Potential impact of accidental releases of hazardous gases on the immediate habitability of a nuclear power plant

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DECLARATION

I hereby declare that the content of this dissertation represents my own work, except those particular cases that are referenced in the text of the dissertation. I also declare that this dissertation has not been submitted to any other educational institution for the awarding of an academic qualification.

This dissertation is dedicated to my loving parents, who always reminded me of the importance of tertiary education. Finally, praise goes out to God for all the blessings brought upon me.

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ABSTRACT

To protect the public and plant operators, the nuclear power industry demands a continuous evaluation of hazards and safety standards. This dissertation provides a history of toxic chemical accidents and the methodologies to evaluate nuclear power plant toxic chemical hazards. The evaluation of hazards may lead to the implementation of preventative measures, i.e., hardware changes, surveillance and procedural changes; the implementation of mitigative measures; the analysis of post-accident conditions to guide accident response; and guidance for the most effective resource allocation to ensure safety.

The evaluation of hazards includes a historical review of toxic chemicals, flammable gas releases, and a compilation of toxic chemicals and flammable gases generally found at or near nuclear power plants. Gases are classified according to their toxicity, weight and flammability to determine which gases are the most hazardous. Biologically, chlorine and ammonia were found to be the most hazardous, while methane gas is the most volatile in terms of flammability.

Methodologies to predict the dispersion of gases were also evaluated. Several computer programs used for predicting the dispersion of toxic gases into the atmosphere were evaluated in terms of their accuracy, applicability and usefulness of derived results.

Generally, credit is not taken for special nuclear power plant measures to mitigate or prevent a release.

The following requirements for nuclear power plant control rooms are not included in this analysis:

- Pressurisation of the control room;
- Automatic isolation in case of a chemical relapse;
- Automatic initiation of filtering with high-grade filters;
- Demanding design, purchasing, fabrication and testing requirements to ensure the operability of installed ventilation during the most adverse accident conditions;
- Internationally accepted limits are used to determine toxicity and physical characteristics;
- Conservative and internationally accepted standards are used to determine dispersion coefficients and receptor location; and
- Conservative and international standards are used to determine the release rate and release amount.

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Nomenclature

Symbol	Description
LD_{50}	The dose of a chemical, which kills 50% of a sample population
t	Time elapsed after a release of pollutant
x	Downwind distance of receptor
y	Horizontal distance from plume centreline to receptor
z	Elevation of receptor
Q	Emission rate from a point source
U	Mean wind speed affecting the plume
$^{\delta}xy$	Crosswind standard deviation of plume at distance y
$^{\delta}xz$	Vertical standard deviation of plume at distance z
$^{\delta}xx$	Downwind standard deviation of plume at a distance x
M	Emission as mass released from point source
C_{xyz}	Pollutant concentration at distances x, y, and z from the source
K	First-order rate constant
KW	Kilowatt
R	Radius affected by an explosion

LIST OF ABBREVIATIONS

The abbreviations used in the document are listed in the following table:

Abbreviation	Term
ALOHA®	Aerial Location of Hazardous Atmospheres
AEGL	Acute Exposure Guideline Level
AFTOX	Air Force Toxic Chemical Dispersion Model
CRH	Control Room Habitability
DEGADIS	Dense Gas Dispersion
EPA	Environmental Protection Agency
ERPG	Emergency Response Planning Guideline (US)
IDHL	Immediately Dangerous to Health and Life
LEL	Lower Explosive Limit
MHI	Major Hazards Installations
MIC	Methyl Isocyanate
NOAA	National Oceanic and Atmospheric Administration
NRC	National Nuclear Commission
NNR	National Nuclear Regulator
QRA	Quantitative Risk Assessment
PSA	Probabilistic Safety Assessment
PSR	Periodic Safety Review
RMP	Risk Management Program (US)
SSC	System Structure and Components
TNT	2,4,6 trinitrotoluene
US EPA	United States (of America) Environmental Protection Agency
US NRC	United States (of America) Nuclear Regulatory Commission
VCE	Vapour Cloud Explosion

GLOSSARY

Term	Definition
Accident	“An unplanned event or sequence of events that may result in an undesirable consequence.” (CCPS, 1996: xxi)
Acute	“Single, short-term exposure (less than 24 hours” (CCPS, 1996: xxi)
Blast	“A transient change in the gas density, pressure, and velocity of the air surrounding an explosion point. The initial change can be either discontinuous or gradual. A discontinuous change is referred to as a shock wave, and a gradual change is known as a pressure wave.” (CCPS, 1996: xxi)
Control room	“A rigid, enclosed room where the operators monitor and control the nuclear plant systems.” (CCPS, 1996: xxi)
Consequence	“The undesirable result of an incident, usually measured in health and safety effects, environmental impact, loss of property, and business interruption costs. For building siting, consequence refers to building damage and occupant vulnerability from the potential effects of an explosion, fire, or toxic material release. Consequence descriptions may be qualitative or quantitative. Consequence is independent of probability.” (CCPS, 1996: xxii)
Consequence-based approach	“The methodology used for building siting evaluation that is based on consideration of the impact of explosion, fire and toxic material release, which does not consider the frequency of events.” (CCPS, 1996: xxii)
Explosion	“A release of energy that causes a blast.” (CCPS, 1996: xxii)
Flammable	“A gas that can burn with a flame if mixed with a gaseous oxidiser such as air or chlorine and then ignited. The term flammable gas includes vapours from flammable or combustible liquids above their flashpoints.” (CCPS, 1996: xxii)
Flammable limits	“The minimum and maximum concentrations of combustible material in a homogeneous mixture with a gaseous oxidiser that will propagate a flame.” (CCPS, 1996: xxii)
Frequency	“The number of occurrences of an event per unit of time.” (CCPS, 1996: xxiii)
Hazard	“An inherent physical or chemical characteristic (e.g., flammability, toxicity, corrosivity, stored chemical energy, or mechanical energy) that has the potential for causing harm to people, property, or the environment.” (CCPS, 1996: xxiii)
Incident	“An unplanned event with the potential for undesirable consequences.” (CCPS, 1996: xxiii)
LFL (lower flammability limit)	The concentration of combustible material in air below which ignition will not occur. It is often referred to as the Lower Explosive Limit (LEL). Mixtures below this limit are said to be “too lean”. (CCPS, 1996: xxiii)
Occupant vulnerability	“The proportion of building occupants that could potentially suffer an injury or fatality if a postulated event were to occur. The level of injury is defined according to the technical basis of the occupant vulnerability model being used. (CCPS, 1996: xxiv)
On-site personnel	Employees, contractors, visitors, service providers, and others present at the facility.

Term	Definition
Overpressure	Any pressure above atmospheric caused by a blast. (CCPS, 1996: xxiv)
Permanent building	“Rigid structures intended for permanent use in fixed locations.” (CCPS, 1996: xxiv)
Periodic Safety Review	“A systematic reassessment of the safety of an existing facility (or activity) carried out at regular intervals to deal with the cumulative effects of ageing, modifications, operating experience, technical developments and siting aspects, and which is aimed at ensuring a high level of safety throughout the service life of the facility.” (IAEA SSG, 2013: 01)
Probability	“The expression of the likelihood of occurrence of an event with units of event/defined period.” (CCPS, 1996: xxiv)
Probit	“A random variable with a mean of 5 and a variance of 1, which is used in various effect models.” (CCPS, 1996: xxiv)
Scenario	“An unplanned event or incident sequence that results in a loss event and its associated impacts, including the success or failure of safeguards involved in the incident sequence.” (CCPS, 1996: xxv)
Toxic material	“An airborne agent that could result in acute adverse human health effects.” (CCPS, 1996: xxvi)
Vapour cloud explosion	“The explosion resulting from the ignition of a cloud of flammable vapour, gas, or mist in which flame speeds accelerate to sufficiently high velocities to produce significant overpressure.” (CCPS, 1996: xxvi)

CHAPTER 1 : INTRODUCTION

The following section describes the basis for evaluating the consequence of the release of toxic chemicals and flammable gas.

1.1 BACKGROUND

Several major nuclear disasters have been recorded in recent history. Radiological and toxic substances often leak into the atmosphere after nuclear and chemical disasters, seriously compromising air quality. Human health is significantly impacted, as in the Chernobyl nuclear disaster in 1986 when thousands of people were exposed to a high radiation dose. The radiological cloud was extensive across Europe, intoxicating many square kilometres of land. In another case, a massive earthquake followed by a powerful tsunami triggered the 2011 Fukushima Daiichi nuclear power plant disaster. The resulting radioactive contamination polluted the surrounding atmosphere and seawater. The Bhopal gas tragedy of 1984 offers an example of toxic chemical gas harming or killing thousands of humans (Shunxiang et al., 2015).

The Fukushima accident has shown the devastation that external hazards could cause to the operational safety of a nuclear power plant. Main classifications of further external hazards in nuclear power plants can range from occurrences related to weather, external floods, strong winds, extra-terrestrial events, aircraft, marine and accidents (including rail and truck) transportation, on-site storage of chemical substances, hazards of facilities in the proximity and further risks caused by humans (Kimura et al., 1987). Numerous nuclear power plants in various countries have experienced earthquakes with intensities that were beyond their seismic design basis. Earthquakes can induce other external hazards, which can include chemical substance releases (Federal Agency for Nuclear Control, 2012). The current study is concerned primarily with the hazards potentially caused by large releases of hazardous substances. Particular attention is given to the storage of chlorine and ammonia and the transportation of substances that can be flammable, such as natural gas in the area of the plant.

Numerous nuclear power plants utilise chlorine to treat water in the circulating water systems as well as in further systems that have an auxiliary function (U.S. Nuclear Regulatory Commission (NRC), 1977). Usually, chlorine is kept on the premises in pressurised cylinders or as liquefied gas in one-ton tanks. In new-build nuclear power plants, chlorine has been replaced by sodium hypochlorite, which fulfils the same function as chlorine in water treatment.

Nuclear plants are typically located in areas separated from densely populated regions. Still, they cannot be too far away from industrial areas as this would increase the cost of power transmission. To facilitate the delivery of natural gas (methane), an essential energy source to some industrial, as well as other facilities, the transportation pipelines may be installed in strategically selected areas. Therefore, as a result of industrial development, pipelines transporting natural gas may occasionally be built close to an existing nuclear power plant.

Based on the characteristic explosion and flammability features of the natural gas cloud, a nearby pipeline could present a significant risk to the mode nuclear power plants operate. If released, it could drift with the wind until either dispersed to concentrations below its flammability limit or encountered by an igniting source. If the gas cloud is ignited, this could cause a jet fire or vapour cloud explosion (VCE), which, in turn, could generate overpressure and thermal radiation to the surroundings. Such an explosion could cause failures in accident mitigation of systems, structures and components (SSCs), and it could also generate explosion fragments or missiles. Natural gas clouds could be considered a potential hazard, mainly because natural gas could displace oxygen and acts as an asphyxiant in a confined environment (Casal, 2008). Asphyxiant concentrations are typically assumed to be in the range of 50 000 to 100 000 ppm (CCPS, 1995).

Loss of containment may lead to a toxic cloud of vapour affecting how habitable a nearby nuclear plant's control room is. Overpressure, due to the explosion of the vapour cloud, and thermal radiation from fireballs and jet fires may also present such a challenge. This happened during the accident in Raunheim (Germany), where excess methane was spilt into the atmosphere. Operators in the control room witnessed a white cloud which gradually expanded across the ground and moved towards the control room. Once this cloud reached the said room, it ignited (CCPS, 1994).

Criterion 19 of Appendix A to 10 CFR 50 necessitates a control room from which safety action may be directed to ensure safety under accident circumstances (U.S. Nuclear Regulatory Commission (NRC), 1981). Currently approved designs for control rooms are assessed in terms of how they protect the operator from both toxic gases and radiation. This review follows the Standard Review Plan 6.4 (NUREG 75/087) and the Standard Review Plan Reference Regulatory Guide 1.78 regarding the habitability of a control room in case of chemicals being released. Moreover, this makes reference to Regulatory Guide 1.95 for protection requirements, specifically from chlorine being released.

The United States Nuclear Regulatory Commission issued an information notice (IE Circular No. 83-62) in 1983 for older plants to be reviewed after several incidences of failed toxic gas (chlorine and ammonia) detectors at control room ventilation system air intakes. Seemingly, several nuclear power plants were established and licensed before the above-mentioned guidelines were instated (U.S. Nuclear Regulatory Commission (NRC), 1983).

The key focus of this dissertation is on the release of a flammable gas, such as methane, resulting from a pipeline accident and an accidental toxic gas release from on-site chlorine and ammonia storage.

To calculate toxic vapour concentration, some conservative assumptions were made, consistent with NUREG 0570 (Wing, 1979) and RMP:

- All of the gas (chlorine or ammonia) in one container is released instantaneously.
- Gas is continuously released from a pipeline linking to an infinite source.
- The released gas moves directly to the control room's air intake.
- The amount of gas released, atmospheric stability, the distance from personnel and control room to the source and duration.

To illustrate why conservative modelling was selected, a problem requiring an estimate of the gas discharge rate from a hole in a storage tank was considered. However, the discharge rate depends on a number of parameters, including (i) the hole area, (ii) the pressure inside the tank, and (iii) the temperature of the gas, to name a few. The complete dynamic solution of this case is problematic, and it is far easier to consider the entire contents of the tank, which would maximise the consequence and insure a conservative result (CCPS, 1995).

Outlier external events, such as beyond-design-basis earthquakes, which might carry serious consequences are becoming increasingly significant, particularly following the Fukushima Daiichi accident (Wheatley S, et al, 2016). Therefore, beyond-design-basis earthquake could result in a rupture of onsite chemical storage tanks. Therefore, the urgency for comprehending the effects of such occurrences is growing, and this needs to be done in such a way that they are incorporated into the plant's safety assessment. Safety assessments are generally performed to ensure that unacceptable consequence will not result from beyond-design basis-accidents. If the risk from beyond-design-basis accidents is unacceptable, preventative measures will be a requirement in order to lower the potential risk.

The worst possible scenario is necessary for the consequence-based method, thus the rules described in IAEA Safety Series No. 98 (*Onsite Habitability in the Event of Accident at a Nuclear Facility*) were followed (IAEA, 1989). The ALOHA® (Areal Locations of Hazardous Atmospheres) model simulated the scales of impact (threat zones) after toxic chemical release. Existing preventative and mitigating measures, which may differ from site to site, were not considered.

1.2 EFFECTS AND CONSEQUENCES ANALYSIS OF FLAMMABLE OR TOXIC LEAKAGES

Consequence analysis was employed to quantify the effects of flammable or toxic chemical leakage by describing their extent, nature and impact on individuals, buildings, equipment and the environment. Firstly, mathematical models are used to estimate the effects by predicting how much thermal radiation is produced by a fire and the explosion's peak overpressures (Schleder, 2015).

This study focussed on chemical cloud dispersion using a simulation tool to compute the downwind concentrations. Modelling cloud formation for flammables predicts where the fire or explosion could occur and how much flammable material there will be. Similar modelling estimates the amount of toxicity by predicting the concentration of a toxic substance in time and space (Schleder, 2015).

Consequence models, as with all models, have uncertainties. By applying conservative values to some of the unknowns, a conservative estimate of the consequence is achieved, thus the design is overdesigned to avoid the hazard (CCPS, 1995).

