STUDY OF TOXIC GAS INGRESS IN NON-PROCESS AREAS

A Thesis

by

ATIF MOHAMMED ASHRAF

Submitted to the Office of Graduate and Professional Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Chair of Committee:	Konstantinos Kakosimos
Co-Chair of Committee:	Luc Vechot
Committee Member:	Mahmoud Amani
Head of Department:	M. Nazmul Karim

August 2016

Major Subject: Chemical Engineering

ABSTRACT

Although the majority of incidents involving toxic gas release in process industries occur outdoors, nearby buildings and its indoor environments are also at high risk. Particularly, non-process areas such as administration buildings are often the least protected, even though they are in the vicinity of potential sources. 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). 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 work 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, wind speed, direction, and pressure on toxic gas ingress is examined. Furthermore, the sensitivity of wind pressure calculation on the toxic gas infiltration rate by using American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) correlation and CFD modelling is studied. Indoor toxic levels are attained using 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 different scenarios and findings is also presented.

To,

Umma & Uppa

For the life I have and their unconditional love and support.

ACKNOWLEDGEMENTS

I sincerely feel obliged to recognize the efforts of my advisor Dr. Konstantinos Kakosimos, who has provided guidance in my research work. I would like to acknowledge my committee members: Dr. Luc Vechot and Dr. Mahmoud Amani. I would also like to thank the Mary Kay O’ Connor Process Safety center for its financial support, without which this work would not have been possible.

I would also like to appreciate the support of all members of Mary Kay O’Connor Process Safety Center extension in Qatar

Finally, I would like to thank Dr. Christos Arygyropolous for his academic as well as moral support and my wife for her incessant encouragement to complete this thesis.

TABLE OF CONTENTS

Page

LIST OF FIGURES

Page

LIST OF TABLES

Page

1. INTRODUCTION

Natural gas is considered to be the fastest growing fossil fuel with nearly 3% growth per year for the past thirty years. The International Energy Agency expects the consumption of natural gas to increase considerably from 2800 to 4700 billion cubic meters between 2004 and 2030. However, nearly 40% of the world's gas reserves contain high levels of Carbon dioxide (CO_2)and Hydrogen Sulfide (H_2S) [1]. 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). This makes sour gas extremely poisonous to living beings in relatively low concentrations. Therefore, it is important that sour gas is extracted in a safe and responsible manner.

The Middle East and Central Asia happen to hold the highest reserve of sour gas fields [1]. As of January 2014, Qatar has the Middle East's largest and the world's third largest and proved reserves of natural gas of which the majority are sour.

In the natural gas industry, H_2S can be found in wells, refineries and in pipelines carrying unrefined petroleum. During extraction hydrogen sulfide may be released into the atmosphere at wellheads, pumps, piping, separation devices, oil storage tank, water storage vessels and during flaring operations [2]. H_2S is considered a broad-spectrum toxin. This means that it can affect several body systems at the same time, with the nervous system being the most susceptible. Exposure to H_2S can cause eye irritation, sore throat, coughing, nausea, shortness of breath, and fluid in lungs. Depending on the concentration of H_2S present in the air, the effects on human can vary greatly. At concentrations below 100 ppm H_2S causes no long term health effects but a single breathe of H_2S gas at concentrations above 1000 ppm will result in fatal effects [3]. The EPA has stated that accidental release of hydrogen sulfide has impacted the public and not just worker at oil and gas extraction sites , as such releases can last for an indefinite period [4].

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. For example, rupture of a pipeline transporting natural gas from offshore to onshore facilities. Such events can produce large scale airborne toxic release which can severely affect large populations.[5]. These are events which have catastrophic consequences but low occurrence. However, in the event of such an accident, 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 is a complex phenomenon which is governed by various factors like meteorological conditions, temperature and pressure differences between the indoor and outdoor environments, building occupant activities e.tc. As a result of ingress of outdoor contamination, the concentration and the consequent dosage inside the building gradually increases. However, this increase is comparatively slower than the increase in the outdoor concentration [6]. Depending upon the concentration of contaminants achieved inside the building, the population is exposed to a certain amount of risk. Therefore it is important to know how much of the released toxic gas infiltrates into the building. This information is also vital to develop mitigation methods for population residing inside a building that is exposed to toxic gas. Hence, this study aims to improve the understanding of toxic gas ingress, particularly H_2Sin a non-process area which is defined as any building which does not house a chemical process.

2. SCOPE OF WORK

Conventional emergency planning derives planning zones based on the distance from the hazard source. These zones are then used as a basis for developing guidelines and training efforts [5]. Regardless of the kind of hazardous material, emergency responders require an estimation of the hazardous cloud footprint as a function of time [7].

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 ingress. Contaminated outdoor air can penetrate into the building through cracks, openings and the ventilation network. Ingress phenomena 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 [8]. Therefore, it is necessary to choose an appropriate tool to study toxic gas ingress.

However, despite the significant risks posed by accident releases in process facilities, there is a lack of data and comparative studies concerning the appropriate models and mitigation methods. A considerable amount of work has been done in this study comparing the results of various models to help and identify the best combination of models to be considered for this work.

The objectives of this research are as follows:

- Develop a hydrogen sulfide gas ingress model into a building employing a combination of multi-zone and CFD models.
- Predict the dispersion of toxic gas concentration inside the building using the developed model.
- Investigate mitigation methods for a non-process building based on the model predictions.
- Explore the need to have defined or comprehensive guidelines for an emergency response plan during a toxic gas infiltration inside the building.

3. LITERATURE REVIEW

The 1982 Lodge Pole incident in Alberta, Canada is perhaps the most significant and well documented hydrogen sulfide release incident that may be found in literature. The sour gas with 28% hydrogen sulfide flowed out at an estimated rate of 150 million cubic feet per day. The rotten egg odor of hydrogen sulfide could be smelled many miles away [9]. In recent times between 1992 and 2011, three major hydrogen sulfide leakage accidents that occurred in China are reported in the literature [10]. 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.

A comprehensive study was conducted on the hydrogen sulfide gas dispersion for different scenarios by the US Department of the Interior. The primary focus of this study was to estimate the aerial extent around a potential release source. The source includes wellhead, pipeline, piping and process vessel in the Pacific Outer Continental Shelf Region (POCSR). The POCSR produce gas containing hydrogen sulfide in concentrations more than 100 ppm [3]. Three hydrogen sulfide concentrations (100, 300 and 1000 ppm), under two sets of atmospheric conditions were addressed in the analysis. The study used EPA's Areal Locations of Hazardous Atmospheres (ALOHA) model for risk assessment to address the potential hazard to the public of a release of sour gas from the offshore pipelines [3].

Based on the available data on hydrogen sulfide incidents in the industry, an extensive preliminary data analysis was done by [9]. Though the main focus of the study was based on geothermal industries, one of the major observations of the study was that there appears to be a lack of adequate knowledge that hydrogen sulfide release could occur and the potential consequences of hydrogen sulfide exposure. This has resulted in inadequate preparedness to deal with the release of toxic gas.

Nevertheless, there is very little literature available on hydrogen sulfide releases in an onshore facility, particularly in a non-process area. Non process areas in this project are defined to be any building which does not house a chemical process.

All buildings operate with their internal atmospheres in some sort of dynamic equilibrium with the outside atmosphere. Ingress of contaminants occurs in areas where the buildings external surface pressure is high in both mechanical and natural ventilated systems. This process is also dependent on meteorological conditions, temperature differences between indoors and outdoors of the building and occupant activities such as opening and closing of windows and doors [11]. The ingress of contaminants through a building is also dependent on the pressure and concentration patterns, as well as the nature of openings on the building envelope. Contamination ingress also varies with time which depends on the building interior and porosity [12]. Therefore, it is of utmost importance to understand and quantify the parameters and dynamics involved with the ingress of outdoor contaminants into building indoors.

Nonetheless, flow of contaminated air into a building is a complex phenomenon. The ingress of air is not only dependent on driving factors such as air conditioning (HVAC), buoyancy, 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 result in uncertainties when trying to quantify these factors [8]. Therefore, it is imperative to choose an appropriate tool to study toxic gas ingress.

Conventionally, assessment of exposure to air pollution has been done using data from fixed ambient air quality monitoring stations. But this does not represent the actual pollution levels experienced by people inside a building. In most circumstances, models are an effective way to examine the potential outcome of a future environmental hazard. Various indoor exposure modeling techniques are available, ranging from simple statistical regression and mass balance approaches, to more complex multi-zone and computational fluid dynamic tools that have correspondingly large input data requirements [13].

Information regarding the dispersion and indoor airflow patterns can also be collected using experimental techniques like tracer gas method [14]. But these methods are often not cost effective and require a lot of physical effort.

Airflow models can be classified into statistical, mass balance (multi-zone), and computational fluid dynamics (CFD). Multi-zone models are generally used to model ventilation, air flow and contaminant transport through buildings. The model represents a building as a network of well mixed zones. Temperature, humidity, mass flow and contaminant concentration are spatially uniform within each zone. These type of models permit multiple indoor source types and characteristics together with complex changes in source emission rate with respect to time [13]. Though various commercial multi-zone models are available, COMIS and CONTAM are the popular ones [13]. Multi-zone models being a complex tool correspondingly requires high data input requirements. Hence, applying to more than a single building can be time consuming and challenging [14]. [15] reviewed both software's COMIS and CONTAM. The paper examined the assumptions considered to ease the calculations to save computing time as well as memory use of the programs at the cost of restricting the models complete capacity. The model's usefulness was found to have been adversely affected in the following cases:

1. Natural ventilation where buoyancy effects dominates mechanically driven flow.
2. Duct system design when losses in T- junction affects the system performance.
3. Control system design when the dynamic transport of pollutant plays a significant role in the simulated system.

CFD models, on the other hand, are used to model the spatial and temporal variations in indoor pollutant concentrations at fine scale (typically 0.01 m to 1 m diameter grid cells) [13]. CFD models can give air velocity and pollutant concentration at individual points in a domain instead of averaged concentration predicted by mass balance models. CFD solves a set of partial differential equations instead of ordinary differential equations solved by mass balance models [16]. Since, CFD is more computationally intensive compared to multi-zone models and it is less often used for whole building analysis or long term transient simulations. However, the considerable improvements in computing power together with improvements in model solution procedures have made CFD a more common design tool [11]. Table 1 shows the comparison between a multi-zone model and a CFD model.

Table 1: Comparison between Multi-zone model and CFD model [17]

Models	**Multi-zone**	**CFD**
Simulation assumptions		
Uniform contaminant concentration in each room	Yes	No
Quiescent or still air in each room	Yes	No
Neglect air resistance in each room	Yes	No
Neglect inflow momentum effect, if any	Yes	No
Instantaneous contaminant transport inside a room	Yes	No
Hydrostatic distribution of pressure inside each room	Yes	No
Simulation capabilities		
Whole building and yearly dynamic simulations	Better	
Modelling building air infiltration	Better	
Computational speed	Better	
Modelling spatial airflow and contaminant concentration		Better
Modelling wind pressure on buildings		Better
Modelling large openings and spaces		Better
Modelling spatial personal exposure		Better

4. METHODOLOGY

Consequences analysis of a hazardous release i.e. H2S 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 [13]. Alternatively, information regarding the dispersion and indoor airflow patterns can also be collected a priori using experimental techniques such as the tracer gas method [14]. 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 [17]. 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 [18] and Quick Urban Dispersion Model (QUIC) [19], respectively. In addition to these tools, a fast empirical model called SLAB dispersion model [20] is also used to model the outdoor dispersion of the H_2S release caused by the pipeline leak.

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 [21]. The model provides information on the time taken for the plume to reach a 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 [22]. These approaches are often time consuming and can be very expensive. [23] 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 [24]. 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. As a result, the wind pressure data estimated by CONTAM may not be realistic. This will also have an impact on the estimation of toxic gas concentration within a particular zone consequent of the ingress phenomena. In such situations, CFD is an appropriate tool to model the wind pressure acting on the buildings as it is able to calculate detailed air properties [17]. Moreover, the available wind pressure correlations in the CONTAM library were found to be building geometry specific and only gave averaged wind pressure coefficients over a building façade. Quick Urban and Industrial Complex (QUIC) dispersion model is a building aware CFD tool that 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. Apart from the wind pressure, the influence of ventilation networks and the nature of openings on ingress of H_2S are also considered.

Below is the detailed description of various models that will be used in this study.

4.1 Modelling of building air quality - 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 zone [14].

CONTAM is a multi-zone indoor air quality ventilation analysis model. It helps to determine airflows which include 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. It also helps to study dispersion of contaminants and predict personal exposure [17].

