu Leon, W. Stuart Dols, and Qingyan Chen. 2010. "Using CFD Capabilities of CONTAM 3.0 for Simulating Airflow and Contaminant Transport in and around Buildings." *HVAC&R Research* 16 (6): 749–63. doi:10.1080/10789669.2010.10390932.