1.3 EXPLOSION, FIRE, AND TOXIC RELEASE PHENOMENA

In this project, an accident is understood as "an unplanned event or sequence of events that result in an undesirable consequence" (Crowl & Louvar, 2011). In the same context, an undesirable outcome can be an explosion, a fire, or a toxic gas release.

Prior to an explosion, fire or toxic release, specific conditions occur. Firstly, various hazards that can result in explosions (viz. fire or toxic substance release is a prerequisite). If the event is an explosion, then flammable, combustible or process circumstances with the ability to generate explosive occurrences must be given. Secondly, a triggering event must be given to set off a series of accidents.

According to Crowl and Louvar (2011), there are three industrial plant accidents i.e., fires, explosions and toxic release. As Table 1-1 (Crowl & Louvar, 2011) demonstrates, fires are the single most frequent, then come explosions and toxic releases; however, a toxic release carries the biggest potential for fatal outcomes (Crowl & Louvar, 2011).

Table 1-1: Three types of accidents

Type of accident	Probability of occurrence	Potential for fatalities	Potential for economic loss
Fire	High	Low	Intermediate
Explosion	Intermediate	Intermediate	High
Toxic release	Low	High	Low

While a toxic release normally leads to limited destruction in terms of plant equipment, the penalty in injuries among staff members, personnel loss and legal compensation, as well as clean-up liabilities may turn out to be severe.

1.4 PROBLEM STATEMENT

The quantification of risk from a beyond-design-basis event at a nuclear plant does not explicitly consider the accidental release of toxic gases that do exist at such plants. Historic periodic safety review (PSR) regulations did not exist in South Africa and, therefore, did not explicitly require an evaluation of toxic chemicals. However, the recently published PSR requires specific external hazards, such as toxic gases, to be included in the safety assessment (National Nuclear Regulator, 2019). Typically, the plant safety analysis report addresses chemical hazards when the plant is commissioned. Still, no mechanism exists that can monitor the addition of chemicals within or outside the plant boundaries.

This oversight could lead to an inaccurate input made available to the decision-makers (for example, emergency preparedness planning). The potential failure to identify weakness in major installations of toxic chemicals, which contribute to the overall level of risk of the installation, is more detrimental. If such components are identified and described more explicitly, this will create opportunity for focusing on improvement which, in turn, could significantly reduce the risk level for accidental hazardous substance release. From a brief review of the Defence Nuclear Safety Board reports (Peter & Winokur, 2011) of several nuclear plants, it is evident that hazardous chemical storage tanks and pipes are typically designed according to general industry codes and standards. This means that they do not necessarily meet the same stringent standards applied to SSCs located on the nuclear island. Unlike nuclear safety vessels and piping, tanks and piping containing toxic or corrosive chemicals are not periodically inspected. Containers for storing chemicals may rupture, which leads to extensive amounts of chemicals being released in case there is an earthquake that exceeds the design criteria of the vessel. This evaluation addresses the consequence of failure for tanks and piping which are not designed or inspected according to rigorous nuclear safety requirements.

In the chemical process industry, emergency conditions are responded to predominantly by isolating the control room and recirculating air via the ventilation system. Most control rooms in the nuclear power industry are pressurised with filtered air in an emergency. Thus, contaminated air could negatively affect the control room’s habitability (IAEA, 1989).

1.5 RESEARCH OBJECTIVES

The objectives of this research comprise the following:

a) To determine the on-site habitability in case a hazardous substance is released, and to perform a consequence-based deterministic assessment which evaluates potential damage to buildings or injuries to personnel (the term on-site habitability includes habitability both within and outside of the control room);

b) To develop accident scenarios (worst-case);

c) To determine the release extent of the explosion/fire for combustible gases;

d) To predict the consequences of the hazardous substance on people outside buildings and structures;

e) To simulate gas dispersion using a computational tool known as ALOHA®;

f) To verify a sample of the dispersion assessment results from ALOHA® with the SLAB® model; and

g) To determine whether the limits of release are exceeded. If so, a more in-depth analysis may be required to evaluate the need for additional preventive measures.

1.6 HYPOTHESIS

Chemical storage vessels or pipelines around a nuclear plant might rupture and let out an extensive amount of flammable or toxic gases if the event is beyond the design criteria of the chemical storage container or pipeline. The impact of such a large flammable or toxic gas release could render the control room and other vital areas inhabitable, which could potentially cause fatalities among employees who might be outside as the accident occurs.

1.7 SCOPE AND LIMITATION

This project does not consider the simultaneous toxic gas release with radiological consequences and, hence, does not argue that such coinciding occurrences do not generate an unacceptable risk levels. It should also be pointed out that the probabilistic nature of the catastrophic chemical spill during transportation and in storage is not considered in this study. The model applications of ALOHA® and SLAB® are used for this study to predict the hazard concentrations. Even though each model has its own assumptions and is limited in some way, such typical limitations discussed across models in the context of this study include the following aspects:

- A flat terrain was taken as the basis. This means that the particularities of a more complicated terrain were not discussed.
- One simulation allows for a single release source.
- No chemical reactions in the plume was regarded.
- The SLAB® model was only be used for the verification of one scenario (chlorine scenario).
- Precautionary measures were not considered, e.g., evacuation, donning facemasks, and mandates to remain inside a building or structure.
- A probabilistic safety assessment (PSA), quantitative risk assessment (QRA) and sensitivity analysis were not performed on the three hypothetical scenarios.
- A particular nuclear site was not selected due to security and confidentiality restrictions.

These limitations resulted in a single set of meteorological conditions to be used to represent the complete dispersion phenomenon.

In Dai’s (2004) comparison of dispersion models, each model’s inherent assumptions and limitations gave different results for the same accidental release scenario. Thus, selecting the correct model is essential, and Dia (2004) recommends that modelling results must be carefully interpreted.

Though the outcomes of the research are helpful in supporting chemical assessment initiatives, they are not intended to signify particular accident scenarios in reactors. Moreover, they should not form part of the Fukushima resolutions or any activities implemented by alternative parties (e.g., updating of nuclear response plans for emergencies).

1.8 RESEARCH METHODOLOGY

The methodology of this study is separated into two phases. The first phase is the review of information that will identify the types of extremely hazardous chemicals utilised at or adjacent to nuclear and industrial facilities.

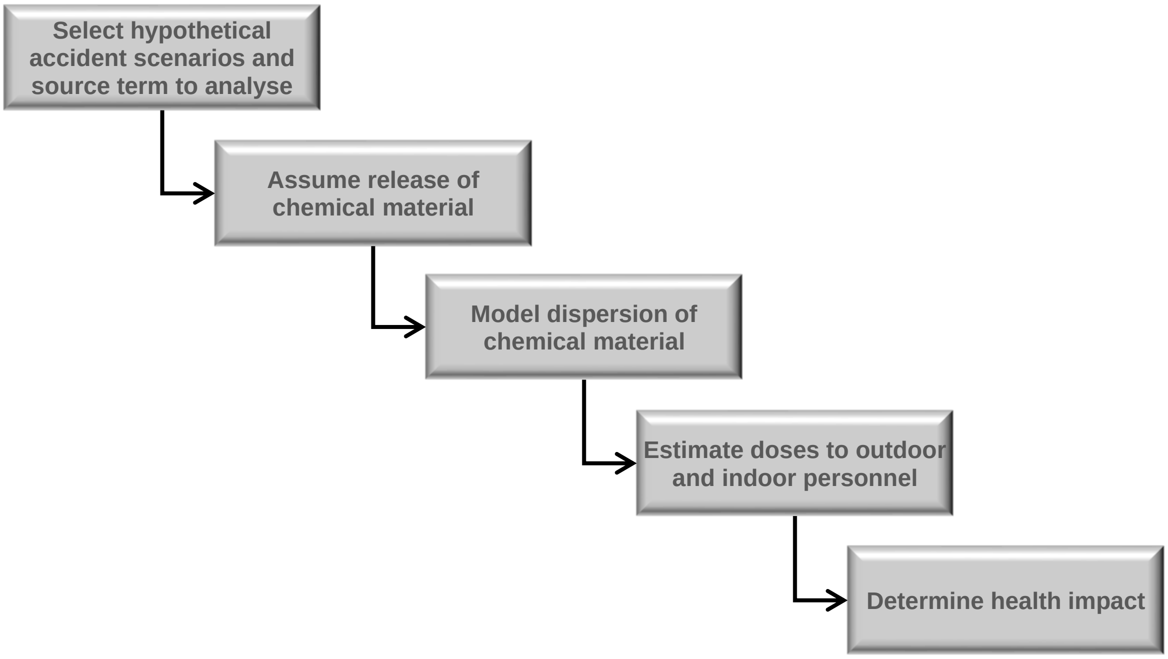


Figure 1-1: Flow chart of study of consequences of a hypothetical severe nuclear accident

The second phase begins with the modelling process of the chemicals that were identified during the first phase for this study to determine the vulnerability of vital areas within a nuclear plant. The modelling was accomplished by using the ALOHA® software, which is available from the US EPA, and it is conceptualised to highlight vulnerable areas. ALOHA® utilises information entered in the program that pertains to the chemical type, state (liquid, solid, gas), storage vessel, release method (hole in the container or valve or pipe) and weather circumstances. The aforesaid information is then used to produce a scenario that could be illustrated graphically. Once the separate scenarios are modelled in ALOHA®, the results were verified using an alternative software (SLAB®) to determine the alignment between the two models (i.e., models that share an identical theoretical background are expected to lead to similar results).

1.9 DISSERTATION CHAPTER CONTENT

The outline of this dissertation is as follows:

- Chapter 1 offers a background to the topic.
- Chapter 2 discusses the literature review related to the topic.
- Chapter 3 deals with the use of dispersion modelling in the analysis of the consequences resulting from an accidental release.
- Chapter 4 discusses the methodology of the models used.
- Chapter 5 displays and discusses these results.
- Chapter 6 outlines the conclusions drawn and provides recommendations.

- The list of references consulted is displayed as the last part of the dissertation.
- The appendices display figures and tables referred to, where applicable, throughout the document.

CHAPTER 2 : LITERATURE REVIEW

Several literature research areas were adopted to support the research objectives. The study considered some of the most documented industrial accidents. These accidents enhanced awareness of chemical distribution and storage dangers, leading to legislation regulating major hazardous installations. Ultimately, accidental emissions of harmful chemicals into the atmosphere should be mitigated and prevented. Each regulation requires similar outputs, such as consequence modelling. The hazards linked to the use of chemicals in nuclear plants are similar to those associated with the same chemicals used in industrial plants. However, in nuclear plants, the concern is that the chemical hazards do not create secondary nuclear hazards. The literature review will not attempt to discuss each subject in its entirety but will highlight the significance of each subject in relation to chemical releases.

2.1 METHODOLOGY OF THE LITERATURE SURVEY

To conduct a consequence modelling process of emissions of extremely harmful substances, an outline of related information needs to be considered. Such a review should cover materials that relate directly to the hazards of chemicals.

To look for the related information, numerous online searches were conducted using the search engine Google and North-West University’s online library search engine. Several technical books related to chemical dispersions were also consulted. Before executing the searches, relevant search terms were identified to aid the search process.

The search terms drawn on in this literature review are:

- External Hazards for Nuclear Plants
- Release of Hazardous Chemicals
- Chemical Explosions
- Control Room Habitability
- Chemical Accidents
- Regulatory Requirements related to Hazardous Chemicals
- Chemical Properties of Toxic Inhalation Hazards
- Air Dispersion Consequences Modelling
- Computer Models used for Air Dispersion

After perusal, every source was included within the annotated bibliography at the end of this project.

2.2 SURVEY OF INDUSTRIAL CHEMICAL ACCIDENTS

Operational experience that can be learned from can be gathered by reviewing events recorded for the most significant chemical accidents.

2.2.1 The Ammonia Accident, Blair, Nebraska, USA, 1970

While filling a large tank with refrigerated liquid ammonia, overfilling occurred, and some 160 tonnes of ammonia entered the atmosphere. Due to the remote location of this accident and the sparse local population, no human life was lost.

The high-pressure jet of ammonia from the leak absorbed oxygen. It caused the ammonia-air mixture, with a density greater than that of ambient air, to settle over an area of approximately 400 km^2 due to the absence of wind. This relative stability of the ambient atmosphere caused water vapour to condense at the top of this cloud, which formed a distinctly visible barrier.

During the period 1994 to 1999, accidents occurred in which hazardous chemicals/gases were released into the atmosphere, mostly involving ammonia and, to a lesser extent, chlorine (Madhusoodan & Dhiman, 2010).

2.2.2 Triomf, Potchefstroom, South Africa, 1973

An ammonia tank at this fertiliser plant, previously known as Triomf, developed a brittle fracture. As a result, it is estimated that approximately 38 tonnes of ammonia was released into the atmosphere, which eventually caused the death of 18 people.

At the time of the accident, the tank pressure and temperature were normal, and no other trigger mechanism could be found during subsequent tests. The investigation extended into the manufacture of the tank, and it was found that the dished ends, which were made of carbon steel, were not subjected to a stress-relief process after welding, hence the brittle fracture.

The gas released from this fracture formed a cloud some 150 metres in diameter and 20 metres high. Initially, the air was stable, but soon afterwards, a wind developed and blew the ammonia cloud towards a township (Mannan, 2004; Madhusoodan & Dhiman, 2010).

2.2.3 Hexachlorophene Manufacturing Plant Accident, Seveso, Italy, 1976

Few chemical incidents can match the severity of the Seveso disaster of 1976. At this hexachlorophene manufacturing plant, the loss of temperature control in a plant process reactor caused the formation of a by-product known as tetrachlorodibenzodioxin. This extremely toxic substance was released through a reactor relief mechanism. A cloud of this toxic chemical dispersed over the town of Seveso, and some 600 people had to be evacuated. The contamination of some areas was so severe that these areas remain abandoned to date.

A condition known as chloracne was diagnosed in approximately 300 people. About 8% of the population suffered from enlarged livers, and nerve damage was diagnosed in a small number of cases. The local environment, including animals, suffered the most damage.

2.2.4 Bhopal Pesticide Plant Accident, India, 1984

The worst industrial accident involving toxic gases took place in Bhopal, India, on 3 December 1984. The plant produced pesticides using methyl isocyanate (MIC), a highly toxic and dangerous compound, as an intermediate. The maximum exposure concentration of MIC vapour over eight hours is 0.02 ppm. Exposure to more than 21 ppm causes severe nose and throat irritation, and significant exposure could lead to death due to respiratory distress (Crowl & Louvar, 2011).

When MIC comes into contact with water, it reacts exothermically. The reaction rate is slow, but without cooling, the reaction temperature increases, ultimately causing MIC to boil and a toxic vapour to be released. The Bhopal disaster occurred when approximately 25 tons of toxic MIC vapour escaped through the scrubber system after a large MIC storage tank was contaminated with water. No plant workers were injured or killed, but the toxic vapour drifted over a nearby town and descended to the ground as it is a heavy gas. More than 2000 civilians died, and the health of an estimated 20 000 people was affected.

The cause of the MIC contamination is unknown, but an operational scrubber would have prevented its release into the atmosphere. Also, inventory levels of hazardous compounds should have been lowered. The accident could have been prevented by regular plant safety assessments and a toxic dispersion analysis (Crowl & Louvar, 2011).