[25] reported a comprehensive study validating the CONTAM model against experimental data which was collected in a controlled environment as well as with field measurement data. CONTAM was found to be in good agreement in both cases.

CONTAM's capability to calculate building airflows and relative pressure between zones of buildings can be utilized for a variety of applications such as [18]:

- Calculating building airflows and relative pressures between zones of the building.
- Assessing the adequacy of ventilation rates in a building.
- Determining the variation in ventilation rates over time.
- Determining the distribution of ventilation air within a building.
- Estimating the impact of envelope air-tightening efforts on infiltration rates.

CONTAM features can be divided into airflow analysis and contaminant analysis. Airflow analysis is based on the algorithm developed in AIRNET, an airflow network simulation program developed by National Institute of Standards and Technology (NIST) [26]. 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 elements is assumed to be governed by Bernoulli's equation [18]:

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

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.

Airflow elements in this project 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:

$$Q = C\left(\Delta P\right)^n \qquad 2$$

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.

Contaminant dispersal model is based on the application of conservation of mass of all species within a control volume (c.v). Control volume is defined as the volume of air which may correspond to a single room, a portion of a room, zones etc. Mathematically, this is expressed as:

$$\left[\rho_i V_i + \Delta t\left(\sum_j F_{i\to j} + R_i^\alpha\right)\right] C_i^\alpha \Big|_{t+\Delta t} \approx \rho_i V_i C_i^\alpha \Big|_t + \Delta t\left[\sum_j F_{j\to i}(1-\eta_j^\alpha) C_j^\alpha + G_i^\alpha + m_i \sum_\beta \kappa^{\alpha,\beta} C_i^\beta\right]_{t+\Delta t} \qquad 3$$

where:

ρ	is the density of air
V	is a given volume
t	is the time
C_i^{α}	is the concentration of contaminant a in c.v. i
$F_{j \to i}$	is the rate of air mass flow from c.v. j to c.v. i
η_j^{α}	is the filter efficiency in the path
G_i^{α}	is the species generation rate
R_i^{α}	is a removal coefficient
$\kappa^{\alpha,\beta}$	is the kinetic reaction coefficient in c.v. between species a and b

In order to analyze airflow or contaminant migration in a building in CONTAM the following steps are followed as shown below:

- Building idealization: Consider the building that is going to be studied
- Schematic representation: Develop a schematic representation of the building
- Define building components: Collect and input data associated with the building components
- Simulation: Set simulation parameters and execute simulation

In order to model airflow and contaminant related phenomenon, CONTAM incorporates assumptions that simplify the model. The following are the assumptions considered in this project:

- Well mixed zones: Treats each zone as a single node, wherein the air has uniform conditions throughout. This includes temperature, pressure and contaminant concentrations.
- Conservation of mass: During steady state simulation, the mass of air within each zone is conserved by the model. During transient simulations, CONTAM provides the option allowing the accumulation or reduction of mass within a zone due to the variation of zone/pressure and the implementation of non-trace contaminants within a simulation.
- Airflow paths: Airflows through various airflow elements provided by CONTAM are modeled using Powerlaw in this project. Powerlaw models establishes a relationship between airflow and pressure difference across the flow path. The discharge coefficient is assumed to be 0.65 for small crack like opening and 0.5 for large openings.

4.2 Fully numerical modeling of release - Quick Urban and Industrial Complex (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 [27]. The simple zero-equation model is based on Prandtl’s mixing length theory[28][29]. 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 [19].

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 discretization 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:

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag*{4}$$

Momentum equations:

$$\frac{\partial \overline{u}_i}{\partial t} = -\frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} - \frac{1}{\rho_i}\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\nu\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)\right] - \frac{\partial \overline{u}_i^{'} \overline{u}_j^{'}}{\partial x_j} \tag*{5}$$

Where

$\overline{u}_i$	is the mean velocity in the *i th* direction
$\overline{u}_i^{'}$	is the turbulent fluctuating velocity
$\overline{p}$	is the pressure
ρ	is the average density
$\overline{u}_i^{'}\overline{u}_j^{'}$	is the turbulence Reynolds stresses
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 [28]. QUIC-CFD model utilizes a 3-D 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.

Being relatively faster than traditional CFD models, QUIC model can be used in various applications related to toxic releases in cities or industrial facilities where turnaround time is very important [27]. QUIC can be applied in the following areas:

1. Vulnerability assessments
2. Training and table top exercises
3. Emergency response

4.3 Fast empirical modelling of release – SLAB EPA, US

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:

$$C(x,y,z,t) = CC(\mathrm{x}).[\mathrm{erf(xa)} - \mathrm{erf(xb)}].[\mathrm{erf(ya)} - \mathrm{erf(yb)}].[\exp(-\mathrm{za}^2) + \exp(-zb^2)] \tag{6}$$

where:

$$xa = \left(\mathrm{x} - \mathrm{xc} + \mathrm{bx}\right) / \left(\sqrt{2}.betax\right) \tag{7}$$

$$xb = \left(\mathrm{x} - \mathrm{xc} - \mathrm{bx}\right) / \left(\sqrt{2}.betax\right) \tag{8}$$

$$ya = \left(y + b\right) / \left(\sqrt{2}.betac\right) \tag{9}$$

$$yb = \left(y - b\right) / \left(\sqrt{2}.betac\right) \tag{10}$$

$$za = \left(z - zc\right) / \left(\sqrt{2}.\mathrm{sig}\right) \tag{11}$$

$$zb = \left(z + zc\right) / \left(\sqrt{2}.\mathrm{sig}\right) \tag{12}$$

Here, *CC(x)*, *b(x)*, *betac(x)*, *zc(x)*, and *sig(x)* are all functions of downwind distance ‘*x*’ whereas, *Xc(t)*, *bx(t)*, and *betax(t)* are all functions of time ‘t’

5. RESULTS AND ANALYSIS

5.1 Description of accident scenario and accidental release modelling

A two level administration building is located 1 km away from a natural gas feed pipeline of 38 inch diameter. High pressure sour natural gas with 0.77% (mass) H_2S impurity was 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 external environment of the building was exposed to H_2S toxic cloud for a period of 1 hour resulting from the pipeline leak. The mass source rate due to full bore rupture was considered as 11,544 kg/s. The accidental release was modelled using the empirical model SLAB. Figure 1 shows the centerline concentration profile of the H_2S toxic plume due to the accidental discharge. Three stability classes C, D and F for wind speeds of 4 m/s, 5 m/s and 3 m/s respectively were considered for modelling. It can be observed that stability F gave the highest concentration compared to other stability classes. The concentration of interest was 1 km away from the source where the building is located. It was observed that F stability class showed a maximum concentration of 660 ppm at 1 km whereas C and D stability class indicated 458 ppm and 515 ppm respectively. This can be attributed to the fact that the F stability provides a stable atmospheric condition for plume dispersion. In all cases the relative humidity (RH) was assumed to be 50%. H_2S concentration in the vicinity of the leak was around 9700 ppm and then gradually decreased to less than 1000 ppm at a distance of 1200 m from the release source. This is due to the fact that as the plume moved further towards the building, the concentration decreased due to dilution with ambient air. It was observed that the extent of dilution was found to have subsided once the plume was beyond 600 m from the release source. The duration of the plume to reach the building was found to be arounds 50 s, according to the SLAB calculations. This duration was considered as the time taken for the plume to hit the first wall of the building. The plume reached the building six times faster than the wind velocity (3 m/s) because of the high release rate due to the full bore rupture and the horizontal jet release assumption considered while modelling the release. In order to provide adequate spatial and temporal coverage of the dispersion domain, the maximum downwind distance was adjusted for the completion of SLAB calculations.

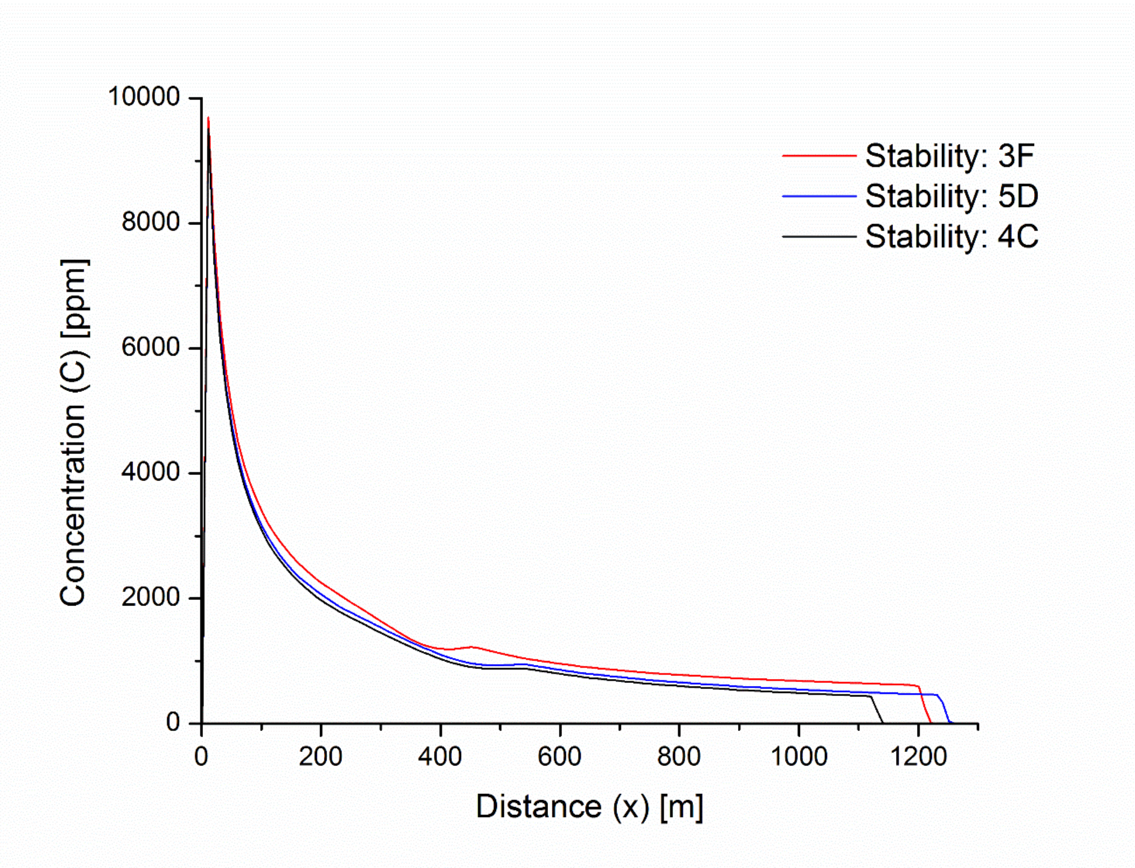
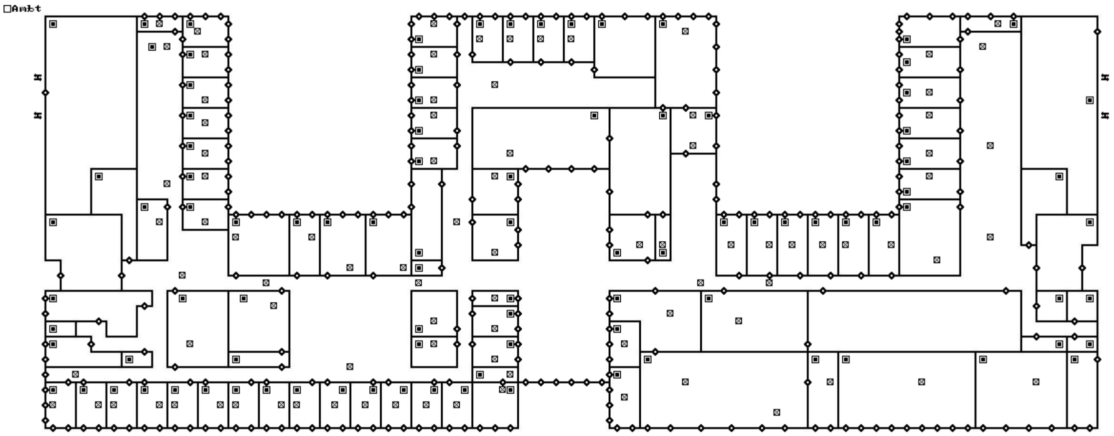