2.2.5 The Siberian Accident, 1989

The Nizhnevartovsk gas pipeline accident occurred on 3 June 1989 in Western Siberia. The accident was caused by a significant leak in the gas line, which was approximately 1 400 kilometres from the pipeline control room and approximately 500 metres from a dual railway line. People living in settlements in the area reported the smell of gas, yet no action followed. The gas had formed two large pockets alongside the railway line. Shortly after the gas was first reported, two trains approached the areas where the gas had settled in opposite directions on the dual line. Both drivers noticed the fog and became aware of a strong smell. The approaching trains caused the mist and gas vapour to mix, forming a flammable cloud. It is believed that a spark from either train ignited the gas mixture, causing several explosions within moments. The fireball quickly spread down the railway line in opposite directions, flattening trees within a four-kilometre radius and shattering windows up to 13 kilometres away from the explosion. Four hundred and sixty-two people were killed, and seven hundred and ninety-six were hospitalised with 70-80% burn wounds (Khan & Abbasi, 1999).

2.2.6 Incidents Involving Chlorine

Chlorine has long been used in water purification systems to kill living organisms. Initially, the nuclear power industry adopted this standard method of treating condenser circulating water to kill organisms. As a result, liquid chlorine was always on hand to be used as needed. As the nuclear industry matured, using elemental chlorine was recognised as tedious and time-consuming due to the hazards involved in its handling. Nowadays, the trend is to use sodium hypochlorite, thereby avoiding the hazards of elemental chlorine. However, the following descriptions of typical incidents involving elemental chlorine are considered generally applicable.

The interesting point is that, in the USA, more deaths have resulted from accidents involving smaller vessels, cylinders and ton containers. One may hypothesise that this is due to the smaller number of safety devices, the increased number of vessels, and the tendency to use such vessels indoors or in enclosures.

A catastrophic spill of chlorine arises from accidents involving large vessels. Small vessels, such as 90-kilogram cylinders, contain too little chlorine to cover a large, confined area with a lethal dose. As a result of the flow-limiting devices in the lines of the larger containers, catastrophic spills will occur (under most circumstances) only by rupture or breaching of the vessel. Breakage of an attached transfer line or one of the angle valves may result in a substantial chlorine release, but the release rate is restricted so that a relatively small area is affected.

Table 2-1 lists some of the more significant chlorine accidents, those involving loss of life or the release of large quantities of chlorine, as compiled by the Chlorine Institute (Simmons, et al., 1974).

Table 2-1: Significant chlorine accidents

Location	Date	Comments
Storage Tanks		
St. Auban, France	12-13-1926	Tank burst, 25 tons, 19 deaths
Near Baton Rouge, Louisiana	05-10-1929	Tank burst, chlorine explosion, 25 tons lost, one death
Zarnesti, Romania	12-14-1939	Tank burst, 25 tons lost, 60 deaths
Rauma, Finland	11-05-1947	Tank burst from overfilling, 30 tons lost, 19 deaths
Walsum, Germany	04-04-1952	Tank failed (an old converted boiler), 15 tons, seven deaths
One-Ton Containers		
Ashokan, New York	07-12-1928	Explosion
Ashokan, New York	07-13-1928	Explosion
Cleveland, Ohio	05-08-1969	Two deaths

2.3 APPLICABLE REGULATORY REQUIREMENTS

2.3.1 Criterion 19 (GDC19)

Appendix A, *General Design Criteria (GDC) for Nuclear Power Plants*, was published by the Atomic Energy Commission in 1971 to provide design criteria (Lobo, 2016). GDC 19 stipulates a control room to safely operate the nuclear power plant under normal conditions and

> "*Adequate radiation protection shall be provided to permit access and occupancy of the control room under accident conditions without personnel receiving radiation exposures in excess of 5 rem whole body, or its equivalent to any part of the body, for the duration of the accident.*" (Lobo, 2016)

A few years later, the NRC Regulatory Guides 1.78 and 1.95 outlined measures for the control room operator's protection from accidentally released hazardous chemicals or chlorine gas, respectively (Lobo, 2016).

In 2003, the United States National Regulatory released a guide (Regulator Guide 1.197) for measuring inleakage in the control room, as well as other areas at nuclear power reactors. Regular inleakage verification ensures that the control room is habitable under normal and accident conditions (Nuclear Regulatory Commission, 2003).

2.3.2 Regulatory Guide 1.78

Regulatory Guide 1.78 discusses protecting the control room from hazardous chemicals released after an accident, either within or outside the nuclear power plant. Assessing control room habitability is key. Guidelines for the screening criteria, such as the distance between the source and the intake, as well as the volume and air exchange rate, are provided. The guide primarily focuses on chemical sources with a toxic effect, but it considers the use of flammable and explosive chemicals on site too. The following are screening criteria for stationary sources (Nuclear Regulatory Commission):

> *"Any hazardous chemical stored on site within 0.3 miles [482 m] of the control room in a quantity greater than 100 pounds [45 kg] should be considered for control room habitability evaluation. Hazardous chemicals should not be stored within the proximity (generally within 330 feet [91 m] or less) of a control room or its fresh air inlets, including ventilation system intakes and locations of possible infiltration such as penetrations. Small quantities for laboratory use, 20 pounds [9 kg] or less are exempt. The maximum allowable inventory in a single container stored at specified distances beyond 330 feet [91 m] from the control room or its fresh air inlet varies according to the distance and the control room type"* (U.S Nuclear Regulatory Commission, 2003).

2.3.3 Regulatory Guide 1.95

Regulatory Guide 1.95 (U.S. Nuclear Regulatory Commission (NRC), 1977) outlined directions for the adequate protection of control room operators from an onsite release of chlorine. Numerous nuclear power plants utilise chlorine for treating water in the circulating water system and further systems with an auxiliary function. The guide stipulates the control room operators need to be kept safe from the harmful effects of a chlorine release accident.

2.3.4 Three Mile Island and Control Room Habitability Requirements

The accident that occurred at Three Mile Island brought about alterations to the policy of the regulatory body among others, a revised Standard Review Plan in July of 1981, NUREG 0800 (U.S Nuclear Regulatory Commission (NRC), 1981). The Standard Review Plan regards an accidental loss-of-coolant-accident as the limiting design basis accident for control room habitability. Nonetheless, other design basis accidents needed to be assessed to decide if they should be more limiting. Licensees assured that the habitability under which systems will run under every outlined circumstance (design basis accidents) to allow the control room operators to remain in the control room to take appropriate actions required by GDC 19 (U.S. Nuclear Regulatory Commission, 2001).

2.3.5 Regulatory Guide 1.91

The 1987 NRC-issued Regulatory Guide (*Evaluations of Explosions Postulated to occur on Transportation Routes near Nuclear Power Plants)* stipulates that overpressures from explosions should not exceed 7 kPa. The relationship $R > 18\ W^{1/3}$, based on estimates of 2, 4, 6 trinitrotoluene (TNT), determines a safe distance, in which R designates the distance (in metres) from an exploding charge of TNT, and W is the mass (in kilograms) of TNT (U.S Nuclear Regulatory Commission (NRC), 2013). Instead of using approximate methods (TNT equivalencies), the current study used outcomes from ALOHA® to model the shock waves and combustion processes inside a gas pipeline using physics principals.

2.3.6 USA Risk Management Plan

Public concern arose from the Bhopal and Bayer CropScience, West Virginia MIC release incidents. This saw the implementation of Section 112(r) of the 1990 Clean Air Act Amendments. Following this, as mandated by Section 112(r), the EPA published rules and guidance for “Risk Management Programs for Chemical Accidental Release Prevention” (Chang & Samsa, 2007).

As a result, the Environmental Protection Agency (EPA) in the USA implemented regulations for risk management programmes (RMP) (U.S. Environmental Protection Agency (EPA), 2009). One of these is a requirement to evaluate the off-site consequences for leaks of harmful substances, and to estimate the total leakage under the worst-case scenario, by isolating weather as well as emission conditions that maximise damage, and varying release scenarios which have a high change of happening. According to the RMP guidelines, the worst-case scenario is a total leakage coming out of the biggest storage container, maximising damaged area.

In line with a risk management planning programme, companies have to produce worst-case and alternative (and more likely) scenarios of a release. Over time, many companies have reassured that such worst-case scenarios were very unlikely. However, the Fukushima accident demonstrated that beyond-design-basis earthquakes do happen. It is also possible that terrorists who intend to cause mass casualties could override safety measures that prevent releases. Catastrophic releases of chemicals through aerial attacks on storage containers or any other unanticipated and inconceivable methods could ensue.

Input parameters to analyse toxic substance worst-case scenarios, as per the RMP, include wind speed and atmospheric stability. Vapour cloud explosion was defined as the worst-case scenario for flammable substances (Kleindorfer et al., 2003).

There is greater flexibility in the way the RMP defines alternative releases compared to worst-case scenarios. One absolute condition for an alternative release scenario is the probability that it will happen more often than a worst-case scenario (Belke, 2001). An offsite endpoint is another condition. Consequence analysis of alternative release scenarios was beyond the scope of the current study.

Table 2-2: Frequency distribution of top 10 RMP chemicals (Belke, 2001)

Chemical	Number of processes	Percentage of total
Ammonia (anhydrous)	8 343	32.5
Chlorine	4 682	18.3
Flammable mixtures	2 830	11.0
Propane	1 707	6.7
Sulphur dioxide	768	3.0
Ammonia (aqueous)	519	2.0
Butane	482	1.9
Formaldehyde	358	1.4
Isobutane	344	1.3
Hydrogen fluoride	315	1.2

2.3.7 South African Major Hazards Installation

South Africa promulgated the Major Hazards Installation (MHI) regulations under the Occupational Health and Safety Act No. 85 of 1993 to deal with installations that might pose a threat to humans and animals (Deartment of Labour (South Africa), 1993). The regulations are applicable to employers, self-employed individuals and users with their own premises, both permanent and temporarily, who have a significantly dangerous installation or an amount of a chemical, which could be a risk that might affect the safety and health of both employees and the community. Nuclear installations are excluded as the National Nuclear Regulator (NNR) has oversight responsibility for such installations.

In South Africa, the status of a facility being an MHI is determined by a number of factors, one of which is the quantity of hazardous chemical stored at the facility.

Fortunately, South Africa has not yet experienced an incident similar in extent to the Fukushima or Bhopal catastrophic disasters. However, if the industrial and nuclear facilities close to population centres produce, retain and use big quantities of dangerous substances, the chances for a tragedy exist, whether caused by an accident or by intentionally released chemicals.

2.4 CHEMICALS STORED AT NUCLEAR POWER PLANTS

Nuclear plants do stock hazardous chemicals similar to those found in industrial plants. However, in nuclear plants, the primary concern is that the chemicals do not create a secondary nuclear hazard. According to the US NRC Regulatory Guide 1.78 (U.S Atomic Energy Commission (AEC), 1974), any hazardous chemical stored on site within 483 m of the control room in amounts above 45 kg ought to be assessed in a control room habitability evaluation. The guide further suggests that smaller amounts for laboratory usage, 9 kg or below, are exempt. The guide also recommends that, if there are numerous chemical containers, merely the failure of the biggest vessel needs to be evaluated. Table 2-3 cites the commonly encountered chemicals found on a nuclear site.

Table 2-3: Toxicity limits (IDHL limits) for some hazardous chemicals (U.S. Atomic Energy Commission (AEC), 1974)

Chemical name	ppm	mg/m^3
Acetaldehyde	2000	3600
Acetone	2500	6000
Acrylonitrile	85	149
Ammonia	300	210
Aniline	100	380
Benzene	500	1600
Butadiene	2000	4400
Butene		asphyxiant
Carbon dioxide	40000	7360
Carbon monoxide	1200	1320
Chlorine	10	30
Ethyl chloride	3800	9880
Ethyl ether	1900	5700
Ethylene dichloride	50	200
Ethylene oxide	800	720
Fluorine	25	50
Formaldehyde	20	24
Halon 1211	20000	
Halon 1301	50000	
Helium		asphyxiant
Hydrogen cyanide	50	55
Hydrogen sulphide	100	150
Methyl alcohol	6000	7800
Nitrogen		asphyxiant
Sodium oxide		2
Sulphur dioxide	100	520
Sulphuric acid		15
Vinyl chloride	1000	2600
Xylene	900	3915

Chemicals such as hydrogen, methane and propane are not listed, but are also common in or near nuclear plants; therefore, they should be added to the list.

The intent of this dissertation is not to conduct a consequences study of all the chemicals listed in Table 2-3 but only a selected few as described in the introduction section. Chemical incidents are categorised into four groups: toxic gas release, fires, explosions and miscellaneous (CCPS, 1996).

2.5 POTENTIAL HAZARDS ASSOCIATED WITH A CHEMICAL RELEASE

During operation, the accidental release of gases from pipelines or storage vessels may occur. After an accidental release, several potential safety hazards may be the result.

2.5.1 Toxic and Asphyxiant Releases

A chemical that is released and does not ignite is followed either by being dispersed or scattered in the atmosphere if it is lighter than air. If it is heavier than air, it will disperse and drop to the ground. In the second situation, the gas is highly concentrated at rather low elevations. Thus, it can have a detrimental effect on the habitability of a nearby control room as well as on neighbouring residents. Not all chemicals are toxic; however, it could pose a potential for asphyxiation due to displacement of the available oxygen.

Asphyxiants are substances that deprive the tissues in the body of the necessary oxygen, thereby causing oxygen starvation (Casal, 2008). Oftentimes, there is no warning and the loss of mental faculties sets in within a few seconds; unconsciousness could occur shortly thereafter. In addition to asphyxiation, some gases have a toxic effect on the human system, either through inhalation, through high vapour concentrations, or by contact of liquefied gas with the skin and eyes.

The release of a hazardous chemical in a nuclear power plant could easily overwhelm the operators on site and make the entrance and exit routes inaccessible for external emergency services. Usually, a nuclear incident or accident is controlled from the control room with the technical support from emergency resources preforming the tactical implementation of the strategy on the plant. However, the control room could become uninhabitable due to an external hazard, such as a chemical release. In addition to toxic and asphyxiant risks, fires and explosions related to the storage of chemicals must also be considered. This study does not address the risk of asphyxiation of inert gases, e.g., nitrogen or argon in a nuclear facility.

2.5.2 Jet Fires

Jet fires, often used as flares in process plants to discard flammable gases safely, are the result of flammable gas combustion or vapour released at high velocity through a restricted outlet. These turbulent diffusion flames incorporate large amounts of air. Because of high heat and flame impingement, accidental jet fires could significantly damage equipment (Casal, 2008).

2.5.3 Vapour Cloud Explosions

VCEs occur when flammable material is released into the atmosphere. The concentration of the combustible component ranges from the higher explosive limit to the lower explosive limit (LEL). At any concentration between these limits, the material within the vapour cloud will form a flash flare or a fireball if it ignites. Overpressures from the sudden detonation of the explosive material could lead to injury or damaged property (Casal, 2008).

According to Casal (2008), dependent on the pressure waves and the distance from the explosion, explosions could result in:

- Explosion damage;
- Thermal damage;
- Missile damage; and
- Personal injury.

CHAPTER 3 : DISPERSION MODELLING OF TOXIC OR FLAMMABLE CLOUDS

Loss of containment from pipes and transportation or storage tanks is the leading cause of industrial accidents relating to gases and other liquids. Mostly, the chemicals involved are harmful to humans and the environment (Crowl & Louvar, 2011). It is important to forecast development predictions in the event of a gas or vapour cloud forming.

Safety measures and emergency contingency plans can be developed by knowing the difference in the substance's concentration at different points in time. Reasonable estimations of how an accident can impact people can also be achieved (Crowl & Louvar, 2011).