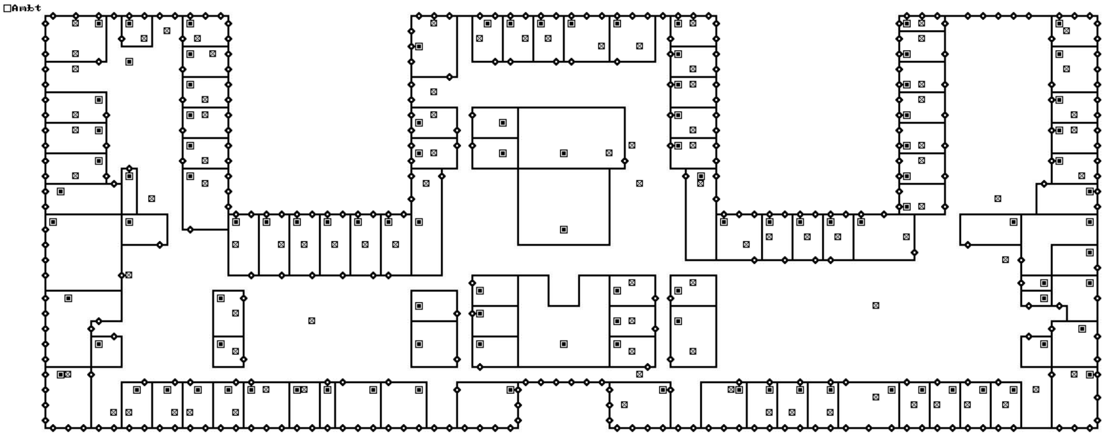
Figure 1: Maximum concentration (centerline) of H_2S plume for different stability classes

5.2 Building geometry

As mentioned in Section 5.1, a two level administration building was chosen for this study. The building was simplified into an idealized building using the multi-zone model CONTAM. The model utilizes different concepts such as walls, zones, airflow paths (openings), levels, etc. to perform simulation and analysis [18]. Figure 2 exhibits the geometry of the administration building. This domain is used in CONTAM to study the effect of meteorological condition, variable wind pressure and ventilation networks 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, CONTAM solves air flow rate between openings as a function of pressure drop along the flow path which is described by Equation 2. The flow coefficient variable in Equation 2 can be calculated using different methods. One method is to utilize the wind pressure acting on the windows calculated based on the ASHRAE formulation for low rise rectangular buildings [22]. The second method is to employ the QUIC dispersion model. The building is composed of 94 rooms on the ground floor and 102 rooms on the first floor. Each floor also contains a corridor which connects with the rest of the rooms in the building. The building has a total area of 3438.95 m^2 where corridors in the first and second floor covers a maximum area of 876 m^2 and 1605 m^2 respectively. All rooms in the perimeter of the building are connected to the outdoor environment through windows. Though every window is considered to be closed at all times in this study, it is assumed to have a leakage area of 1.73 cm^2/m. A leakage area of 187.5 cm^2 per door is also assumed in the scenario which assumes the whole building to be sealed from the outdoor environment [24]. Apart from windows, other components such as doors and ventilation network were also considered to study the ingress of toxic gas.



a) Ground floor



b) First floor

Figure 2: Idealized building layout of the building as incorporated in CONTAM

5.3 Indoor toxic levels

The effect of three parameters on the indoor toxic levels were considered in this work; meteorological, wind pressure and ventilation networks. Considering the large size of the building, only the corridor area on the first floor are shown in the results. The corridor area is chosen over other rooms because it occupies a majority of the area in the building and was found to influence the ingress concentrations the most. Hence, toxic levels attained in the corridor area is assumed to be the worst case scenario in this study.

5.3.1 Effect of wind direction

Wind direction was found to influence the ingress phenomenon as well as the dispersion of gas inside the building. In order to consider a worst case scenario, the building was exposed to the outdoor toxic cloud with the entrance doors open and the HVAC system switched on the entire duration of simulation. It is observed from Figure 3 that 90^0 wind direction was found to be most vulnerable to the building. This is because the direction of wind is normal to the entrance doors of the building which is directly connected to the corridor area. The HVAC air inlets which supplies the outdoor air for ventilation is also located normal to the 90^0 wind direction. This results in an increased infiltration of gas inside building. Since the leak is assumed to last for 1 hour, the maximum concentration attained inside the corridor gets close to the outdoor toxic levels during the duration of the leak. The positions of the entrance doors and the HVAC air inlets with respect to the 90^0 wind direction also results in a faster decay rate of the indoor toxic levels after 60 min. Keeping the entrance doors open and the HVAC system switched on one would assume the toxic levels would decay quickly once the leak is contained. On the contrary, it took around 30 min for the indoor toxic level to go below Acute Exposure Guideline Limits -3 (60 min) limit (AEGL-3) of 50 ppm.

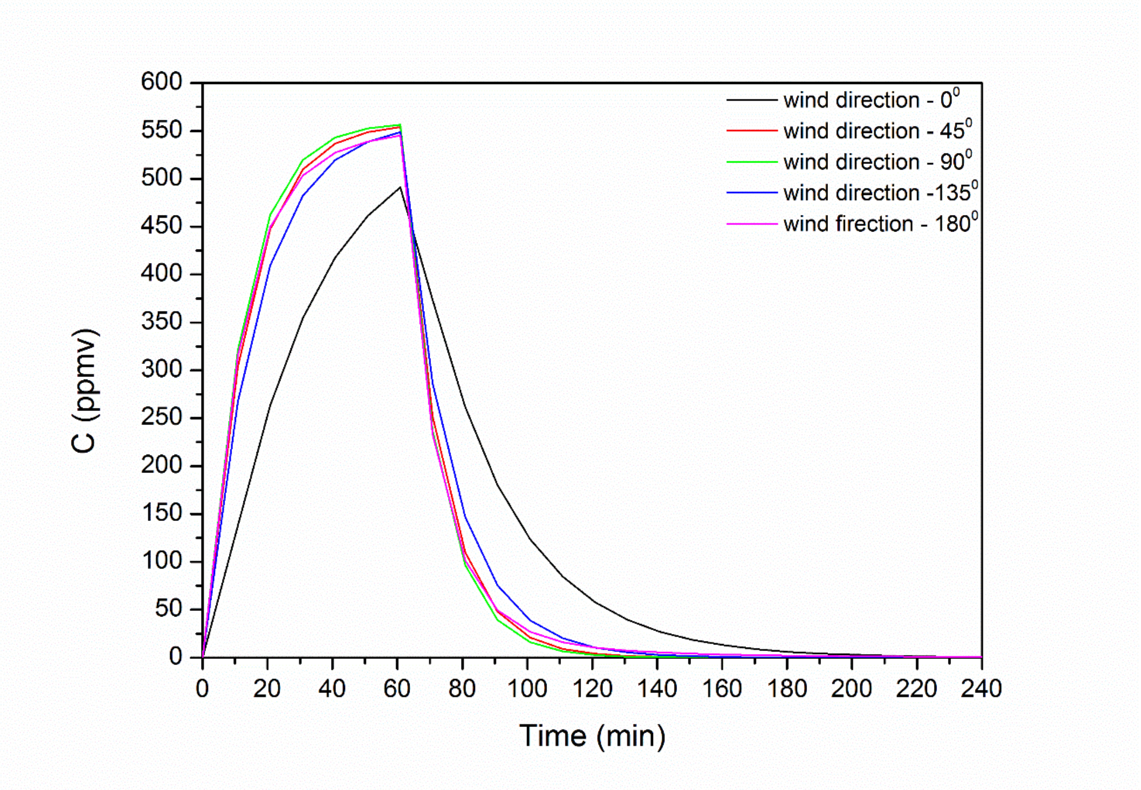


Figure 3: Effect of wind direction on the indoor toxic level

5.3.2 Effect of wind pressure

Wind pressure acting on the exterior of the building influences the infiltration of the air from the outdoor environment to the indoor environment. In order to compute building ingress, CONTAM solves air flow rate between openings as a function of pressure drop along the flow path which is described by Equation 2. The flow coefficient variable in Equation 2 can be calculated using different methods. One method is to utilize the wind pressure acting on the windows calculated based on the ASHRAE formulation for low rise rectangular buildings [22]. However, this method can be assumed to be generic since it caters only to a specific building geometry. The second method is to employ the

QUIC dispersion model to calculate the flow coefficient variable by taking into account the actual geometry of the building. In this study, ASHRAE correlation for low rise rectangular buildings was considered in the CONTAM multi-zone model to calculate the variable wind pressure acting on the exterior facade of the building. The wind pressure profile based on the ASHRAE correlation is depicted in Figure 4. The correlation produces wind pressure coefficients averaged over a building façade as function of wind direction [22].

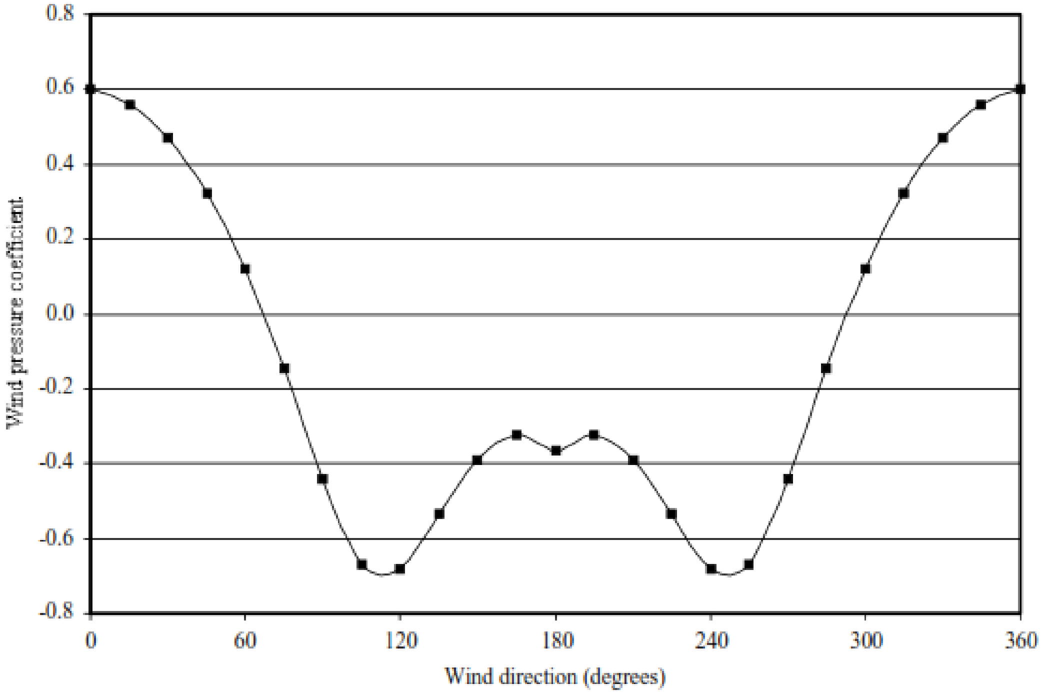
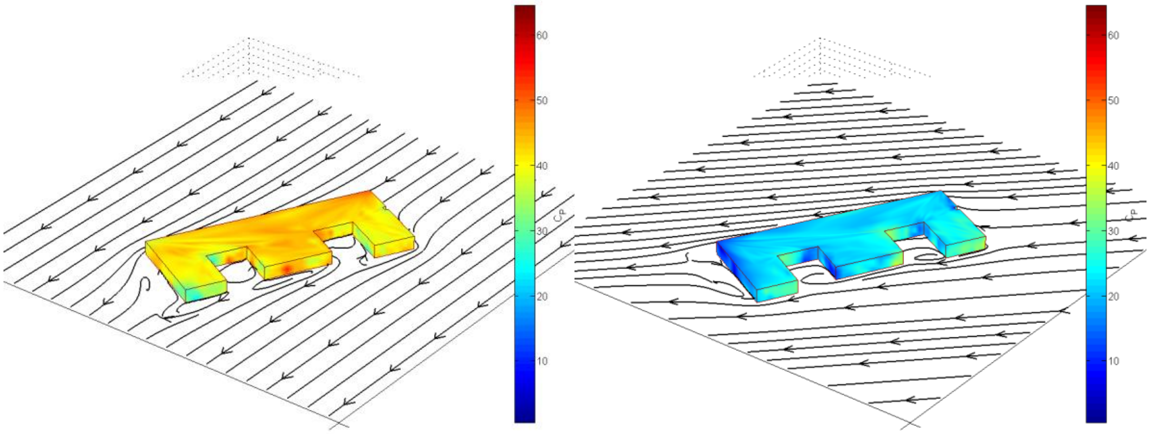


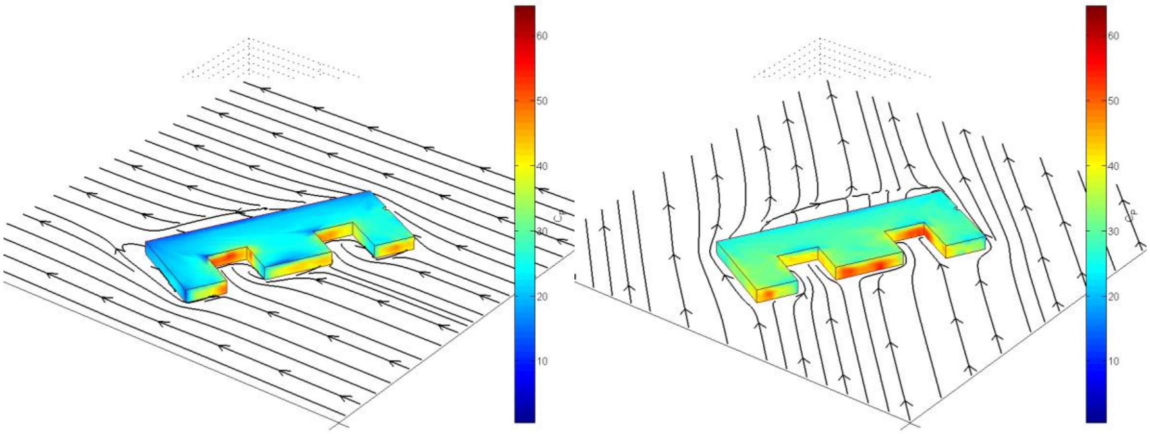
Figure 4: Wind pressure profile based on ASHRAE correlation for low rise rectangular shaped buildings [22]

However, more accurate variable wind pressure data was obtained using the QUIC-CFD model. QUIC takes into account the building geometry while calculating the wind pressure acting on the building openings. Figure 5 presents the relative pressure field developed on the building for various wind directions.