This chapter provides aspects for consideration for gas or vapour cloud development modelling for accidental releases.

3.1 DISPERSION ANALYSIS

According to Casal (2008), the pattern of dispersion of airborne material depends on three fundamental characteristics (Casal, 2008: 195):

- the meteorological factors – such as wind, atmospheric stability, humidity;
- the terrain – urban, suburban, rural in addition to elevation; and
- the physical properties and characteristics of the released material. The characteristics of the chemicals released ultimately determine the shape, magnitude, and severity of the plume.

For a given scenario, dispersion analyses are sets of mathematical equations based on which a pollutant cloud's development, its function and the timespan of the release can be estimated. Based on the duration of the release, emission can be categorised as either instantaneous or continuous.

The "Gaussian" and Heavy "Gas Dispersion" models are used to estimate chemicals' dispersion patterns (Casal, 2008). Whist the Gaussian model is frequently used, incorporating meteorological and terrain variables, current models for the dispersion of heavier-than-air gases are rather complex and these situations are currently under-researched (Casal, 2008). The "Gaussian" model assumes that atmospheric turbulence is random and dispersion in the horizontal and vertical planes follows a downwind direction.

According to CCPS (1995), in general, the main steps for consequence modelling include (refer to Figure 3-1):

- Conceptualising the release scenario;
- Characterising the array of potential environmental conditions;
- Conducting chemical accident release modelling;
- Conducting an impact analysis; and
- Implementing mitigation measures as required.

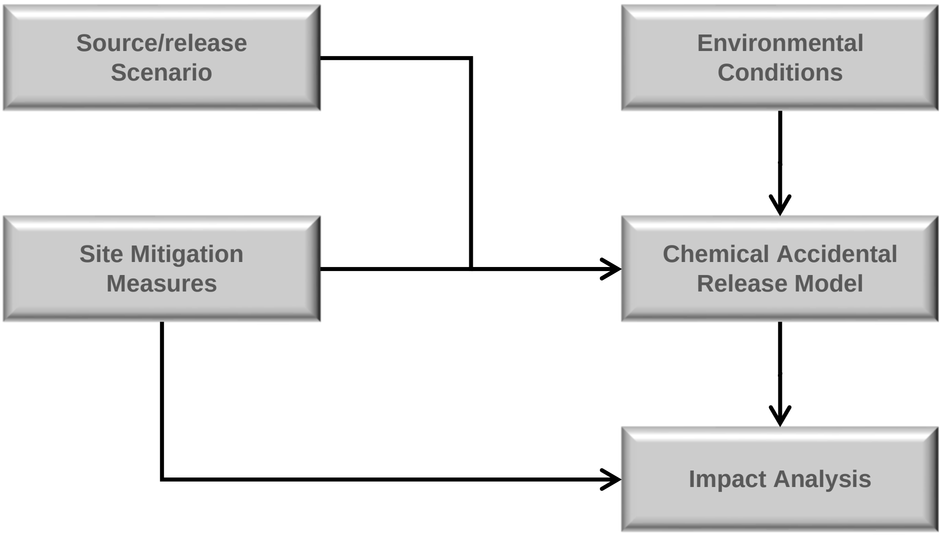


Figure 3-1: Major components of chemical accident analysis (Casal, 2008)

3.2 SOURCE TERM

Casal (2008) asserts that accidents usually happen due to loss of containment of a hazardous substance that can be either gas or liquid and this can occur continuously over a period of time in case of a leak or instantaneously in the case of a rupture. Continuous release of a liquid hazardous substance can create a jet of liquid, which can form a pool of liquid that may also evaporate to form a gas cloud. In such cases, it is necessary to estimate the mass flowrate and duration of release to ascertain the total amount of hazardous substance released.

Furthermore, it is important to note that in both continuous and instantaneous hazardous substance release, the release substance interacts with its immediate environment and this interaction influences the form of release, which can lead to the formation of a pool, create a dispersion or may be ignited immediately (Van den Bosch et al., 1997). The characteristics of the release are determined by the ambient circumstances (namely state, pressure, temperature and other) (Schleder, 2015).

The cloud dispersal can be evaluated once the substance's discharge, pool spreading and vapourisation (in the event of a pool) and cloud formation can be evaluated according to the source term (Casal, 2008).

3.2.1 Leak Rates

The flow of liquid through a hole in a tank (Casal, 2008):

$$Q = C_D A \sqrt{2\left(\frac{P_{cont-P_0}}{\rho}\right)} \quad \text{..} \; (3.1)$$

where:

Q is the liquid mass flow (kgs^{-1})

C_D is the discharge coefficient (normally 0.62)

P_{cont}	is the pressure above the liquid (Pa)
P_0	is the outside pressure (Pa)
A	is the cross-sectional area of the pipe (m^2)
ρ	is the density (kg.m^{-3})

It is important to note that for this study, it was assumed that when an accident occurs the leak or rupture will be continuous and this is a conservative assumption bearing in mind of the possibility of major and rupture failures that would quickly depressurise and burn with less intensity (Nilsson, 2009).

3.2.2 Flow of Gas Through a Hole

$$\dot{m} = 0.8AP\sqrt{\frac{M\gamma}{zRT}\left(\sqrt{\frac{2}{\delta+1}}^{\frac{\gamma+1}{\gamma-1}}\right)} \quad \text{...} \; (3.2)$$

where:

m	is the mass flow rate (kg/s)
γ	is the ratio of heat capacities
P	is the pressure in (Pa)
A	is the cross-sectional area of the orifice (m^2)
δ	is the scaled distance (m)

The mass of flammable gas was set out to be the total amount to gas that would leak out. This was under the assumption that the flammable gas cloud would travel in the direction of the wind during which it would interact with a source of ignition.

3.2.3 Evaporation from Aqueous Solutions

Following a historical survey featuring 139 cases (Casal, 2008), the most frequent substances involved in such phenomena included methanol (76 of the cases), formaldehyde (8%), ammonia (7%), hydrogen cyanide (4%) and nitric acid (3%). The following expression has been suggested for this situation:

$$E_{pool} = \frac{k \times P_{ev} \times M}{R \times 10^3 \times T} \quad \text{...} \; (3.3)$$

where:

E_{pool}	is the evaporation rate (kgm^{-2}s^{-1})
k	is a mass transfer coefficient (ms^{-1})
P_{ev}	is the vapour pressure of evaporating substance (Pa)
M	is the molecular weight (kgkmol^{-1})

R is the ideal gas constant (Jkmol^{-1}K^{-1})

T is the temperature of the solution (K)

The mass transfer coefficient may be calculated using the subsequent expression (Casal, 2008):

$$k = 0.0048 \times u_w^{7/9} \times D_{pool}^{-0.11} \times Sc^{-2/3} \quad \text{..................................} \quad (3.4)$$

where:

u_w is the wind speed (ms^{-1})

D_{pool} is the pool diameter (m)

Sc is the Schmidt number

3.2.4 Continuous and Instantaneous Releases

A number of aspects are employed in assessing if an instant release is instantaneous or continuous. For instance:

- When the time needed for the cloud to reach a certain locale is more extensive than the release's duration, , it is considered an instantaneous emission. An instance might be the explosion of a tank containing a pressurised gas. After the release, the pollutant is carried away from the source by the wind (Casal, 2008).
- When the duration of the release is longer than the time the cloud needs to reach a particular location, it is considered a continuous emission. An instance might be the plume from a stack. After the release, the pollutant is moved further away from the source by the wind in a characteristic plume-like manner (Figure 3-2).

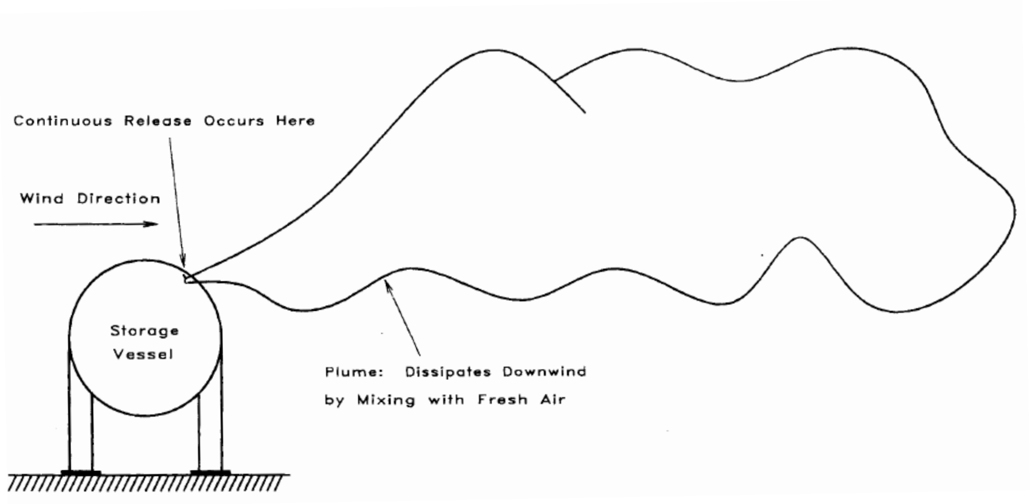


Figure 3-2: Plume formed by a continuous release of material

3.3 DISPERSION MODELS FOR NEUTRAL GASES (GAUSSIAN MODELS)

Gaussian dispersion equations are employed for describing the dispersion of gas into the atmosphere whose densities resembles that of air. This type of modelling is the most frequently used one, and it can include meteorological and terrain circumstances into its analysis. The main presumption of this model suggests that atmospheric turbulence occurs randomly and that its distribution is normal (Casal, 2008) in the vertical and horizontal planes following a downwind direction. A central limitation of this model is that it is normally only valid for a distance of 0.1 to 10 km from the point of its release (Crowl & Louvar, 2011).

Atmospheric dispersion modelling refers to the mathematical simulation of air pollutants' dispersion into the ambient atmosphere. This modelling is conducted using computer programs to resolve mathematical equations and algorithms that can simulate how pollutants disperse. These models are employed to gauge the downwind concentration of air pollutants emitted from sources. In general, a dispersing cloud of vapour would follow a downwind direction and it would expand laterally and vertically. A gas cloud with a higher density than air also spreads under gravity because it sinks and is able to move upwind to a limited extent.

The maximum concentration of toxic substances in the atmosphere happens at the point of release, which is not always at ground level. Concentrations downwind are lower as a result of turbulent mixing with fresh air and toxic substances dispersing.

Two types of neutral buoyancy pollutant dispersion models are normally utilised, namely the plume and puff models (CCPS, 1996). The plume model outlines the steady-state concentrations of substances released from a continuous source of which a characteristic example is gases being released from industrial stacks. The puff model outlines the temporary concentration of substances from a singular release of a fixed amount material. An instance might be the explosion of a container containing a pressurised gas.

3.4 CONTINUOUS EMISSION – PLUME MODEL

According to the "Consequences Analysis of Chemical Releases published by Center for Chemical Process Safety in 1995, the basic assumptions, which are associated with this model, are:

- Substance continues to escape for more than a minute;
- Steady-state conditions are assumed – concentrations only averaged over a given period;
- Pollutant takes on neutrally buoyant characteristics;
- Constant wind speed at all locations;
- Vertical crosswind distributions are known and Gaussian;
- Negligible mass diffusion in the x-direction; and
- No deposition and gravitational settling of the pollutant.

The following equation expresses all the relationships mentioned above. Concentration is given at a point downwind (x), crosswind (y), and at a height (z) above the ground, as a result of an emission at an effective height (H) above the ground:

$$C_{x,y,z} = \frac{G}{2\pi u \sigma_x \sigma_y \, \sigma_z} exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \times \left\{exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \text{..........(3.5)}$$

where:

G	is the total mass of the material being released (mass/time)
C	is the time average concentration (mass/volume)
$\sigma_x \sigma_y \, \sigma_z$	are the coefficients in the x, y, and z directions (length)
y	is the crosswind direction (length)
z	is the distance above the ground (length)
u	is the wind speed (length/time)
H	is the release height above the ground (length)

To apply the above equation, the values of the standard deviations or dispersions coefficients (also known as Pasquil-Gifford dispersion coefficients) σ_y and σ_z are required. These are functions of the distance downwind from the point of emission and the atmospheric conditions. Accordingly, these functions can be calculated (for 100 m < x <10 000 m) by utilising the expressions displayed in Table 3-1. A distinction is drawn between urban and rural regions. Urban areas have a higher level of turbulence given that there are buildings; therefore, the plume is dispersed faster compared to rural areas (Casal, 2008).

Table 3-1:
Equations for the calculation of the dispersion coefficients σ_y and σ_z
for a continuous emission (the distance x is in metres) (Casal, 2008)

Stability class	**σ y(m)**	**σ z(m)**
Rural conditions		
A	$0.22x(1 + 0.0001x)^{-0.5}$	$0.20x$
B	$0.16x(1 + 0.0001x)^{-0.5}$	$0.12x$
C	$0.11x(1 + 0.0001x)^{-0.5}$	$0.08x(1 + 0.0002x)^{-0.5}$
D	$0.08x(1 + 0.0001x)^{-0.5}$	$0.06x(1 + 0.0015x)^{-0.5}$
E	$0.06x(1 + 0.0001x)^{-0.5}$	$0.03x(1 + 0.0003x)^{-1}$
F	$0.04x(1 + 0.0001x)^{-0.5}$	$0.016x(1 + 0.0003x)^{-1}$
Urban conditions		
A-B	$0.32x(1 + 0.0004x)^{-0.5}$	$0.24x(1 + 0.0001x)^{+0.5}$
C	$0.22x(1 + 0.0004x)^{-0.5}$	$0.20x$
D	$0.16x(1 + 0.0004x)^{-0.5}$	$0.14x(1 + 0.0003x)^{-0.5}$
E-F	$0.11x(1 + 0.0004x)^{-0.5}$	$0.08x(1 + 0.0015x)^{-0.5}$

3.5 INSTANTANEOUS EMISSION – PUFF MODEL

The assumption in the puff model is that a chemical escapes into the atmosphere within sixty seconds or less. In an instantaneous release, the concentration at a certain locale is dependent on the position (x, y, and z), on the source's effective height (H) as well as in the time (t). The concentration may be estimated with this expression (CCPS, 1995):

$$C(x,y,z,H) = \frac{m}{(2\pi)^{1.5}} exp\left(-\frac{(x-ut)^2}{2\sigma_x^2}\right) \times [\mathrm{exp}\left(\frac{-(z-H)^2}{2\sigma_z^2}\right) + \theta exp\left(\frac{-(z+H)^2}{2\sigma_z^2}\right) \ldots\ldots\ldots\ldots (3.6)$$

where:

x,y,z	location of interest relative to source (m)
x-Ut	downwind distance from puff centre (m)
y-Ut	crosswind distance from puff centre (m)
z-Ut	vertical distance from puff centre (m)
m	emission as mass related from point source (g/s)
U	mean wind speed affecting the plume (m/s)
θ	reflection value, usually a value of 1 is assumed

The dispersion coefficients σ_x, σ_y, and σ_z in the case of an instantaneous release may be calculated from the expressions shown in Table 3-2.