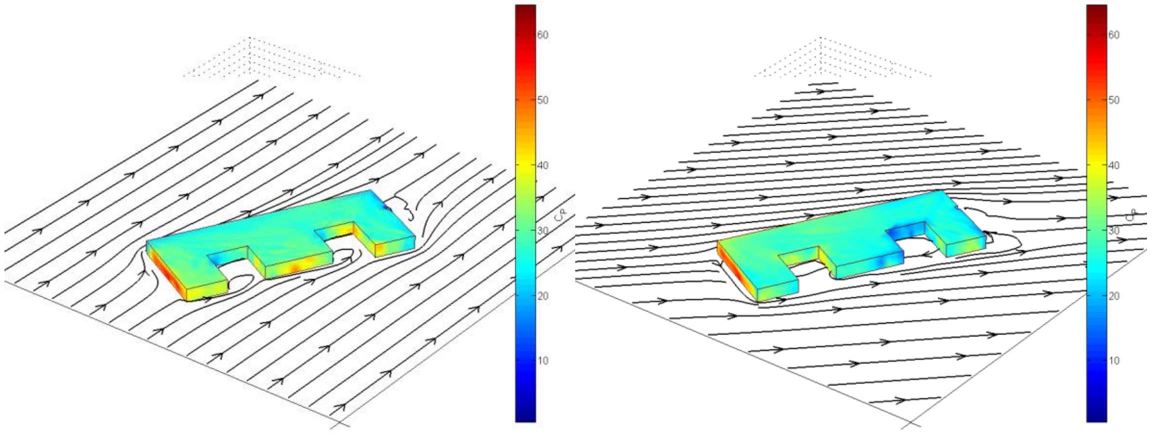
South West

West



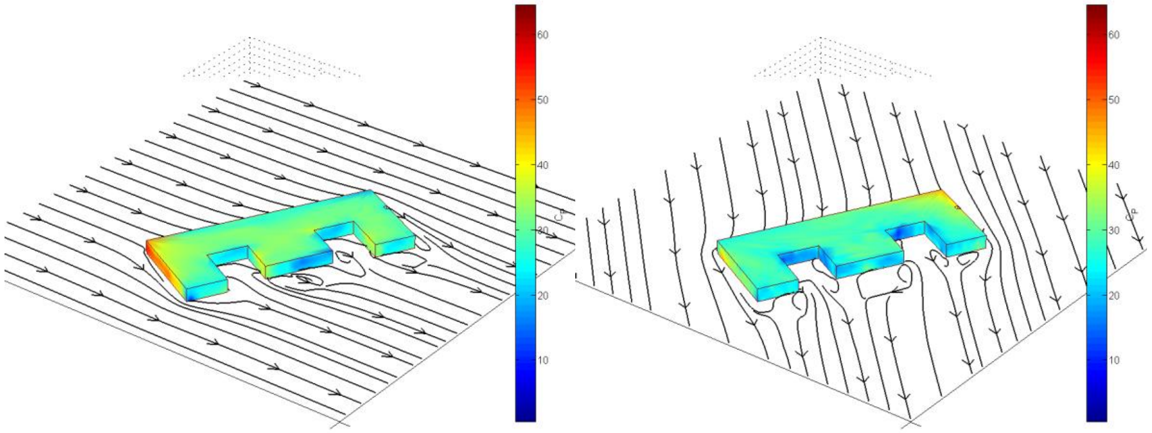
North West

North



North East

East



South East

South

Figure 5: Plot of relative pressure fields on the building wall for various wind directions

A more detailed study of the developed pressure coefficients followed in order to demonstrate the applicability of the ASHRAE formulation of the need for a more advanced approach. The pressure coefficient for a number of locations (points) on the building has been calculated for various wind directions. Figure 6 shows the location of these points and Figure 7 the pressure coefficients. From Figure 7 it was clear that although the range of the pressure coefficient is within the ASHRAE recommendations, the wind direction dependence was not similar. This was expected because of the complex building geometry. This behavior is expected to be more intense by the inclusion of the surrounding buildings and the use of the fully numerical wind flow model. Since the wind pressure coefficients calculated using the ASHRAE correlation does not even follow the same pattern compared to the predictions attained using QUIC CFD, its application on the chosen building can be questionable.

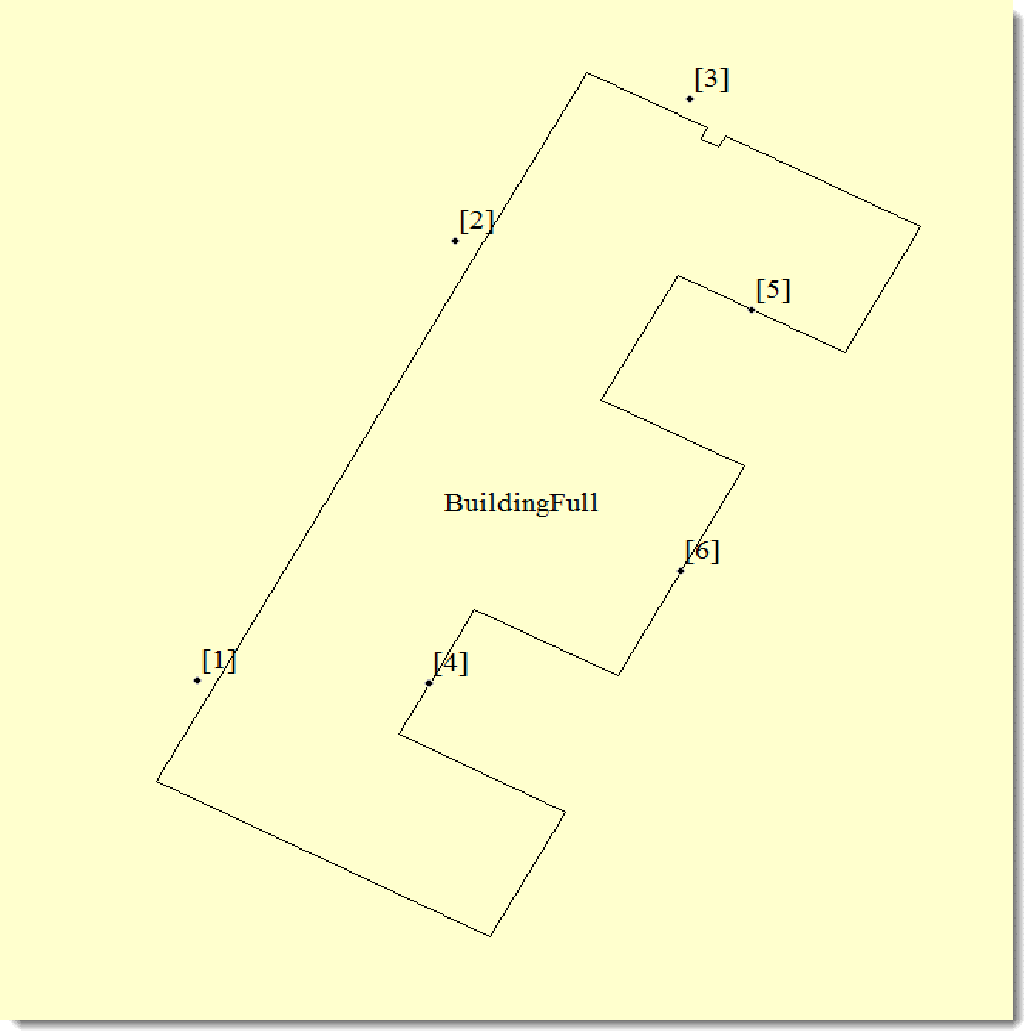


Figure 6: Location of points used to calculate pressure coefficients

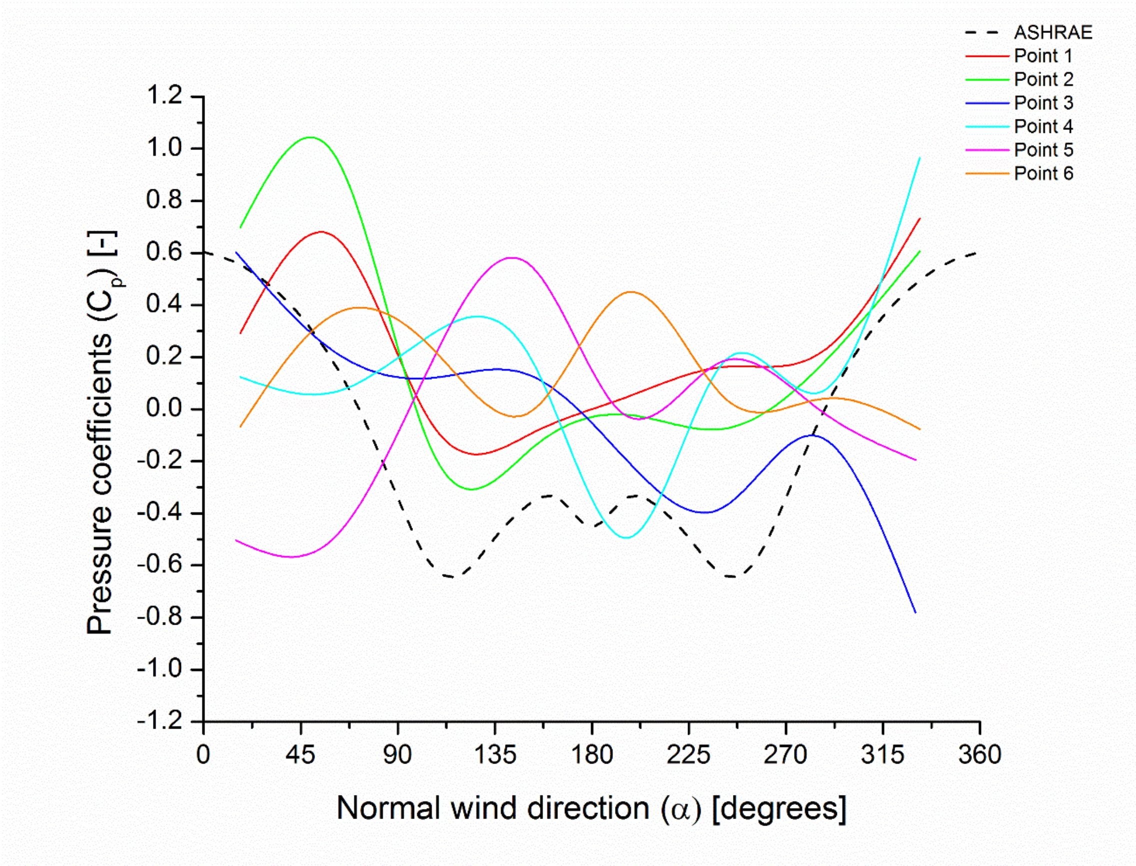


Figure 7: Comparison of pressure coeffcients w.r.t wind direction (QUIC Vs ASHRAE calculation method)

Subsequently, the wind pressure data obtained from QUIC were imported into the CONTAM model as a WPC file to study the effect of wind pressure on toxic gas ingress. Figure 8 compares the toxic gas concentration in the corridor area and a typical office room in the building based on the wind pressure calculated by QUIC and ASHRAE correlation. The concentration profile attained inside the room was shown to vary significantly with respect to the wind pressure calculation method. QUIC method showed a faster rate of ingress and higher concentration in the room compared to the ASHRAE method. However, comparing the concentration profiles of the corridor area for both calculation methods does not seem to differ. This is due to the t that corridor covers a large area and CONTAM considers the area as a single zone. Therefore, the well mixed assumption of the model cannot be deemed realistic.

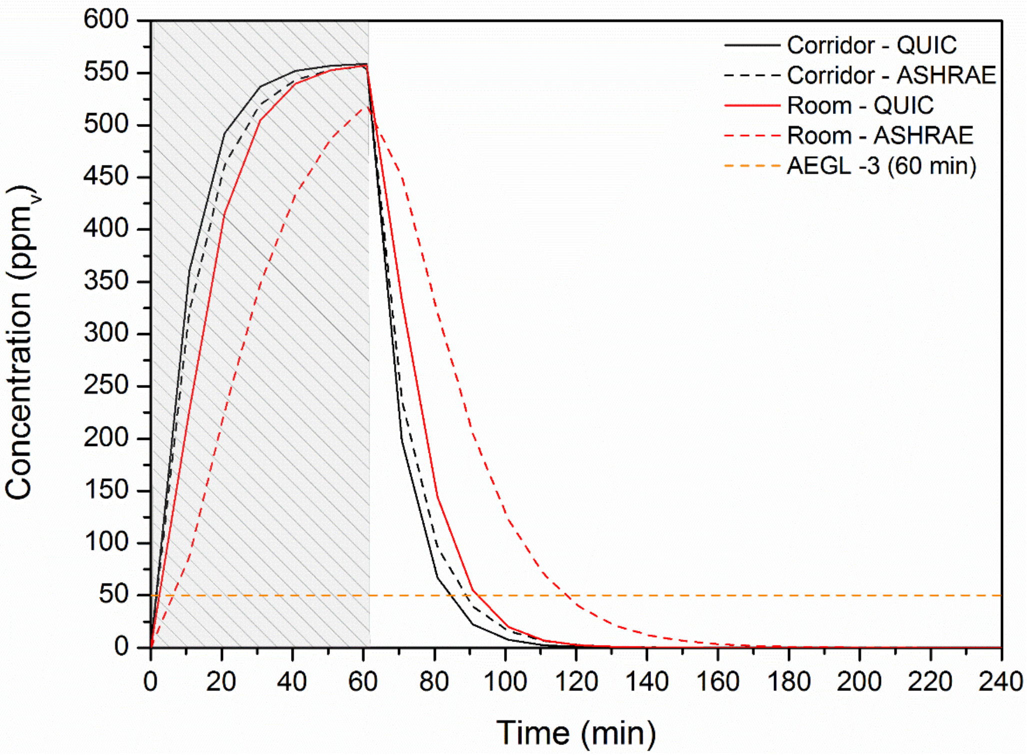


Figure 8: Effect of wind pressure on indoor toxic levels

The effect of wind pressure on the airflow rates between zones inside the building were also studied. For comparison, airflow rates between the corridor area and 8 rooms from different areas of the building were compared. The chosen rooms are depicted in Figure 9. Figure 10 exhibits the airflow rate prediction between the corridor (green) and rooms (red) by both models. It is observed that QUIC predicts an airflow in all the rooms surrounding the corridor area except room ‘h’ whereas ASHRAE correlation fails to predict in rooms ‘a’ and ‘h’. Since room ‘h’ is only connected to the ambient atmosphere through a window and not the corridor both models fails to predict an airflow between the corridor and the room. In all cases QUIC predicts a higher flowrate compared to ASHRAE especially for rooms ‘a’ and ‘d’ where the flowrates predicted by QUIC are an order of magnitude higher than the ASHRAE predictions. Subsequently, this will be reflected in the contaminant concentration data obtained for a particular zone and eventually the mitigation strategies. 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. Difference in airflow rates prediction by the ASHRAE model can be attributed to the fact that the correlation used in the model caters only to low rise buildings. However, the building chosen for this study is a two level building.

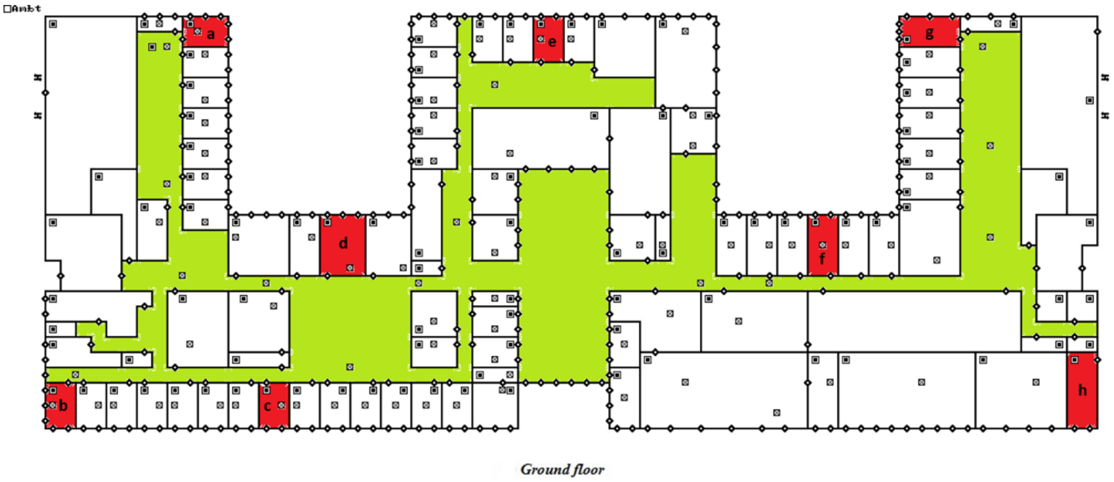


Figure 9: Selected rooms (red) and corridor (green) for airflow rates comparison

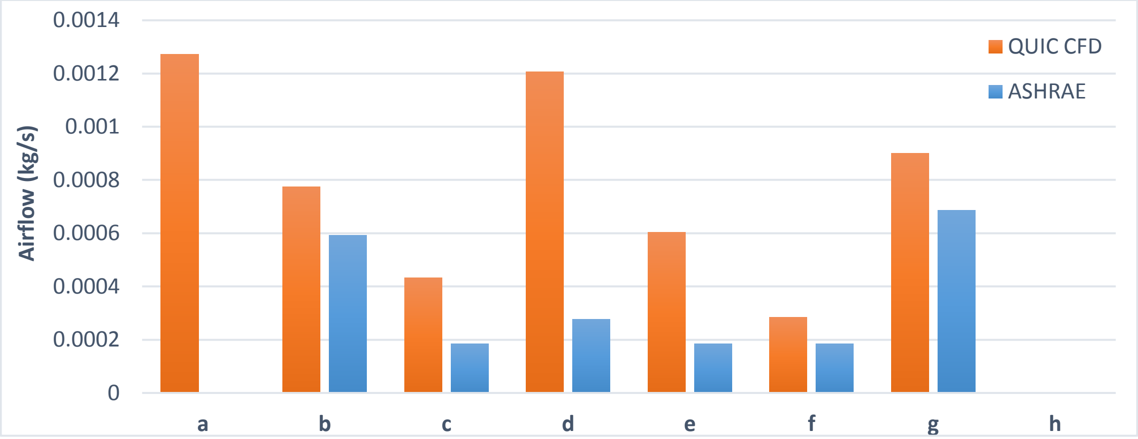


Figure 10: Comparison of airflow rates between corridor and rooms based on QUIC CFD and ASHRAE models

5.3.3 Effect of ventilation network (HVAC)

Mechanical ventilation or forced ventilation systems such as HVAC form an integral part of a building. Therefore, it is 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 release. Table 2 describes the various scenarios considered in order to study the effect of HVAC on indoor toxic levels.

Table 2: Scenarios description

Scenario	**HVAC**	**Entrance door**
1	On	Open
2	On	Closed
3	Off	Closed
4	Off	Open
5	On-Off	Closed

As mentioned in the earlier section 5.3.1, the worst case scenario was considered keeping the HVAC switched on and the entrance doors open during the entire duration of the simulation. This corresponds to Scenario 1. Scenario 1 also takes into account the effects of both mechanical and natural ventilation that occurs inside the building. Scenario 2 takes into account only the forced ventilation since ingress occurs only through the HVAC system. In Scenario 3, a sealed building is mimicked by shutting down the HVAC system and keeping the entrance doors closed during the entire duration of simulation. In Scenario 4, only natural ventilation is accounted by keeping the entrance doors open and the HVAC system switched off. Considering the worst case scenario (Scenario 1), it was found that it took approximately 2 min for the concentrations to reach 50 ppm (H_2S AEGL-3 (60min)). Hence, the HVAC system was configured to shut off after 2 min in the case of Scenario 5. Scenario 5 resembles a typical emergency response practice in the event of an outdoor toxic release. Figure 11 describes the effect of ventilation on the concentration profile in the corridor area by comparing Scenario 2, 3 and 4 respectively. Ventilation was found to be the dominant variable while trying to model the ingress of toxic gas into the building. Comparing Scenario 2 and Scenario 3, the presence of forced ventilation resulted in a significantly higher concentration levels in the corridor. Conversely, Scenario 3 which considers a sealed building, shows minimal infiltration of the released toxic gas. This was mainly due to the fact that in Scenario 3, infiltration takes place only due the assumed leakage area for the doors and windows. However, in the case of Scenario 4, which considered only the natural ventilation by shutting down the HVAC system, the concentration profile achieved inside the corridor is similar to Scenario 2 which considered only the forced ventilation. This indicated that the presence of any kind of ventilation, either forced or natural can compromise the integrity of building, thereby exposing its indoor population to risk of H_2S exposure.

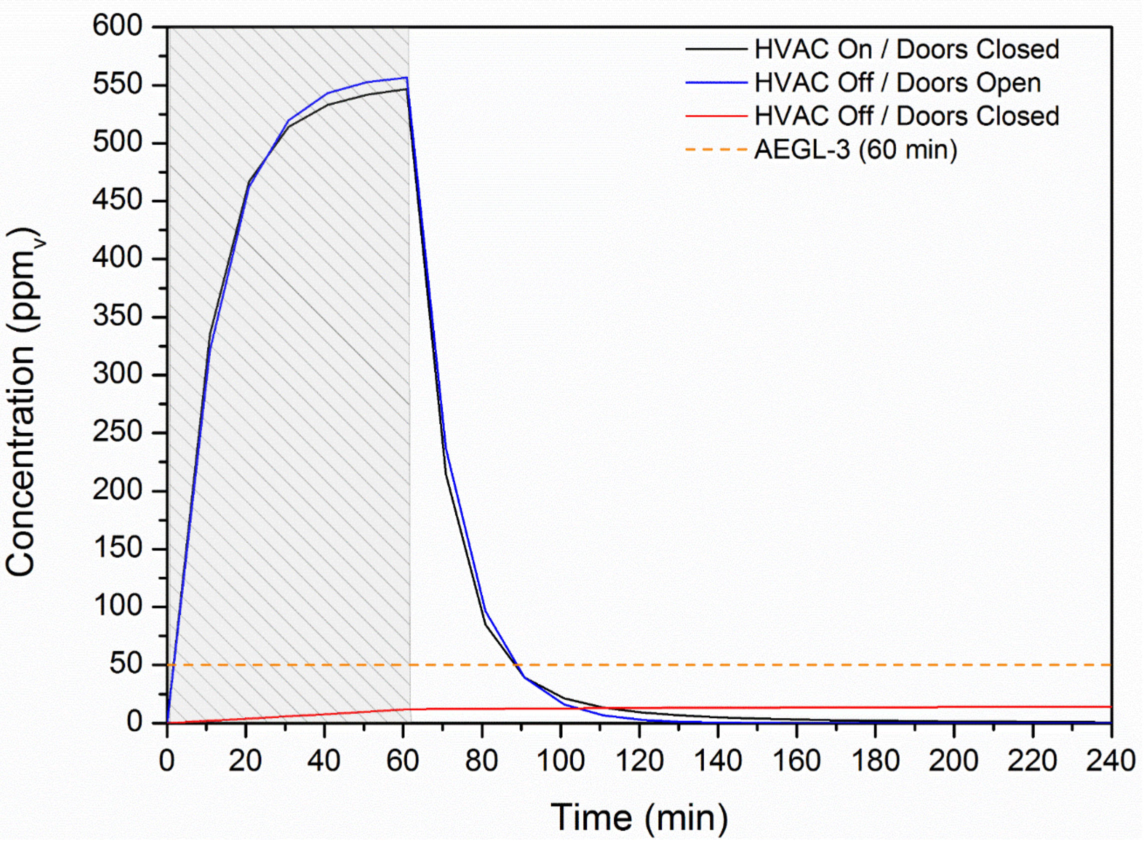


Figure 11: Effect of ventilation on indoor toxic levels

5.4 Assessment of mitigation methods

Toxicity is the ability of a substance to produce an unwanted effect when the chemical has reached a sufficient concentration at a certain site in the body [30]. A dose-response model is usually used to base various toxicological considerations. Acute toxicity data is commonly used to establish dose-response curves. However, for computational purposes the response versus dose curves is not preferred [31]. Conversely, analytical equation like Probit (probability unit) equations which helps to estimate exposure of various types of chemicals is more convenient [32]. A probit variable is normally distributed and has a mean value of five and a standard deviation of one [21]. With respect to inhaled toxic gas, the dose can be presented as a specified gas concentration administered over a period of time.