Table 3-2:
Equations for the calculation of the dispersion coefficients σ_x, σ_y and σ_z for an instantaneous release (distance x is in metres) (Casal, 2008)

Stability class	σ_x or σ_y (m)	σ_z(m)
A	$0.18x^{0.92}$	$0.6x^{0.75}$
B	$0.14x^{0.92}$	$0.53x^{0.73}$
C	$0.10x^{0.92}$	$0.34x^{0.71}$
D	$0.06x^{0.92}$	$0.15x^{0.70}$
E	$0.04x^{0.92}$	$0.10x^{0.65}$
F	$0.02x^{0.89}$	$0.05x^{0.61}$

3.6 DISPERSION MODELS FOR HEAVIER-THAN-AIR GASES

The density of a material influences its dispersion in the atmosphere, especially initially. Numerous hazardous substances, which could be emitted if there is an accidental loss of containment, are heavier than air, as outlined by Casal (2008):

- If the material's molecular weight is greater than air, for example, chlorine gas.
- If the material is a cold gas or it cools as it evaporates, for example, liquefied natural gas.

- If an aerosol and vapour mixture with an average density greater than that of the vapour releases after a pressurised liquid is strongly depressurised and flashing occurs. The cooling of the evaporating droplets will keep the cloud cooler for longer.
- If the material undergoes chemical reactions that change its molecular weight during dispersion.

Because the gas are denser than air, it will sink immediately after release, moving upwind and downwind. The mechanism for mixing with air is entirely different from a neutrally buoyant release.

The SLAB® or Box model estimates the overall cloud characteristic, including radius, mean height and mean temperature (Ermak, 1990). The more rigorous computational fluid dynamics model solves the three-dimensional conservation equations; however, the problem must be substantially defined and the computation needs moderate computing capacity. According to the Health and Safety Executive Report (Britter & McQuaid, 1988), dense gas releases were modelled using dimensional analysis, incorporating the fundamental equations to simplify the problem to dimensionless groups. Most mathematical models that simulate flammable and toxic dense gas cloud dispersion use specialist computer codes because of the simulation’s complexity. There are, however, versatile models that are publicly available, such as SLAB® and ALOHA® (Ermak, 1990).

ALOHA® offers built-in algorithms that allowed for the appropriate model (Gaussian or heavy gas dispersion) to be selected (NSC (US), 1996). In the current study, the model selection was case specific and dependent on the atmospheric conditions, as well as chemical properties and features.

3.7 PARAMETERS AFFECTING ATMOSPHERIC DISPERSION MODELLING

1. Wind Speed – An increase in wind speed results in the plume becoming more extended and narrower. The chemical is carried downwind more rapidly and subsequently diluted faster by a larger quantity of air decreasing ground-level pollutant concentrations. An increase in wind speed may also limit plume rise and affect ground-level concentrations reversely. The direction of the wind can be understood as the direction from where the wind is coming.
2. Atmospheric Stability – The six classes of atmospheric stability are outlined in Table 3-3. The extent of a pollutant from a release is determined by the atmospheric stability together with wind speed. For example, a dense gas would have the greatest endpoint at night when atmospheric conditions are stable and the wind speed is low, as would a buoyant gas in high wind speeds (Burger, 2016). In a neutral atmosphere, air pockets and the surrounds cool at the same rate.

Table 3-3: Classification scheme for atmospheric stability (Burger, 2016: 2-11)

Stability class	Stability classification	Description
A	Very unstable	Calm wind, clear skies, hot daytime conditions
B	Moderately unstable	Clear skies and daytime conditions
C	Unstable	Moderate wind, slightly overcast daytime conditions
D	Neutral	Strong winds or cloudy days and nights
E	Stable	Moderate wind, slightly overcast night-time conditions
F	Very stable	Low winds, clear skies, cold night-time conditions

3. Ground Conditions – Otherwise referred to as surface roughness, buildings, trees and water bodies contribute to increasing (in the case of building and trees) or decreasing (lakes and open areas) mechanical mixing. Figure 3.4 illustrates how wind speed varies with height depending on congestion conditions. Turbulence from high congestion will reduce wind speed, and the highest velocity is reached at a higher elevation than a low area (open terrain) (Casal, 2008).

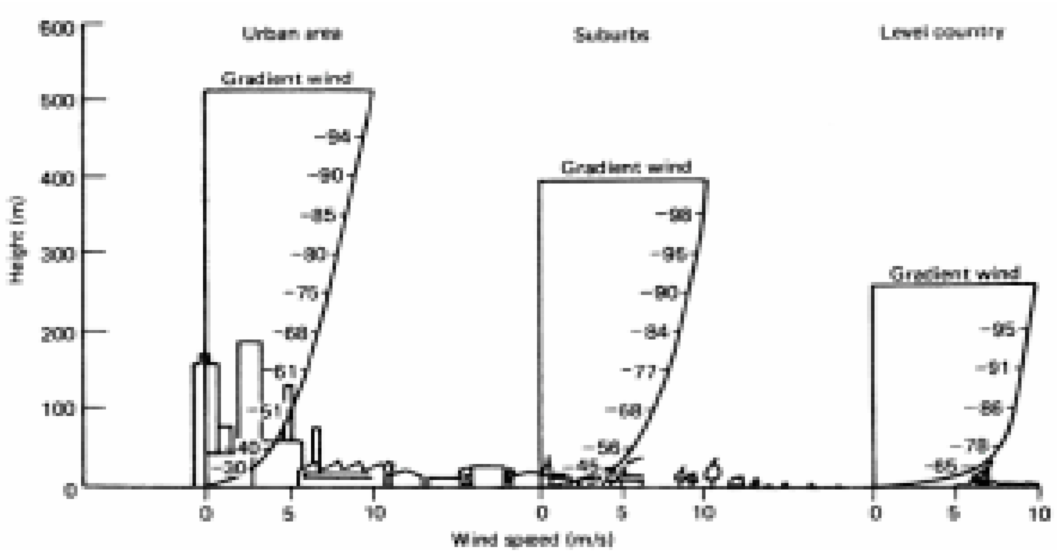


Figure 3-3: Variation of wind velocity with height (Casal, 2008)

4. Height of Release – The hight of the release has a notable effect on ground-level concentrations. While the height of the release increases, ground-level concentrations decrease as the plume rise needs to disperse across a greater distance.
5. Momentum (a result of the pollutant release velocity) and buoyancy (a result of the release temperature) of the initial material released – these parameters affect the effective height of the release.

3.8 DOSE AND PROBIT EQUATION

According to Casal (2008), doses of toxicants being inhaled are commonly defined in terms of concentration per unit time of exposure raised to the power *n* multiplied by duration exposure ($c^n t$). During most accident scenarios, in which toxic chemicals are emitted into the atmosphere, the concentration at a certain time ranges as a function of time. Moreover, the concentration would also change depending on a person's position, particularly if the person is outdoors (i.e., can leave the situation). As such, the dose of a chemical is articulated as follows (CCPS, 1995):

$$D = \int_0^t [c(t)]^n \, dt \ldots\ldots (3.7)$$

The probit equation for lethality in the case of inhalation of a toxic substance has the following general expression:

$$Y = a + b \times ln \int_0^t [c(t)]^n \ldots\ldots (3.8)$$

In practical purposes, the subsequent expression is commonly substituted for the above expression:

$$Y = a + b \times ln(C^n t) \ldots\ldots (3.9)$$

Where Y is the probit value*,* *a*, *b* and *n* are constants, *C* signifies the concentration of the substance (in molar ppm or mg/m^3), and *t* designates the exposure time (in minutes). The coefficient *n* relates to the mechanism of toxicity on the bodily organs that are being affected by a certain chemical.

Probit equation parameters for individual gases are usually derived from animal experiments; thus, accurate concentrations and deviation values are rarely available from historical toxic accidents. Probit data is available from several sources (Casal, 2008).

The following table gives *a*-, *b*- and *n*-values for ammonia and chlorine.

Table 3-4: Constants for lethal toxicity probit equation (Casal, 2008).

Substance	***a***	***b***	***n***
Ammonia	– 15.6	1	2
Chlorine	– 6.35	0.5	2.75

When the *n*-value is not available, a default value of 2.2 can be used. For spreadsheet computations, a more useful expression for performing conversion from probits to percentage is given by:

$$P = 50\left[1 + \frac{Y-5}{|Y-5|} erf \left\langle \frac{|Y-5|}{\sqrt{2}} \right\rangle \right] \ldots\ldots (3.10)$$

where "erf" designates the error function (Casal, 2008).

3.9 EFFECTS AND CONSEQUENCE ANALYSIS OF FLAMMABLE SUBSTANCES

The extent and nature of unwanted effects on humans, buildings, equipment and the environment due to flammable or toxic material releases, such as explosions, fires and toxicity, are defined by consequence analysis (Schleder, 2015).

Flash fires happen when vapour clouds, with a concentration between the lower and upper flammable limit, encounter an ignition source. Vapour can burn above the initial liquid pool from which the vapour evaporated and is ignited by a flame travelling back to the spill. Thermal radiation from flash fires and pool fires can injure, sometimes fatally, people within the burning gas cloud's range. Explosions could occur from the vapour cloud's ignition under turbulent conditions produced by congested or semi-confined areas, resulting in fatalities from exposure to the overpressure (Schleder, 2015).

The first step of consequence analysis is to model the effects of the accidental release. This involves predicting the thermal radiation emitted by the fire, the explosion's peak overpressures, the fragment's trajectory or the dispersion concentration. Predictions involve estimating how much material was involved in the accidental release and its rate of release using source term models based on fluid dynamics and heat transfer (Casal, 2008).

The current study's main focus was modelling cloud formation and dispersion from the accidental release of flammable substances, thereby enabling predictions for where a fire or an explosion may occur and how much material will be in a given area. Similar modelling for accidental toxic substance release provides valuable insight into toxicity levels in time and space.

3.9.1 Radiation Effects

The effects of radiation are assessed by utilising the point source radiator method. This method assumes that fire is a point source of heat, which is located at the core of the flame, and that it radiates a proportion of the combustion heat (Casal, 2008).

$$\frac{L}{d}=\frac{5.3}{C_T}\sqrt{\frac{{}^{T_f}/_{T_i}}{\alpha_T}\left[C_T+(1-C_T)\frac{M_a}{M_f}\right]}\ldots\ldots\ldots\ldots (3.11)$$

where:

L	is the length of the turbulent flame (m)
d	is the diameter of the jet (m)
C_T	is the fuel mole fraction in a stoichiometric fuel-air mixture (unitless)
T_f, T_i	are the adiabatic flame temperature and jet fluid temperature (K)
M_a	is the molecular weight of air (mass/mole)
M_f	is the molecular weight of the fuel (mass/mole)
α_T	is the mole of reactant per mole of the product (unitless)

The point source view factor is provided by:

$$F_T = {}^{1}/_{4\pi x^2} \quad (3.12)$$

where:

F_T is the point source view factor (m^2)

x is the distance from the point source (m)

Radiant flux at the receiver is determined by:

$$Er = \tau\varphi m \Delta F_T \quad (3.13)$$

where:

E_r is the radiant flux at the receiver (kJ/m^2)

m is the mass flow rate of the fuel (kg/s)

τ is the atmospheric transmissivity (unitless)

φ is the fraction of energy converted to radiation (unitless)

3.9.2 Estimation of Overpressure: TNT Equivalency Method

A frequently used approach for assessing damage generated by a particular explosion is the estimation of the TNT equivalency, namely, the mass of TNT that would lead to identical degrees of damage. In explosions of vapour clouds, one can calculate the mass equivalent to TNT using the following expression (CCPS, 1995):

$$W_{TNT} = \propto \frac{M\Delta H_c}{\Delta H_{TNT}} \quad (3.14)$$

where:

M is the mass of fuel in the cloud (kg)

ΔH_c is the lower heat of combustion of the fuel (kJ kg^{-1})

$\propto$ is the explosion yield factor and

ΔH_{TNT} is the blast energy of TNT (4680 kJ kg^{-1})

Once the value of the equivalent mass TNT, W_{TNT} is established, the scaled distance needs to be calculated (Crowl & Louvar, 2011):

$$d_n = \frac{d}{M^{0.33}} \quad (3.15)$$

where:

d_n is the scaled distance (m kg$^{-1/3}$)

d is the real distance between the centre of the explosion and the point where the overpressure needs to be estimated (m) and

M is the charge mass (kg)

The techniques described above allow for determining radiation or overpressure levels resulting from fires and explosions at any distant point away from the source.

3.10 PROBIT ANALYSIS

Probit analysis predicts any adverse health effects, and their extent, or fatalities after an accidental release. A biological response to toxic gases is normally distributed, and this distribution is transformed into a linear form, a probit equation, which takes the following form (Casal, 2008):

$$Y = a + b \times ln(C^n t) \text{...} (3.16)$$

Where Y is the probit value, a, b and n are constants. C is the molar concentration of the chemical (ppm) and t is the time of exposure (in minutes).

3.10.1 Vulnerability to Thermal Radiation

The most effect method of analysing the effects of thermal radiation or the dose of a toxic substance on individuals or on property is employing probit equations (Casal, 2008). There are a number of probit equations for gauging the effects thermal flux has on people, which are shown below.

First-degree burns:

$$Y = -38{,}83 + 3.0186 ln\left(tI^{4/3}\right) \text{......................................} (3.17)$$

Second-degree burns:

$$Y = -43{,}14 + 3.0186 ln\left(tI^{4/3}\right) \text{......................................} (3.18)$$

Lethality:

$$Y = -36{,}38 + 2.56 ln\left(tI^{4/3}\right) \text{..} (3.19)$$

where t is the (effective) exposure time in seconds, and *I* is the radiation intensity in Wm^{-2}.

The expressions above do not consider protection that clothing may offer. Unless ignited, clothes do offer some protection. In the case of ignition, clothing may lead to severe burns, which carries a high probability of death. The threshold value for clothes igniting (t = 20 s) is approximately 35 kW/m^2 (Uijt de Haag & Ale, 1999).

In the event of thermal radiation exposure, a person can suffer skin burns. The degree of the burns depends on the raidation intensity, measured in kWm^{-2}, and the dose. Exposure to jet fire thermal radiation could be fatal, and this applies to all living organisms (Burger, 2016).

Figure 3.5 extracted from Burger (2016) illustrates first- and second-degree burn damage to human skin from less-severe exposure to jet fire flames.

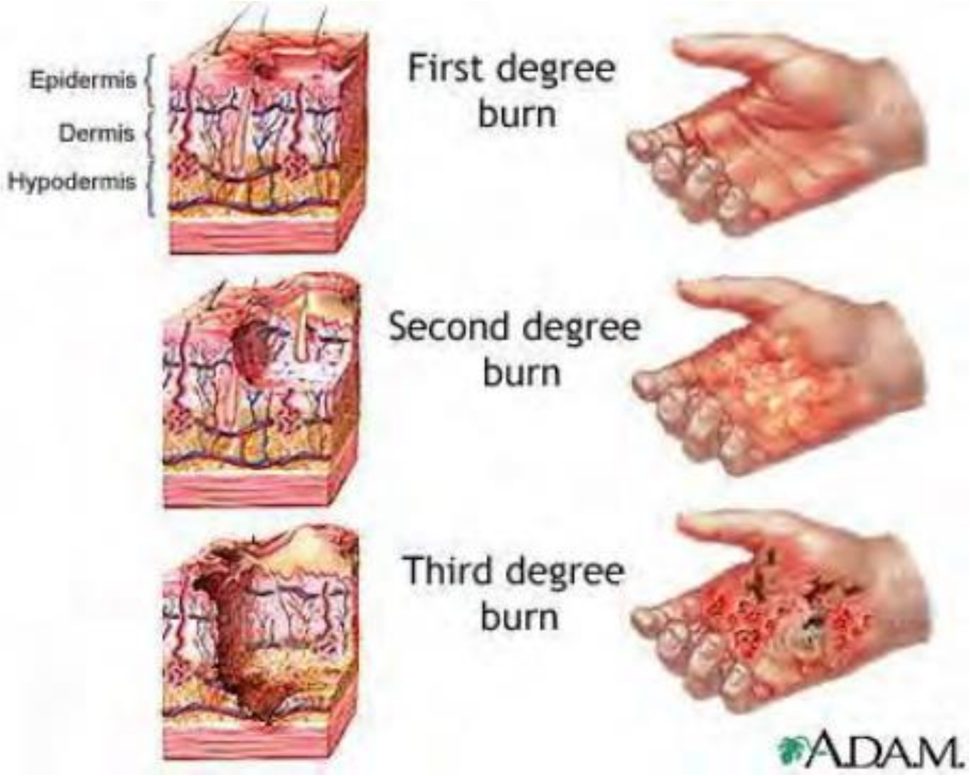


Figure 3-4: Levels of burns (Health Partners, n.d.)