Equation 13 describes the probit equation which gives the best fit for percentage fatalities versus concentration duration using log probability plots or standard statistical packages.

$$Y_i = A + B\ln\left(V_i\right) \tag{13}$$

$$V_i = C^n t \tag{14}$$

where:

Y_i	is the probit function
A and B	are constants
V_i	is the causative variable
C	is the concentration in ppm
t	is the duration in minutes

The probit approach has been used for at least 30 years to determine the consequences of toxic gases. They have been developed for a wide range of toxic materials including H_2S. Recognized bodies like TNO and HSE UK have published their own probit functions (Table 3). However, there is no clear pattern on either of them indicating a higher or lower concentration for a given lethality level. But TNO probit is recommended for all studies unless a particular probit is specified [33]. Hence, this work utilized the TNO probit function which is given by Equation 15. The causative variable which calculates the toxic dosage follows Equation 16. The probit is converted to percentage fatalities (*P*) using Equation 17 [34].

Table 3: Constants for UK HSE and TNO probit functions

Material	**HSE Probit**			**TNO Probit**		
	A	B	n	A	B	n
Hydrogen Sulfide	-30.08	1.16	4	-10.87	1	1.9

$$Y_i = -10.87 + \ln\left(V_i\right) \qquad 15$$

$$V_i = \left(C_i\right)^n t + V_{i-1} \qquad 16$$

$$P = 50\left[1 + \frac{Y_i - 5}{|Y_i - 5|} erf\left(\frac{|Y_i - 5|}{\sqrt{2}}\right)\right] \qquad 17$$

Apart from the probit method, another method called Toxic Load (TL) approach was used in this work to model the dosage resulting from H_2S exposure. TL method was developed by the EPA and is based on the AEGL limits. TL is integrated from zero using actual evolving contaminant concentration history [35]. This is described by Equation 18.

$$TL(t) = \int_0^t TL_{rate}\left(t'\right) dt' \qquad 18$$

$$TL_{rate}(t) \equiv \frac{dTL}{dt} = \frac{1}{t_b}\left[\frac{C(t)}{C_{t_b}}\right]^n \qquad (19)$$

where:

n is the power exponent (-0.23 for H_2S)

T is the time in seconds

t_b is the reference AEGL time band exposure step

C is the concentration in ppm

TL results are normalized to a value of 1 above which indicates life threatening or death conditions prevail. Therefore if the TL value for a particular case is closer to 1, the likelihood of a fatality is higher.

Both approaches used for dose response modelling were tested for two different types of evacuation scenarios as depicted in Figure 12. The first scenario involved escaping outside the building in the horizontal or vertical direction in the event of a release. The second scenario considered assumed a shelter in place during the entire period of release. The average speed of a person escaping outside the building is assumed to be 1.4 m/s.

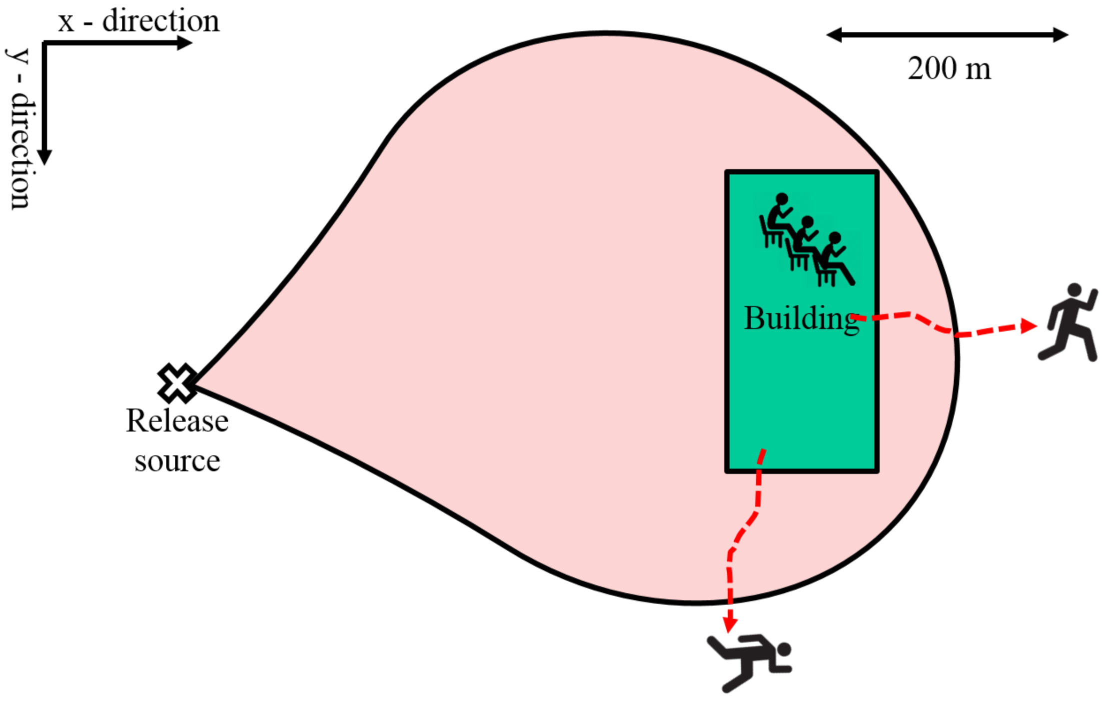


Figure 12: Evacuation scenarios

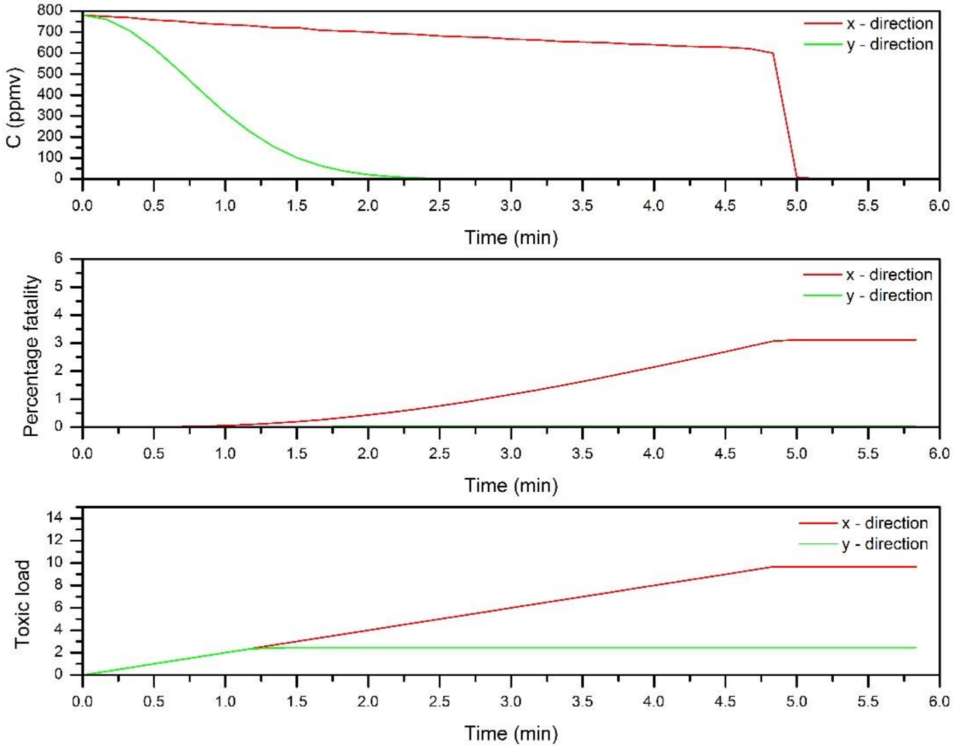


Figure 13: Comparison of percentage fatalities based on probit and TL method for the first scenario

The number of fatalities for the first scenario was calculated using both dose response techniques and compared in Figure 13. While probit predicts a 3 % fatality for moving in the x direction in the event of a release, it predicts no fatalities if the same person was to go in the y direction. However, TL values reach 1 in almost half a minute for both directions. This means that the person is exposed to a fatal environment in less than one minute making it unsuitable to escape outside. Probit underestimates lethality because it does not take into account short term exposures; for e.g. as in the case of AEGL limits. Conversely, TL is based on AEGL limits. A variation can also be found of probit results depending on the parameters chosen; for e.g. between TNO and HSE UK (Table 3). It is also an added advantage that AEGL limits are mainly applicable to vulnerable groups like the general population which accounts for a non-process building [35]. In order to overcome this inconsistency the probit concentrations for the same time period as the AEGL -3 values found in Table 4 were compared in Figure 14. It can be observed from Figure 14 that the threshold concentrations calculated by probit is significantly larger than the AEGL-3 concentrations for the same time period. For e.g. at 60 min, AEGL-3 predicted 50 ppm as the threshold concentration compared to 300 ppm by probit. This means that probit will only calculate a fatality if a person is exposed to 300 ppm for one hour. This is predominantly the reason why probit underestimated lethality in Figure 13 compared to the TL method which followed the AEGL-3 values. Since the AEGL- 3 values for H2S fits the power law, the probit function expressed in Equation 15 was adjusted for the power exponent 'n' to match the power law profile followed by the H2S AEGL – 3 values. The comparison is depicted in Figure 15. It was observed that when n was adjusted to 2.74, the adjusted probit was consistent with the AEGL – 3 profile. For e.g. at 60 min, both AEGL-3 and the probit threshold concentration was found to be 50 ppm.

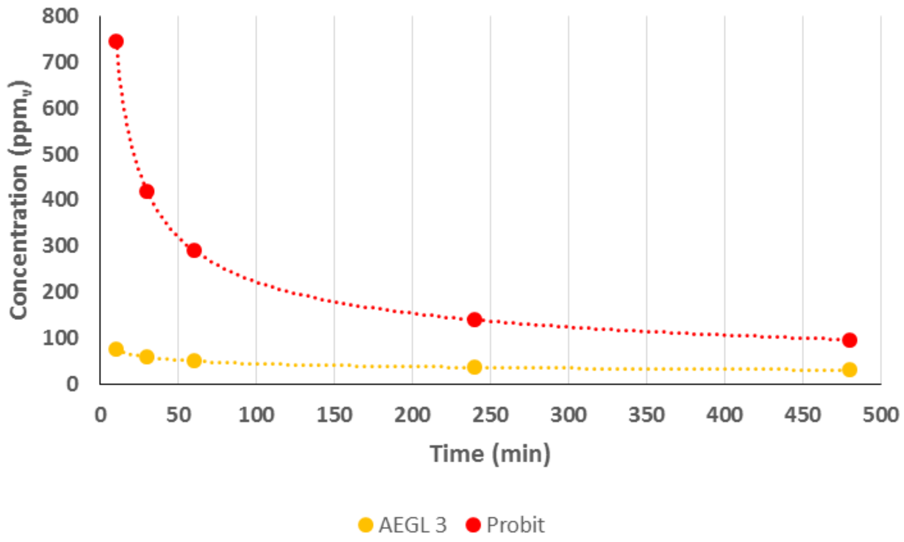


Figure 14: Comparison of threshold concentrations based on AEGL-3 and probit

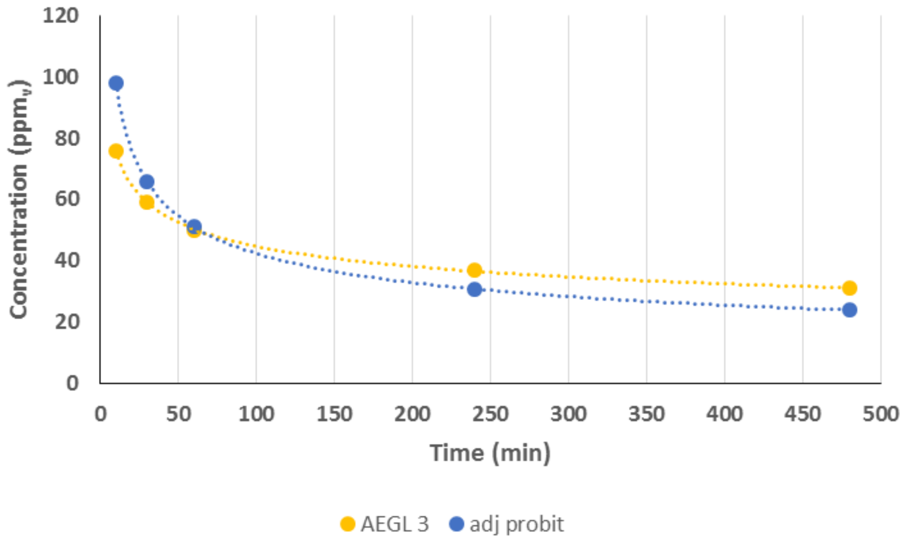


Figure 15: Comparison of threshold concentrations based on AEGL-3 and adjusted probit

Table 4: AEGL-3 values for H_2S

Time (min)	10	30	60	240	480
Concentration (ppm)	76	59	50	37	31

The adjusted probit was compared to both dose response models as shown in Figure 16. It can be seen that adjusted probit shows a 100 % fatality in half a minute which corresponds to the TL value of 1 for the same time.

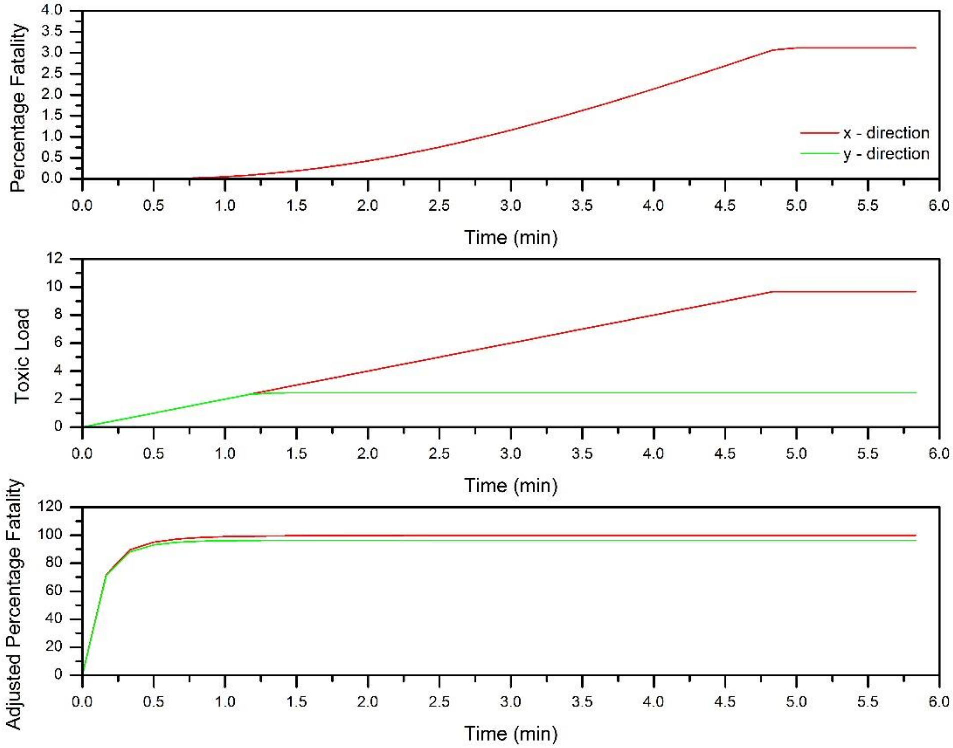


Figure 16: Comparison of adjusted probit with probit and TL dose response models for the first scenario

Figure 16 clearly depicts that escaping outdoor is not a feasible option. Therefore the second scenario considered was staying inside the building as exhibited in Figure 12. Since the corridor was found to be the most vulnerable area inside the building, the indoor toxic level of the corridor on the ground floor is considered for assessment. As the corridor area covered the largest area inside the building, the probit function was approached as a weighted probit which gave the probability of dying and being at a particular location at a given time. Equation 20 below describes the weighted probit.

$$Y = Y_i . X_j \qquad 21$$

$$X_j = \frac{v_i}{\sum v_i} \qquad 22$$

where:

X_j	is the probability of being at a particular location
v_i	is the volume of the individual room
Y	is the weighted probit
Y_i	is the probability of fatality

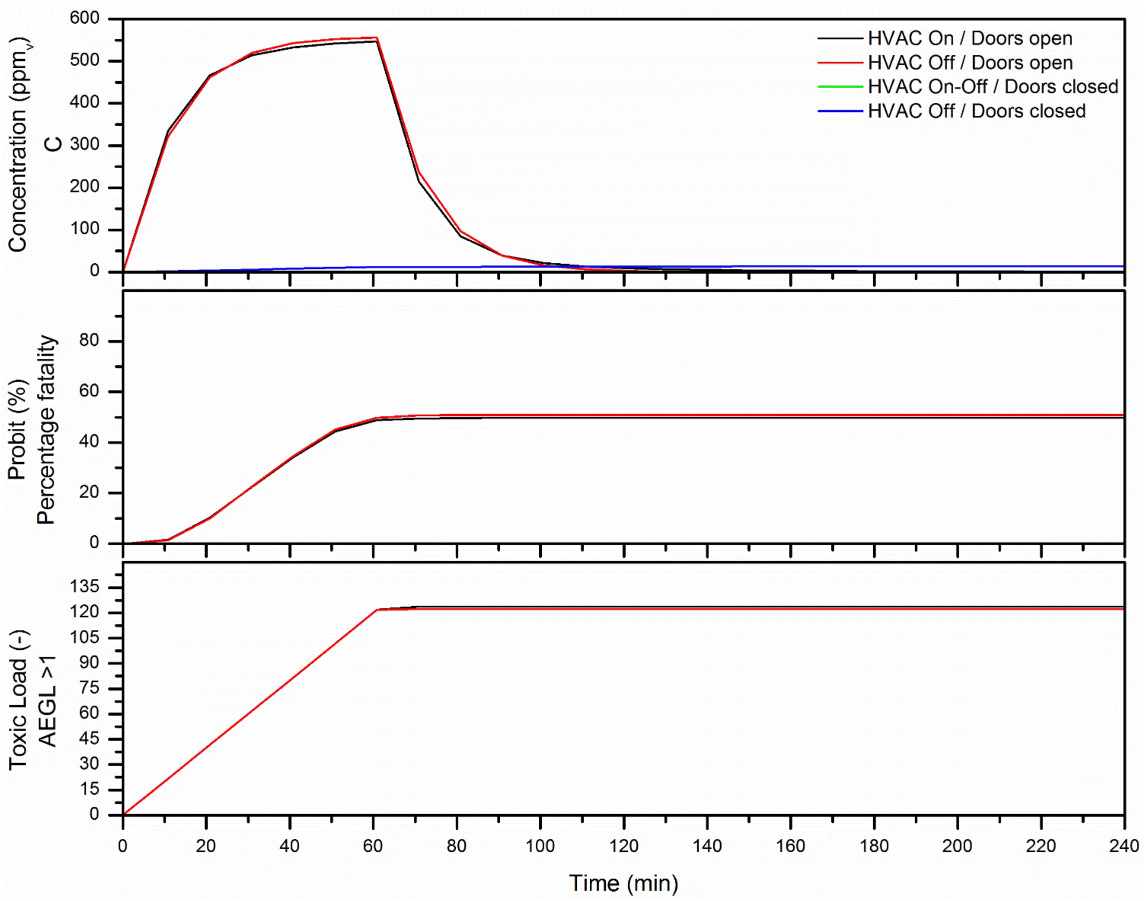


Figure 17: Comparison of percentage fatalities based on probit and TL method for the second scenario

Since ventilation was found to be the most dominant factor while modelling the ingress of released toxic gas, different scenarios described in Table 2 was considered as mitigation methods. Each scenario involving HVAC produced different toxic levels in the corridor. The corresponding toxic levels were utilized to model the dosage using the probit and TL method. Figure 17 compares the results of both dosage calculation techniques. Shutting down the HVAC system in Scenarios 3 and 5 deters the indoor toxic concentrations to reach fatal levels. As a result no fatalities were reported for both these scenarios in either dose response models. For Scenarios 1 and 4 which is considered as a worst case scenario, probit predicts around 50% fatality whereas TL predicts a probability of 100% fatality in less than 1 minute. The reason is because TL calculation method is based on the toxic levels in the corridor while probit is based on the weighted probit which gives the combined probability of a fatality and being at a certain point in the corridor. In all cases, Scenarios 3 and 5 were found to be the most suitable mitigation methods as no fatalities were calculated. This is mainly because the building is considered to be sealed by shutting off the HVAC and entrance doors thereby limiting the ingress of toxic gas. The toxic levels recorded in the corridor in both scenarios 5 were solely due the leakage areas attributed to the windows and doors.

The probit calculated for the second scenario was adjusted for n = 2.74 to produce the adjusted probit. However, the weighted probit was omitted and actual the concentration profile used for TL calculations were utilized to calculate the adjusted probit for comparative reasons. Figure 18 compares the adjusted probit with probit and TL. In contrast to the trends presented in Figure 17, adjusted probit starts to capture fatalities around 10 min complementing the TL predictions.

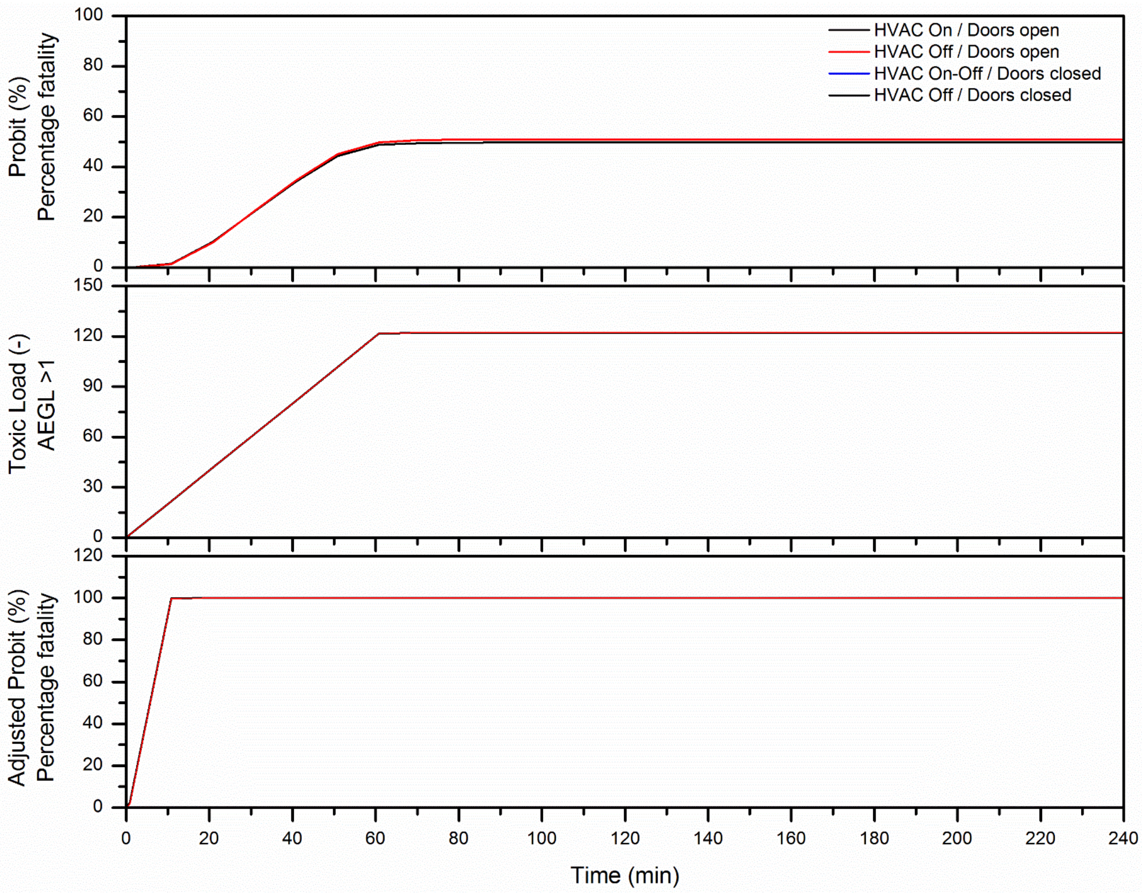


Figure 18: Comparison of adjusted probit with probit and TL dose response models for the second scenario

Considering all the mitigation methods for the second scenario, Scenario 3 and 5 is realized to be most plausible option as no fatalities were recorded in either dose response models. Scenario 1 and 4 represented the worst case scenarios displaying high toxic levels inside the corridor resulting from the exposure of the corridor area to the outdoor toxic environment through the open entrance doors and operational HVAC system. Both scenarios resulted in a high percentage of fatalities should everyone stay inside the building as described by the second scenario.