Table 3-5 gives the level of damage for different thermal fluxes on people.

Table 3-5: Approximate levels of damage for different thermal fluxes (Casal, 2008)

Radiant heat level (kW/m^2)	**Physical effect (effect depends on exposure duration)**
1.2	Received from the sun at noon in summer.
2.1	Minimum to cause pain after 1 minute.
4.7	Will cause pain in 15-20 seconds and injury after a 30-second exposure.
12.6	Significant probability of fatality for extended exposure. High chance of injury.
23.0	Likely fatality for extended exposure and probability of fatality for instantaneous (short) exposure.
35.0	Significant probability of fatality for instantaneous exposure.

3.10.2 Consequences of an Explosion for Buildings and Structures

The damage generated by an overpressure wave on a building is influenced by the peak overpressure, turbulence and robustness of the installation. Data gathered from real cases (CCPS, 1996) are used for gauging the effects overpressure may have on buildings and structures. These are commonly articulated as a function of peak overpressure. Of particular interest in this project is the ‘distance’ effect, which involves limited damage to structures and broken breakage of windows, rather than the formation of craters. Table 3-6 gives such detailed information.

Table 3-6: Damage to buildings and structures (blast) (Casal, 2008; EPA (US), 1996; Burger, 2016)

Peak overpressure (kPa)	Damage	Peak overpressure (bar)
0.15	Annoying noise.	0.0015
0.2	No structural damage; the occasional breaking of large window panes already under strain.	0.02
0.3	Loud noise similar to a sonic boom, occasional glass failure.	0.03
0.7	Small windows breaking.	0.007
1 – 1.5	The typical threshold for glass breakage.	0.01
2	Probability of 0.95 of no severe damage beyond this value; some damage to house ceilings; 50% of window glass broken.	0.02
3	Limited minor structural damage.	0.03
3.5 – 7	Windows usually shattered, occasionally damage to window frames.	0.035 – 0.07
5	Minor damage to house structures.	0.05
7	The collapse of the roof of a tank.	0.07
8	Partial demolition of houses made uninhabitable.	0.08
7 – 15	Corrugated asbestos shattered. Corrugated steel or aluminium panels fastenings fail followed by buckling; wood panel fastenings fail; panels blown in.	0.07 – 0.15
10	The steel frame of clad buildings slightly distorted.	0.1
15	The partial collapse of walls and roofs of houses.	0.15
15 – 20	Unreinforced concrete or cinderblock walls shattered.	0.15 – 0.2
18	The lower limit of structural damage. 50% destruction of brickwork of houses.	0.18
20	Heavy machines in industrial buildings suffer little damage; steel frame building distorted and pulled away from foundations.	0.2
20 – 28	Frameless; self-framing steel panel building demolished; rupture of oil storage tanks.	0.2 – 0.28
20 – 40	Large trees falling down.	0.2 – 0.4
30	The cladding of light industrial buildings ruptured. Panelling is torn off.	0.3
35	Breakage of wooden telephone poles; most buildings destroyed; except for concrete reinforced shear wall buildings; “platting” of cars and trucks pressed inwards.	0.35
35 – 40	The displacement of a pipe bridge, failure of the piping.	0.35 – 0.4
35 – 50	Near-complete destruction of houses.	0.35 – 0.5
40 – 55	The collapse of a pipe bridge.	0.4 – 0.55
50	Loaded tank cars/train wagons overturned; brick walls, 20 – 30 cm thick collapse.	0.5
50 – 55	Unreinforced brick panels, 25 – 35 cm thick, fail by shearing or flexure.	0.5 – 0.55
60	Loaded train boxcars completely demolished.	0.6
70	Probable destruction of buildings; heavy machine tools moved and badly damaged.	0.7

3.11 Simulation Tools for Cloud Dispersion Analysis

The development of computer programs by private and public companies that can simulate vapour cloud scenarios allows for a technological and modernised approach to rapid risk analysis. The following sections review popular simulation systems, available in the public domain, which are based on the described mathematical models (Jones et al., 1989).

3.11.1 ALOHA® (Areal Locations of Hazardous Atmospheres), United States Environmental Protection Agency

ALOHA® , developed by the National Oceanic and Atmospheric Administration (NOAA) and the EPA's Chemical Emergency Preparedness and Prevention Office as a source-term and time-dependent model, estimates the release rates of chemicals from time-dependent sources, such as leaking gas pipes, leaking tanks and evaporating puddles, by simulating the dispersion of dense and less dense gases, and gases from the source. With a library of approximately 1 000 common hazardous chemicals, ALOHA® can simulate key hazards, such as toxicity, flammability, thermal radiation (heat) and overpressure (explosion blast force), from uncontrolled and excess chemical releases that could result in toxic gas dispersion, fires and explosions (NSC (US), 1996).

The graphical user interface generates various graphical formats, including threat zone plots of the area downwind of the accidental release, using weather inputs from portable monitoring stations, where concentrations are expected to be above a user-set threshold and source-strength plots of the release rates. Concentrations at any point beyond the release point can be viewed. Furthermore, ALOHA® predicts indoor concentrations using filtration rates based on building type, wind speed and air temperature (NSC (US), 1996).

ALOHA® is explicitly designed for users responding to chemical accidents, as well as for emergency response, planning, training and academic purposes. Therefore, ALOHA® should be equally suited to emergency response and planning processes at nuclear power plants. The heavy dispersion calculations employed in ALOHA® are rooted in the ones used for the DEGADIS model (Havens & Spicer, 1989), which will be discussed below. However, ALOHA® is limited to estimating concentrations downwind at distances beyond 10 km from the point of release. Furthermore, ALOHA® can be used for site characterisation of industrial settings. Dimensions of tanks, pipes and other fixtures can be described and saved as text or ALOHA®-runnable files. Different accident scenarios can then be simulated to derive worst-case possibilities.

The ALOHA® software program also features guidelines for acute exposure (AEGLs) for a wide range of chemical substances, which serve as "exposure guidelines designed to help responders deal with emergencies involving chemical spills or other catastrophic events where members of the general public are exposed to a hazardous airborne chemical" (NSC (US), 1996). The guidelines were conceptualised by the National Academy of Sciences, and they are drawn on extensively in a wide range of chemical-modelling programs.

3.11.2 DEGADIS (Dense Gas Dispersion)

The PC-based DEGADIS (acronym for DEnse GAs DISpersion) software program was developed by Dr Jerry Havens and Dr Tom Spicer at the University of Arkansas for the United States Coast Guard and the United States Environmental Protection Agency (US Environmental Protection Agency (EPA), 2019). The purpose of this program was to determine the end-point distances in the dispersion of toxic substances. It can further determine the lower flammable limits for toxic and flammable substances (Havens & Spicer, 1989). The program may be utilised to gauge short-term ambient concentrations, as well as the exposed area of the threshold values for the release of toxic substances. Its input requirements cover a diverse range of variables, such as release duration, instantaneous or continuous release, buoyancy and elevation of releases, However, it does not provide for high pressure/velocity releases, e.g., from pressure relief valves. Moreover, the properties of most chemical substances need to be provided by the user. Output abilities do not include source calculations or the characteristics of a release.

The program does not have graphical representations; the plume centreline information is given in a table. The output includes elevation, mole fraction, concentration, density, temperature and the dispersion coefficient values at downwind distances. For finite-duration releases, off-centreline distances for a pair of defined concentrations are given at each downwind distance. These are at specified receptor heights and concentrations versus time histories (Heaven & Spicer, 1989).

3.11.3 SLAB® (An Atmospheric Dispersion Model for Denser-Than-Air Releases), Lakes Environmental Software

SLAB®, developed by Dr Donal Ermak of the Lawrence Livermore National Laboratory, models spatial and temporal dispersion for denser-than-air toxic chemical releases. It estimates short-term ambient concentrations and area of exposure to above-threshold concentrations. The software does not incorporate wind shifts or the effects of terrain steering, thus assumes a uniform wind field. It models continuous, finite-duration and instantaneous releases from various release types: ground-level evaporating pool, elevated horizontal jet, stack or high vertical jet and instantaneous volume. As with DEGADIS, SLAB® outputs are in tabular format (Ermak, 1990).

SLAB® is not source-term and it cannot process real-time meteorological data, so meteorological parameters are user inputs. It does not have a chemical database, relying on external input. Furthermore, source type and source, spill and field properties are data inputs. The model simultaneously simulates several meteorological conditions in one run. Mixing heights and the depths of the turbulent boundary layers are used. These are significant for elevated releases. Each modelling run outputs instantaneous, spatially averaged cloud parameters, time-averaged cloud parameters and time-averaged concentration values at the plume centreline and at five off-centreline distances at four user-specified heights and the height of the plume (Ermak, 1990).

SLAB® modelling software has a user-friendly interface and is fast, allowing several thousand runs. The key input parameters are further discussed in Section 4.4.2.

3.11.4 Air Force Toxic Chemical Dispersion Model

AFTOX (Air Force Toxic Chemical Dispersion Model) is also PC-based, Gaussian puff/plume model with the ability to estimate downwind concentrations from an accidental release for neutral buoyant releases (Environmental Protection Agency (EPA), 2019). The program was conceptualised based on the USA Air Force's toned for updating its toxic gas capability for potential accidental omissions. The AFTOX model has been evaluated and refined against many test cases and field studies. The model further presumes a flat atmospheric flow field without any obstacles, such as constructs or trees.

The program features an option for continued heated plumes from stacks. It has a library featuring 129 substances but is fit to use for different substances too. This model is applicable to a wide range of accidental emission scenarios and process analyses. It is also applicable to plan for emergency responses involving highly toxic industrial chemicals. For every instance of a release, AFTOX presumes that the plume distribution is Gaussian, both in the directions of downwind and crosswind. It employs Pasquill-Gifford dispersion coefficients with certain alterations to allow for average timing that is specified by the user. Its outputs include concentration contour plots as well as toxic corridors. They further feature concentrations at indicated locations, as well as maximum concentrations at specific elevation levels and particular times.

3.11.5 US Nuclear Regulatory Commission's Control Room Habitability Code

HABIT (US NRC's Control Room Habitability Code), incorporating several programs, aims to improve the habitability of control rooms by evaluating instantaneous dangerous accidental chemical releases within two minutes. According to Regulatory Guide 1.78 (U.S. Atomic Energy Commission (AEC), 1974), a two-minute effect corresponds with a maximum concentration chemical accident. HABIT, therefore, differentiates between maximum concentration-duration chemical accidents and continuous releases, and does not cover the entire assessment prescribed by the Regulatory Guide (U.S. Atomic Energy Commission (AEC), 1974).

The ARCON86 code, developed by the Pacific Northwest National Laboratory contracted to the UN NRC, was an advancement on other dispersion models being more robust. ARCON96 derives from relative atmospheric concentrations in buildings published in Revision 1 to NUREG/CR-6331 (Ramsdell & Simonen, 1997). It is only available via special request to the US NRC.

3.12 HEALTH CRITERIA

Level of Concern defines the concentration above which a gas may be hazardous to an average person. Level of Concern was used in the current study to estimate the footprint (geographic area) potentially affected by an accidental chemical release. The chlorine and ammonia Levels of Concern were based on AEGLs (acute exposure guideline levels), which were developed under the National Research Council's Committee on Toxicology. They guide national and local authorities and private companies in the event of accidental spills or potentially dangerous releases (CCPS, 1996).

According to Chang and Samsa (2007: 25-26), “the AEGLs for exposure times of 10, 30 and 60 minutes and four and eight hours are defined as:

- AEGL-3 (red area on the modelling plume) refers to the airborne concentration, expressed as parts per million (ppm). It means that the general population, including susceptible individuals, could experience life-threatening health effects or death.
- AEGL-2 (orange area on the modelling plume) refers to the airborne concentration, expressed as ppm. It means that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.
- AEGL-1 (yellow area on the modelling plume) refers to the airborne concentration, expressed as ppm. It means that the general population, including susceptible individuals, could experience discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are reversible upon the termination of exposure”.

Because AEGLs were developed robustly, they are the preferred guideline. Emergency Response Planning Guideline (ERPG) values are the go-to when AEGLs are not available for certain chemicals. Three-tiered ERPG levels are defined for a one-hour averaging time (American Industrial Hygiene Association, 1991).

Immediately Dangerous to Life and Health (IDHL) – “An atmospheric concentration of any toxic, corrosive or asphyxiant substance that poses an immediate threat to life or would cause irreversible or delayed adverse effects or would interfere with an individual’s ability to escape from a dangerous atmosphere”. IDHL levels were designed by the National Institute for Occupational Safety and Health (NIOSH, 1994).

Emergency Response Planning Guidelines, Level 3 (ERPG-3) – “the maximum concentration in air below which it is believed nearly all individuals could be exposed for up to one hour without experiencing or developing life-threatening health effects.” ERPGs were established by the American Industrial Hygiene Association.

Definitions for terminology such as “life-threatening” may be subjective and not entirely transparent. For many individuals, an exposure that lasts a number of hours at IDHL or ERPG-3 concentrations would be required for a healthy person to result in a fatality.

CHAPTER 4 : METHODOLOGY FOR THE CONCENTRATION QUANTIFICATION OF THE ACCIDENTAL RELEASE OF HAZARDOUS SUBSTANCES

The physical processes of an accidental release (rate and size) must be established to determine the consequences of loss of containment. Other aspects of the release also add valuable information to a consequences analysis, such as the spread, evaporation and dispersion of toxic and asphyxial vapours from the resulting airborne cloud from a liquid release. If there is an ignition, estimating the fire's burning rate and thermal radiation transfer or explosion overpressures are necessary (Casal, 2008).

The magnitude of an accidental release is quantified based on the consequences to all living organisms and structures in the surrounding environment. Consequences could be described by comparing predicted gas concentrations, thermal radiation or overpressures to short-term guideline values (described in Section 3.12) or using a dose-response analysis correlating the accidental release's intensity with the degree of injury or damage it could cause (Casal, 2008).

Hazardous substances will be selected, based on ranking in terms of usage, toxicity, flammability and frequency of involvement in accidental releases. A substance should be preferably ranked high up the order in one or the other category. It should also be representative of the three most common types of releases. Thus, three chemical substances were selected for this study.

The three case studies served as the basis for consequences modelling to firstly estimate the concentration of said hazardous substance at the time of the incidents, disregarding the probability (deterministic approach), and quantifying the likely impact it may have on the operators.