6. CONCLUSION AND RECOMMENDATIONS

The ingress of toxic gas into the building from outdoors is a complex phenomenon which is dependent on various factors like buoyancy, variable wind properties, leakage characteristics of the building, ventilation systems etc. This work aimed to study and quantify the dynamics involved with the ingress of contaminants in a non-process area. Non-process area in this work was defined to be any area which does not house a chemical process.

Initially a two level administration building was chosen as the non-process area for case study. The chosen building was assumed to be situated inside the perimeter of a functioning natural gas plant. This building located 1000 m away from the source of release was exposed to a H_2S toxic gas cloud for 1 hour. The release was assumed to be due to a full bore rupture of pipeline carrying natural gas. In order to meet the objective of developing a toxic gas ingress model into a non-process area a combination of three different models were utilized; a multi-zone model called CONTAM, a heavy gas dispersion model called SLAB and a CFD model called QUIC. The influence of meteorological properties, ventilation system and wind pressure calculation method on the toxic gas ingress was investigated. Finally, based on the indoor toxic levels achieved inside the building two evacuation scenarios were proposed and assessed.

Ingress of toxic gas was found to be sensitive to meteorological conditions and by the presence of mechanical ventilation. Plume dispersion was modeled for stability classes C, D and F. Stability class F was found to be the worst case scenario as it provides stable conditions for plume dispersion. Four different scenarios were considered to study the effect the ventilation network on the toxic levels attained inside the building. In all cases the corridor area was realized to be the most susceptible area in the building. However, its large area was found to have limitations on the well mixed assumption of the CONTAM model. It was found that presence of a functioning HVAC resulted in a rapid increment of toxic level equivalent to the outdoor plume in the corridor area. Disabling the ventilation system at the moment of release and closing the entrance doors assisted in capping the toxic level inside the corridor at safe levels. It was also found that HVAC was the most dominant variable while modeling the ingress of contaminants.

The influence of wind pressure and its calculation method on the ingress phenomena was examined by comparing the wind pressure calculated using ASHRAE correlation and QUIC-CFD modelling. Comparison of both calculation techniques showed that there is an inconsistency in the wind direction dependency even though the pressure coefficients calculated fall within the same range for both methods. A comparison of the airflow rates between the corridor area and the surrounding rooms indicated that wind pressure modelled using QUIC predicted higher airflow rates in rooms compared to the ASHRAE correlation predictions. This behavior 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 toxic levels in the corridor and a typical office room in the building was compared for both calculation techniques. In comparison to the ASHRAE method, QUIC displays a higher maximum concentration and a faster decay rate.

Two evacuation scenarios were proposed and were assessed based on the dose Probit and Toxic Load (TL) dose-response modelling procedures. The probit method followed the TNO parameters. However, it was found that both models did not complement each other because probit was not based on short term exposure limits like AEGL whereas TL method is based on the AEGL limits. Therefore, this work proposed an adjusted probit by adjusting the power exponent (n) of the existing probit method by a factor of 2.74. The adjusted probit was found to be consistent with the TL method results on comparison. The first scenario assumed people escaped outdoors during the release in horizontal and vertical directions. It was found to be not feasible to escape outside in either direction based on the predictions by the adjusted probit and TL method. The second evacuation scenario considered people to stay indoors during the entire period of the release. Since ventilation was found to be the most influential factor while modelling ingress, various mitigation strategies were implemented and compared. The mitigation method, which recommended sealing the building was found to be me the most suitable choice as neither models predicted any fatalities. This is due to the fact that sealed building limit the toxic levels prevent to reach fatal levels inside the corridor.

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 model can be used to get a preliminary understanding of the potential present consequences and the recommend mitigation methods that needs to be implemented within seconds. The sensitivity analysis on the governing variables of the ingress phenomenon can also provide a basis in order to achieve realistic results. Based on the assessment of mitigation methods considered in this case study, it is recommended to provide a shelter in place inside the building as escaping outdoor during the release was found to be not feasible.

The following recommendations are suggested for future works:

- The results of the modelling work showed that the multi-zone model approach was found to be inappropriate for large areas like the corridor area. Large zones in CONTAM domain can be further divided into smaller zones while modelling ingress in non-process areas.
- Multi-zone model does not take into consideration the impact of flow obstacles like pipe and tanks that can be present around the building. CFD modelling of the outdoor and indoor environment can address these issues and provide more accurate results.
- Conducting tracer gas experiments will allow validation of the proposed model. It will also help to develop a custom CONTAM library for Qatar which can be easily adapted by various interested parties.

BIBLIOGRAPHY

[1] Total E&P, “Sour Gas, A History of Expertise,” 2007. [Online]. Available: http://www.total.com/sites/default/files/atoms/file/total-sour-gas-history-expertise.

[2] L. Skrtic, “Hydrogen Sulfide, Oil and Gas, and People’s Health,” Msc diss., University of California, Berkeley, 2006.

[3] T. Chambers and J. A. Johnson, “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 Rep. 2009-021, Apr. 2009.

[4] L. Driver and E. Freedman, “Report to Congress on Hydrogen Sulfide Air Emissions Associated with the Extraction of Oil and Natural Gas,” US EPA., Research Triangle Park, NC, Final Rep. EPA-453/R-93-045, Oct. 1993.

[5] W. R. Chan, P. N. Price, A. J. Gadgil, W. W. Nazaroff, G. Loosmore, and G. Sugiyama, “Modeling Shelter-In-Place Including Sorption On Indoor Surfaces,” in *84th American Meteorological Society Annual Meeting*, 2004.

[6] K. Sirén, “The Protection Ability of the Building Shell Against Sudden Outdoor Air Contamination,” *Build. Environ.*, vol. 28, no. 3, pp. 255–269, Jul. 1993.

[7] M. Pontiggia, G. Landucci, V. Busini, M. Derudi, M. Alba, M. Scaioni, S. Bonvicini, V. Cozzani, and R. Rota, “CFD Model Simulation of LPG Dispersion in Urban Areas,” *Atmos. Environ.*, vol. 45, no. 24, pp. 3913–3923, Aug. 2011.

[8] B. Kandola, “Smoke Hazard Assessment on Offshore Oil and Gas Installations,” *Fire Saf. Sci.*, vol. 4, pp. 1233–1244, 1994.

[9] F. Danielsson, R. Fendler, M. Hailwood, and J. Shrives, “Analysis of H_2S - Incidents in Geothermal and other Industries,” OECD Rep., Sep. 4, 2009.

[10] Z. Jianwen, L. Da, and F. Wenxing, “Analysis of Chemical Disasters Caused by Release of Hydrogen Sulfide-Bearing Natural Gas,” *Procedia Eng.*, vol. 26, pp. 1878–1890, 2011.

[11] D. J. Hall and A. M. Spanton, “Ingress of External Contaminants into Buildings – A Review,” Envirobods Ltd., UK, Rep. ADMLC/2012/01, Dec. 2012.

[12] D. Hall and A. Spanton, “Internal and External Building Exposure to Air Pollutants and External Contaminants,” 2013. [Online]. Available: http://iaqm.co.uk/download/presentation/Hall_Spanton_DMUGDec2013Presentation%20(3).pdf

[13] J. Milner, S. Vardoulakis, Z. Chalabi, and P. Wilkinson, “Modelling Inhalation Exposure to Combustion-Related Air Pollutants in Residential Buildings: Application to Health Impact Assessment.,” *Environ. Int.*, vol. 37, no. 1, pp. 268–79, Jan. 2011.

[14] Y. L. Chen and J. Wen, “Comparison of Sensor Systems Designed using Multizone, Zonal, and CFD Data for Protection of Indoor Environments,” *Build. Environ.*, vol. 45, no. 4, pp. 1061–1071, Apr. 2010.

[15] D. Lorenzetti, “Assessing Multizone Airflow Simulation Software,” Lawrence Berkeley Natl Lab., Berkeley, CA, Doc. LBNL-49578, Jan. 2002.

[16] P. Kassomenos, A. Karayannis, I. Panagopoulos, S. Karakitsios, and M. Petrakis, “Modelling the Dispersion of a Toxic Substance at a Workplace,” *Environ. Model. Softw.*, vol. 23, no. 1, pp. 82–89, Jan. 2008.

[17] L. L. Wang, W. S. Dols, and Q. Chen, “Using CFD Capabilities of CONTAM 3.0 for Simulating Airflow and Contaminant Transport in and around Buildings,” *HVAC&R Res.*, vol. 16, pp. 749–763, 2010.

[18] G. N. Walton and W. S. Dols, “CONTAM User Guide and Program Documentation.” Gaithersburg, MD, 2013.

[19] M. Nelson and M. Brown, “The QUIC Start Guide (v 6 . 01).” Los Alamos Natl Lab., Doc. LAUR-13-27291, Sep. 2013. [Online] Available: http://www.lanl.gov/projects/quic/open_files/QUICv6.01_StartGuide.pdf

[20] D. Ermak, “User’s Manual for SLAB: An Atmopheric Dispersion Model For Denser Than Air releases.” Lawrence Livermore Natl Lab., Livermore, CA, Doc. UCRL-MA-105607, Jun, 1990. [Online]. Available: https://www3.epa.gov/scram001/models/nonepa/SLAB.PDF

[21] A. Barrett, “Mathematical Modeling and Decision Analysis for Terrorism Defense: Assessing Chlorine Truck Attack Consequence and Countermeasure Cost Effectiveness,” PhD diss., Carnegie Mellon University, Pittsburgh, Pennsylvania, 2009.

[22] A. K. Persily and E. M. Ivy, “Input Data for Multizone Airflow and IAQ Analysis.,” National Institute of Standards and Technology, Gaithersburg, MD, Rep. NSTIR 6585, Jan. 2001.

[23] M. V. Swami and S. Chandra, “Correlations for Pressure Distribution On Buildings and Calculation of Natural-Ventilation Airflow,” *ASHRAE Trans.*, vol. 94, pp. 243–266, 1988.

[24] R. A. Sheldon, “Fundamentals of Green Chemistry: Efficiency in Reaction Design,” *Chem. Soc. Rev.*, vol. 41, p. 1437, 2012.

[25] F. Haghighat and A. C. Megri, “A Comprehensive Validation of Two Airflow Models - COMIS and CONTAM,” *Indoor Air*, November 2015, pp. 278–288, 1996.

[26] G. N. Walton, “AIRNET - A Computer Program for Building Airflow Network Modelling,” National Institute of Standards and Technology, Gaithersburg, MD, Rep. NISTIR 89-4072, Apr. 1989.

[27] A. Gowardhan, E. R. Pardyjak, I. Senocak, and M. J. Brown, “A CFD-Based Wind Solver for an Urban Fast Response Transport and Dispersion Model,” *Environ. Fluid Mech.*, vol. 11, pp. 439–464, 2011.

[28] L. Prandtl, “Report on Investigation of Developed Turbulence,” *ZAMM*, vol. 5, pp. 136–139, 1925.

[29] C. D. Argyropoulos and N. C. Markatos, “Recent Advances on the Numerical Modelling of Turbulent Flows,” *Appl. Math. Model.*, vol. 39, pp. 693–732, 2014.

[30] B. Plog and P. Quinlan, *Fundamentals of Industrial Hygiene*. Itasca, Ill.: National Safety Council, 2012.

[31] D. Crowl and J. Louvar, *Chemical Process Safety Fundamentals with Applications*. Englewood Cliffs, NJ.: Prentice-Hall, 2011.

[32] B. Zhang and G. Chen, “Quantitative Risk Analysis of Toxic Gas Release Caused Poisoning—A CFD and Dose–Response Model Combined Approach,” *Process Saf. Environ. Prot.*, vol. 88, no. 4, pp. 253–262, Jul. 2010.

[33] The International Association of Oil and Gas Producers, “Vulnerability of Humans,” Risk Assessment Data Directory Rep. 434-41, Mar. 2010

[34] D. Crowl and J. Louvar, *Chemical Process Safety: Fundamentals with Applications*, Third Edit. Upper Saddle River, NJ: Paul Boger, 2001.

[35] J. P. Boris and G. Patnaik, “Acute Exposure Guideline Levels (AEGLs) for Time Varying Toxic Plumes,” Naval Research Laboratory, Washington, DC, Rep. NRL/MR/6003-14-9493, Sep 2014.