Models to estimate the impact from accidental releases were selected based on applicability, desired outcome and ease of availability. A discussion of the model's capabilities and limitations, including its various input parameter requirements, will be discussed in this chapter.

4.1 CRITERIA FOR THE SELECTION OF HAZARDOUS SUBSTANCES

Three substances and release types representative of neutrally buoyant dispersion, dense phase dispersion, and a fire and explosion event were selected to quantify the concentration of the release, as well as the potential impact on control room operators.

4.2 BASIS FOR SELECTING HAZARDOUS SUBSTANCE

The following criteria were considered for selecting the chemical substances to be used in the dispersion and consequences analysis:

- General usage of the hazardous substance on or near nuclear power plants. This should support the likelihood that the accidents' frequency is coupled with storage volumes and will serve as a guideline for selection.

- Frequency of involvement in accidents. The more frequently the substance is involved in an accident release, the more likely it will surface again in the future.
- The severity of past accidents, that is deaths, injuries and the loss of property, serves as a guideline according to which substance was selected for investigation.
- Toxicity of chemicals. The more toxic, the more likely a substance was to be used in this study. This analysis is for acute consequences, not long-term effects (cancer).

4.3 CHEMICALS TO BE USED AS A BASIS FOR MODELLING

The following substances were selected for modelling and estimating exposure parameters, and to illustrate the usage of dispersion modelling. The justification for the use is that in one or the other category (usage, production, accident frequency), it features as high ranking, and it was representative of three different common types of release scenarios (dilute, dense and flammable). The toxicity to humans also played a significant role in the selection.

4.3.1 Chlorine

Chlorine is the most toxic of all the gases listed in Regulatory Guide 1.78 (U.S. Atomic Energy Commission (AEC), 1974) based on its toxicity value. Furthermore, the release of chlorine into the atmosphere is of particular concern since it disperses at ground level. The effects various concentrations of chlorine have, are given by Branscomb et al, 2010. Chlorine has a characteristic sharp, penetrating odour above 3,5 ppm. At higher concentrations, the severely irritating and painful effects make it unlikely that any person will remain in the immediate area. Low concentrations cause irritation to the mucous membranes and the respiratory system, as well as the skin (Branscomb et al, 2010).

The high number of chorine processes results primarily from the common uses of chlorine to disinfect water. To maximally alleviate the bio-fouling phenomenon in the cooling water system of thermal (nuclear) power plants, adding chlorine is a method widely used in most countries for its simplicity and convenience. In China, it is the most extensively used method in thermal (nuclear) power plants. Chlorine is usually stored on the site of nuclear power plants in one tonne cylinders (U.S. Nuclear Regulatory Commission (NRC), 1977).

4.3.1.1 Nature of Hazard from Chlorine Storage

At normal room temperature and atmospheric pressure, chlorine has a greenish-yellow colour and it is a non-combustible gas with an irritatingly pungent smell. It is heavier than air, which means that the gas will settle within low areas when it is released into the outside.

Hazards from chlorine come from the loss of containment, which may be the result of leakage, pipe rupture or vessel rupture. If chlorine enters the air, it becomes highly hazardous. Chlorine poses a significant health hazard if human beings are exposed to high concentrations. Small doses may cause irritation in the eyes and skin, as well as in the respiratory tract. Larger quantities of chlorine gas, such as exposure to 1000 ppm, can lead to death after a few deep breaths (Branscomb et al, 2010). If very high concentrations are inhaled, chlorine disintegrates in the lungs and forms hydrochloric acid, which burns the tissue of the lungs, thereby leading to pulmonary oedema (Branscomb et al, 2010). In essence, this causes drowning since liquid floods the lungs. The extent poisoning by chlorine is dependent on the amount of gas, setting and duration of exposure, as well as other circumstances (Branscomb et al, 2010).

4.3.2 Ammonia

The dispersion into the atmosphere study for ammonia is of significant interest for a dual reason. Firstly, ammonia is a widely used chemical with numerous applications based on the chemical and physical qualities it has. Secondly, this chemical is extremely toxic, corrosive, flammable, and under certain circumstances, it is an explosive chemical.

According to Peter and Winokur (2011), the Defence Nuclear Board staff evaluated the existing controls at the Hanford nuclear site for the ammonia system and found the following deficiencies:

- “Control Room Habitability – The Board concluded that the design of the ventilation system for the main control room is insufficient to protect workers following an ammonia release. The Board’s staff also identified a chance that ammonia concentrations can rise above levels established as “immediately” hazardous to life and health resulting from large quantities of ammonia being released from the storage containers or an accident with a tanker truck.
- Seismic event – The Board concluded that the controls for a seismic incident inadequately protect workers if there is an earthquake larger than seismic design basis criteria. Such an earthquake could lead to a large release of ammonia from storage containers, resulting in multiple fatalities among employees who are outdoors as the accident happens or it can affect any staff being evacuated to the outside.”

Ammonia is generally stored on the sites of nuclear power plants where it is primarily used for pH control of the secondary circuit inventory of the nuclear plant. Up to 22 000 litres stored in tanks can be found on nuclear sites. These tanks are periodically refilled by tanker trucks (Peter & Winokur, 2011).

4.3.2.1 Nature of Hazard from Ammonia Storage

The majority of instances involving spilling and leaking of ammonia are brought about by equipment failure o or mishandling by staff (Peter & Winokur, 2011). For instance, storage containers are susceptible to accidental incidents that could lead to a more serious danger to personnel in the proximity of the tanks. The most terrible accident scenario would be a ruptured tank that instantaneously spills its entire load of ammonia onto the ground.

Depending on the concentration, ammonia is less toxic than chlorine: exposure above 50 ppm of ammonia leads to mild irritation in the nose or throat (Branscomb et al, 2010). Exposure to 700 ppm or above results in coughing and severe eye irritation (Branscomb et la, 2010). Exposure to greater amounts may result in blindness and further kinds of severe or even fatal injuries. Ammonia at 5 000 to 10 000 ppm is rapidly fatal to humans (Branscomb et al, 2010). As stated previously, toxic chemical storage vessels are not subject to the demanding design and inspection requirements that nuclear vessels are.

4.3.3 Natural Gas

Lastly, natural gas via pipelines has been involved in numerous chemical accidents. Natural gas (methane) was selected for this study since more gas pipelines are being laid close to the boundaries of nuclear power plants.

Natural gas consists of a mix of hydrocarbons of which the main component is methane (CH_4). It is categorised as a dangerous chemical because of its physio-chemical qualities, which can affect people’s health and property, as well as the environment. It is a colourless and odourless gas of easy ignition; thus, it is flammable and explosive (Cameo Chemicals, n.d.).

Natural gas is a buoyant and a flammable gas, and it is lighter than air (relative density of 0.6). When it is released outside, the non-ignited gas has a tendency to disperse quickly at an altitude. Upon release, ignition can be possible. In this case, the gas would burn in a jet (or torch) flame. Released inside an enclosed area, both explosions or flash fires are a possibility.

Being non-toxic, natural gas only poses an asphyxiation risk close to the accidental release in the event of overexposure. Otherwise, dizziness, drowsiness, headache, excitation, excess salivation, vomiting and unconsciousness could occur. In sufficiently ventilated areas, such as outdoors, the asphyxiation hazard is significantly reduced since natural gas is buoyant and will rapidly dissipate (Burger, 2016). An explosion or fire caused by a rapturing natural gas line releasing a toxic gas could release carbon dioxide, carbon monoxide, water vapour, small quantities of sulphur dioxide or unburnt hydrocarbons (Burger, 2016).

The ERPG, IDLH, threshold limit values, and other guidelines for sulphur dioxide are outlined in Table 4-1.

Table 4-1: Toxicological properties of high dosages of sulphur dioxide

Physiological or toxic effects	Concentration (ppm)	Exposure period
Emergency Response Planning Guideline (ERPG)-1	0.3	1 hour
Normal detectable odour range	0.7	
Eight-hour time-weighted threshold limit value	2	8 hours per day 40 hours per week
Minor eyes, nose and throat irritation	2	
ERPG-2	3	1 hour
15-minute short-term threshold limit value	5	15
Respiratory irritation and nosebleeds	10	
Bronchospasms in normal individuals	10 - 20	
ERPG-3	15	1 hour
Eye irritation and may lead to chronic respiratory symptoms	20	
Immediately dangerous to health and life	100	30 minutes
LC_{50} (human, derived from animal studies)	400 – 2 200	30 minutes

Finally, the substances and its corresponding release characteristics should be representative of the three major forms of dispersion dynamics, which are:

- Neutrally buoyant (substance density that resembles that of air) type of release (aqueous ammonia);
- Dense (gas substance density higher than air density) release (chlorine); and
- A release of a flammable substance, ignition and explosion (natural gas as methane).

Chemicals selected based on the criteria stated above will be subjected to a worst-case hazard assessment to indicate its potentially harmful effects on humans.

4.4 MODEL SELECTION

The desired output, applicability and screening capability determined the model selection. Intermediate models, for example, ALOHA®, are more appropriate as screening tools as the flow of information is usually easier to follow. Two intermediate models, available in the public domain, were compared with similar input parameters for verification of the results. Regulatory models, for example, the “HABIT” model, requires extensive quality assurance and difficult to obtain outside the United States (Ramsdell & Stage, 1998).

Although the input data requirements and level of sophistication increase with the more advanced models, a more complex model does not necessarily lead to more accurate predictions.

4.4.1 ALOHA® Tool

The ALOHA® model was selected for the simulation since this software was designed to respond before situations of chemical emergencies (Tseng et al., 2012). It was developed by a group of mathematical equations that describe the transport phenomena (advection and diffusion) or Gaussian dispersion of continuous and buoyant air pollutants (Jones et al, 1989). This dispersion model was established together by the United States Environmental Protection Agency (US EPA), Chemical Emergency Preparedness and Prevention Office and NOAA. ALOHA® can model dangerous hazards, such as toxicity, flammability, thermal radiation (heat), and overpressure (explosion), linking to the accidental release or leak of substances that may cause the dispersion of toxic gases and explosions.

ALOHA® models gas (neutral, buoyant or dense gases) cloud dispersion into the atmosphere after an accidental release. Overhead views illustrate threat zones in which the levels of concern are exceeded using AEGLs (CCPS, 1996).

The AEGLs gauge the level of concentration at which the majority of individuals – including at-risk candidates such as the elderly, sick or very young children – will start to suffer health effects upon exposure to a specific dangerous chemical over a certain time. For a particular exposure time, a chemical carries three-tiered AEGL values, and each one corresponds with a specific level of health consequences:

- “**AEGL-3** (red area on the modelling plume) refers to the airborne concentration, expressed as parts per million (ppm), of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.”

- “**AEGL-2** (orange area on the modelling plume) refers to the airborne concentration expressed as ppm, of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.”
- “AEGL-1 (yellow area on the modelling plume) refers to the airborne concentration, expressed as ppm, of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.”

ALOHA® can be used in emergencies, meeting these criteria as per ALOHA® Manual (U.S. Nuclear Regulatory Commission (NSC), 1996):

- *“Operates on common computers*: The model has to run rapidly on small and transportable computers (PC or Macintosh), which have to be financially feasible for the majority of users.
- *User-friendly*: The program needs to be clear and simple to use in order for more inexperienced responders to utilise it in high-pressure situations with a low likelihood of error.
- *Reliable:* The user interface has been developed to reduce errors by operators; the program checks and cross-checks every entry prior to moving on to options for solutions.
- *Accuracy:* ALOHA® is only a tool, and its usefulness depends on the accuracy of the information entered into the model and the accurate interpretation and application of the data. Algorithms and physics represent a compromise between accuracy and speed so that good results are available quickly enough to be of immediate use.”

4.4.1.1 ALOHA® Inputs

To maximise usefulness, ALOHA® demands a minimum quantity of information, which the user may enter with ease utilising a detailed graphical interface. The inputs, as given by National Safety Council (NSC (US), 2019) are:

1. Geographic location and time: Location is needed to assess incoming solar radiation, while elevation is employed to calculate ambient air pressure;
2. Site definition: The roughness of the ground is required for calculating dispersion. Information pertaining to a specific building is utilised for predicting concentrations indoors, as well as its doses;
3. Chemical definition: Chemical selection determines the material’s physical and chemical properties; for example, in this project, carbon dioxide (CO_2);

4. Atmospheric data: The atmospheric parameters which are relevant to ALOHA® include (a) stability class, (b) inversion height, (c) wind speed, (d) air temperature, (e) ground roughness, (f) cloudiness and (g) humidity; and
5. Source definition: The source may be (a) direct, the proposed source is a continuous or instantaneous release point, (b) a puddle of evaporating liquid on the ground, (c) tank and (d) pipe.

4.4.1.2 ALOHA® Outputs

ALOHA® simulates a cloud of pollutant gas dispersing into the atmosphere. The main output is a diagram illustrating a plan overview of the relevant area within which it predicts the gas concentration in the air and where it will reach hazardous levels. This diagram is known as a hazardous footprint. This footprint indicates that the user-defined hazardous concentration (e.g. IDHL) will be exceeded for the particular footprint width and length at some time after the release. ALOHA® will be utilised to model neutral buoyant gas (ammonia), as well as the heavy gas (Cl_2) release.

4.4.1.3 Limitations and Assumptions in the Consequence Analysis

Conservative presumptions were employed in the consequence analysis. These include the following:

- A constant flow of mass at the maximum possible initial rate of evaporation for the modelled wind speed has been employed, while, in practice, the rate of evaporation would sink over time as the concentration levels in the solution decrease.
- Worst-case stability class (F) atmospheric conditions were used, which almost exclusively occur during night-time hours, and maximum night-time ambient temperature of 25°C was used in the modelling.
- It is assumed that the prevailing wind direction from the source was towards the area of interest (control room).
- The ALOHA® model considers enclosed buildings only, which contrasts with a nuclear control room.
- A flat terrain is assumed, in other words, the effects of complex terrain (e.g., hilly areas) were not considered. ALOHA® model assumes tank walls to be 1 cm thick steel.
- Only one chemical in the tank. No multi-component cases are considered.

4.4.2 SLAB® Tool

SLAB® is a computer model that simulates the dispersion of denser-than-air releases into the atmosphere. Due to the complex nature of the physical properties of the cloud after a release incident of natural gas from a pipeline, it was decided to employ SLAB® for its ability to simulate the initial heavy gas cloud characteristics and then to compare the results with the ALOHA® simulation results for the chorine scenario.

The SLAB® executable model necessitates an input file (“INPUT”) that contains all the parameters required to run the dispersion model. An area total of 30 possible input parameters are needed for running SLAB®. Said input parameters are entered in a fixed format, as described in the SLAB® User’s Manual (Ermak, 1990). The input data (Section 3, page 43, of the User’s Manual) includes (a) model parameter options, (b) release gas physical and chemical properties, (c) spill characteristics, (d) output field parameters and (e) ambient meteorological properties.

While most of the input parameters are a direct supply of information, such as the molecular weight, heat capacities, storage temperature, release size, wind speed and others, some parameters need to be calculated before supplying these in the INPUT file. These include the fraction of liquid that may be present on release (CMEDO), the temperature of the material at the point of release (TS), and the effective source area (AS). There are six different values for the ambient wind speed, ambient temperature, relative humidity and the stability class, corresponding to six different graphs. The complete INPUT file is presented in Table 4-2.

Table 4-2: Input file variables (Ermak, 1990)

Source Type	≡ IDSPL
Sub-step Parameter	≡ NCALC
Molecular Weight of Source Material (kg)	≡ WMS
Vapour Heat Capacity at Constant Pressure (J/kg.K)	≡ CPS
Boiling Point Temperature (K)	≡ TBP
Initial Liquid Mass Fraction	≡ CMEDO
Heat of Vaporization (J/kg)	≡ DHE
Liquid Heat Capacity (J/kg.K)	≡ CPSL
Liquid Density of Source Material (kg/m^3)	≡ RHOSL
Saturation Pressure Constant	≡ SPB
Saturation Pressure Constant	≡ SPC
Temperature of Source Material (K)	≡ TS
Mass Source Rate (kg/s)	≡ QS
Source Area (m^2)	≡ AS
Continuous Source Duration (s)	≡ TSD
Instantaneous Source Mass (kg)	≡ QTIS
Source Height (m)	≡ HS
Concentration Averaging Time (s)	≡ TAV
Maximum Downwind Distance (m)	≡ XFFM
Heights of Concentration Calculation (m)	≡ Z(1)
Heights of Concentration Calculation (m)	≡ Z(2)
Heights of Concentration Calculation (m)	≡ Z(3)
Heights of Concentration Calculation (m)	≡ Z(4)
Surface Roughness Height (m)	≡ ZO
Ambient Measurement Height (m)	≡ ZA
Ambient Wind Speed (m/s)	≡ UA_1
Ambient Temperature (K)	≡ TA_1
Relative Humidity (%)	≡ RH_1
Stability Class	≡ STAB

An output file (PREDICT) is produced upon completion of a SLAB® execution. The primary output in the file is the time-averaged concentration provided in different formats for further use or interrogation. The average concentration based on time is articulated as the time-averaged volume fraction, which has values in the range of 0.0 to 1.0. This value can then be multiplied by 1 000 000 to get the value of the relevant concentration in parts per million. The results are given from an observer’s or receptor’s point of view situated at the downwind distance *x*, the crosswind distance *y* from the mean cloud centreline and the height *z* above ground level.

The SLAB® model was only selected as a comparison tool for the chlorine scenario due to its applicability, specifically for heavier-than-air (chlorine) dispersion modelling.

4.5 RELEASE SCENARIOS

In this section, three hypothetical worst-case scenarios are set up for each chemical substance, namely chlorine, ammonia and methane.

4.5.1 Modelling Parameters

As was previously discussed, the RMP rule (U.S. Environemntal Protection Agency (EPA), 1996) necessitates the use of particular parameters in the offsite consequence analysis modelling. The analysis done in this project used these parameters:

- For ammonia, chlorine and methane, the worst-case scenario considers a release which is sudden and as a result of which, the entire contents of the biggest container or pipeline are leaked. For modelling, it was presumed that the timespan of the release was ten minutes. The release may be out in the open or within a building.
- According to the RMP rule, the worst-case conditions for weather consider an atmospheric stability category F, with a wind speed of 1.5 m/s, unless it could be demonstrated that said circumstances have not been applicable at the site over the last three years. Furthermore, in the absence of detailed meteorological data for a particular site, two common weather conditions (stability and wind speed) used in many QRA studies are F and 1.5 m/s, which is typical for still night-time conditions.
- The toxic endpoints were 200 ppm for ammonia, 3 ppm for chlorine and 50 000 ppm for methane, irrespective of the exposure duration.
- US EPA guidance also recommends assuming urban conditions (ground roughness of 100 cm) for a site area with many obstacles.
- In the absence of guidance for selecting a relative humidity percentage, the use of a medium value seemed reasonable.

4.5.2 Dense Gas Dispersion Modelling – Chlorine Release

A hypothetical worst-case scenario considers the failure of a cylinder that contains 90 kg chlorine and the vessel empties within ten minutes of the incident.

Table 4-3: Hypothetical chlorine source input (WCS)

Parameters	Input
Release Quantity (kg)	90
Release Time (min)	10
Release Height (m)	0

Table 4-4: Hypothetical meteorological input parameters at the time of chlorine release (WCS)

Parameter	Input
Ambient Temperature (°C)	29
Wind Speed (m/s)	1.5
Wind Direction	NE
Relative Humidity (%)	50
Atmospheric Pressure (atm)	1
Atmospheric Stability	F
Ground Roughness (m)	1

The AEGLs shown in Table 4-5 have been conceptualised by the National Academy of Sciences and serve as indicators of the effects on health linked to selected chemical exposure.

Table 4-5: Acute exposure guidelines for chorine (ppm) (U.S. Environmental Protection Agency (EPA), 2019)

Chlorine (ppm)			
	10 Minutes	**30 Minutes**	**60 minutes**
AEGL-1	0.5	0.5	0.5
AEGL-2	2.8	2.8	2
AEGL-3	50	28	20

Despite these exposure limits having been set by the National Research Council's committee of toxicology, other limits have been put in place by industry or governments that give more detail pertaining to the particular health effects resulting from exposure to such substances at varying levels of concentration (also refer to Branscomb et al).

In ALOHA®, each of the three levels of AEGL: AEGL-1, AEGL-2 and AEGL-3 are established for exposure periods of ten minutes, 30 minutes and 60 minutes, respectively.

4.5.3 Neutrally Buoyant Dispersion Modelling – Ammonia Release

In this context, it can be presumed that a solution of 25% ammonia was accidentally released during a postulated seismic event, and the aqueous ammonia formed a pool of liquid on the ground in an area without dikes. In reference to atmospheric dispersion modelling, the difference between aqueous and anhydrous ammonia is that aqueous ammonia evaporates slowly from a pool. In contrast, the anhydrous ammonia is a blend of vapour and liquid droplets that is initially denser than air. By contrast, the vapour from a pool of aqueous ammonia is neutrally buoyant, or even marginally lighter than air. As such, using the Gaussian dispersion model for a neutrally buoyant plume is suitable. In this instance, the dispersion modelling analysis was conducted with ALOHA®. Details of the conditions surrounding the release and representative meteorological conditions based on worst-case weather conditions (F stability, 1.5 m/s wind speed) as defined by the US EPA are summarised in Table 4-6 and Table 4-7, respectively (U.S. Environmental Protection Agency (EPA), 1996).

Table 4-6: Hypothetical aqueous ammonia source input (WCS)

Parameters	Input
Release Quantity (litres)	22 712
Release Rate (kg/min)	9.01
Release Area (m^2)	40
Enclosed Building (control room - 0.5 air change per hour) distance from release source (m)	100

Table 4-7: Hypothetical meteorological input parameters at the time of chlorine release (WCS)

Parameter	Input
Ambient Temperature (°C)	25
Wind Speed (m/s)	1.5
Wind Direction	NE
Relative Humidity (%)	50
Atmospheric Pressure (atm)	1
Atmospheric Stability	F
Ground Roughness (m)	1

During the hypothetical worst-case scenario, the aqueous ammonia spill was presumed to evaporate in the form of gas via laminar transfer. The ALOHA® model examined the effects of the designated wind speed and atmospheric turbulence force that moved the released molecules as a gas through the air.

Table 4-8: Acute exposure guidelines for ammonia (U.S. Environemntal Protection Agency (EPA), 2019)

Ammonia release in (ppm) over time			
	10 minutes	**30 minutes**	**60 minutes**
AEGL-1	30	30	30
AEGL-2	220	220	160
AEGL-3	2 700	1 600	1 100

4.5.4 Natural Gas (Methane)

For this study, natural gas was modelled as a pure component (methane). The physical properties used in the simulations are given in Table 4-9.

Table 4-9: Properties of methane gas (Crowl & Louvar, 2011)

Property	Value
Molecular weight (g/mol)	16
Relative density of the gas (atmospheric temp. and pressure)	0.6
Heat of combustion (MJ/kg)	50
Flammable range (vol. % in air)	5 to 15
Ratio of specific heats (Cp + Cv)	1.32
Flashpoint	-218°C
Flame temperature	2 200 K
Fracture of energy converted to radiation	0.2

The leak size is required to determine the natural gas' mass flow rate. According to Burger (2016) three kinds and forms of leaks are (see Figure 4-2):

a) “Splitting of the pipeline in a tangential direction, mostly caused by earth movements or by being passed over by heavy construction equipment or similar machines;

b) Splitting of the pipeline in an axial direction over a relatively short section with simultaneous widening crosswise to the pipe axis (fish mouth rupture).

c) Splitting of the pipeline in the upper vertex over several metres.”

For the current study, a guillotine break in the gas pipeline causing a large release under pressure and the leaking substance in contact with an ignition source were assumed. The release conditions, including the flammable material's mass and when ignition occurs, could lead to a localised fire or a vapour cloud explosion.

Figure 4-1: Carlsbad explosion crater 19 August 2000 (National Transport Safety Board (NTSB), 2003; Burger, 2016)

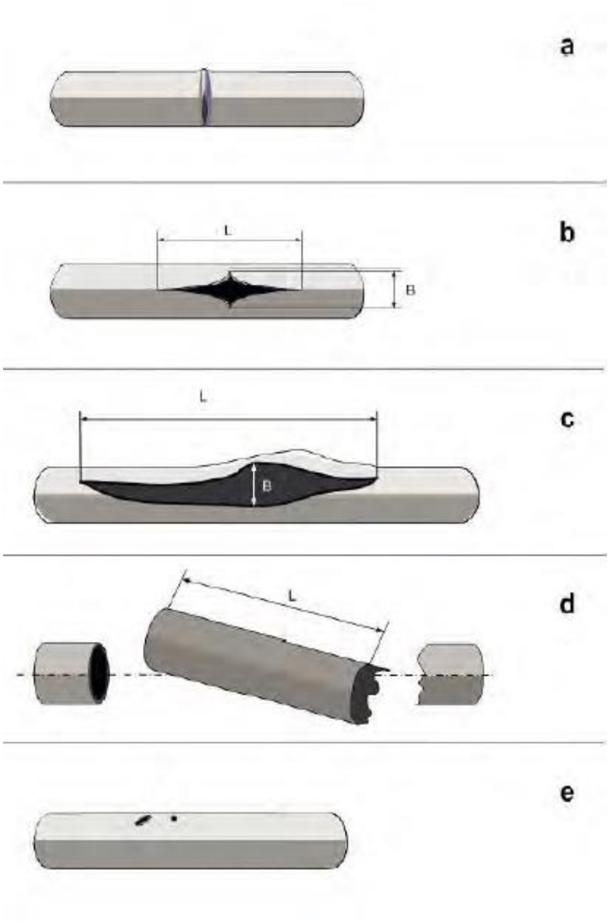


Figure 4-2: Typical types of leaks in high-pressure pipelines

Legend: (a) splitting of the pipeline in a tangential direction;
(b) Splitting of the pipeline in an axial direction;
(c) Splitting of the pipeline in the upper vertex;
(d) A guillotine break; and

(e) An oval or circular penetration (after Konersmann et al. 2009; Burger, 2016)

Lastly, for a risk to exist, individuals need to be located in the range of harm (consequence distance) of the fire or the explosive event. The proximity to the event determines whether injuries occur and what their impact may be.

Office of Response and Restoration (2013) states that ALOHA® thermal radiation levels of concern for thermal radiation are as follows:

- **4 kW/m^2**, pain within 60 seconds;
- **5 kW/m^2**, second-degree burns after 60 seconds;
- **10 kW/m^2**, potentially lethal within 60 seconds.

Table 4-10: Hypothetical methane source input (WCS)

Parameters	Input
Operating pressure (bar)	26
Pipe diameter (mm)	300
Pipe length (m)	> 1000
Depth of cover (mm)	900
Guillotine break (mm)	300
Enclosed building (control room - 0.5 air change per hour) distance from release source (m)	1000

Table 4-11: Hypothetical meteorological input parameters at the time of methane release (WCS)

Parameter	Input
Ambient temperature (°C)	25
Wind speed (m/s)	1.5
Wind direction	NE
Relative humidity (%)	50
Atmospheric pressure (atm)	1
Atmospheric stability	F
Ground roughness	Rural

According to the RPM (U.S. Environmental Protection Agency (EPA), 2009), to conduct an analysis of the worst-case consequence for flammable chemicals, one can utilise a TNT-equivalent model (i.e., a model that gauges the explosive effects of a flammable chemical by comparing it to the effects of the high explosive TNT. This is grounded on the available combustion energy in the vapour cloud. The ALOHA® simulation was used as the model to compute overpressure and thermal radiation.

CHAPTER 5 : MODELLING RESULTS AND DISCUSSION

The following sections provide modelling outputs, calculations and results of the consequence analyses conducted for chlorine, aqueous ammonia and methane gas.

5.1 SCENARIO 1: CHLORINE

Scenario 1 is grounded on an accident scenario in which 90 kilograms of chlorine are released from a cylinder over ten minutes. The dispersion analysis does not account for a prevailing wind direction and, therefore, assumes an equal opportunity of the chlorine vapour cloud dispersing in any possible direction. The scenario was modelled utilising both the ALOHA® and SLAB® software for comparison purposes. The ALOHA® software program contains AEGLs for many substances. These guidelines serve as "exposure guidelines designed to help responders deal with emergencies involving chemical spills or other catastrophic events where members of the general public are exposed to a hazardous airborne chemical" (NSC (US), 1996).

The modelling results of scenario 1 show that AEGLs values are exceeded on-site. ALOHA® predicts the outside concentration within the control room building to be approximately 313 ppm, but it predicts the indoor concentration (inside control room) to be 27 ppm. Figure 5-1 shows a decrease in the maximum downwind concentration when the distance increases as a result of dilution as it moves further from the source.

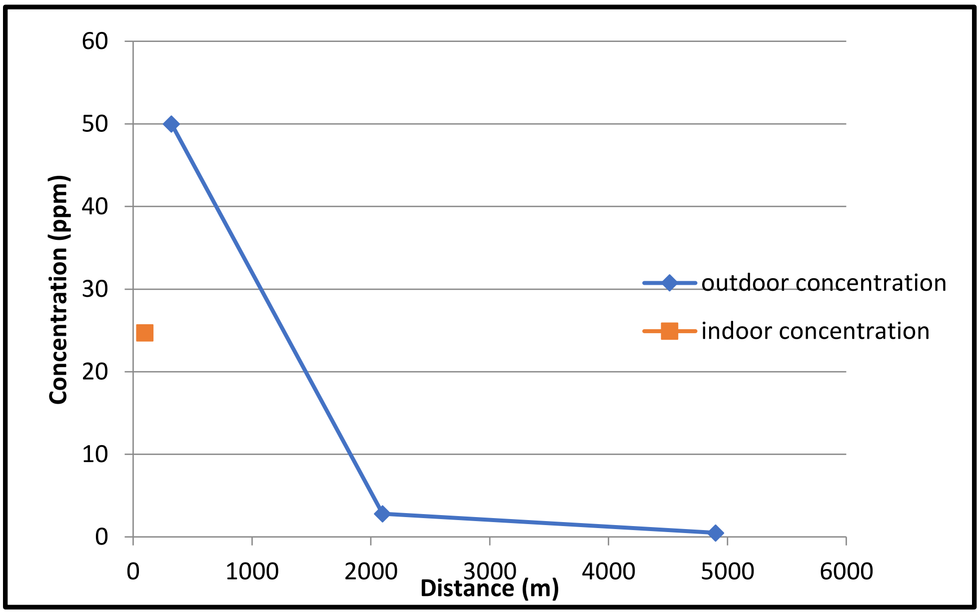


Figure 5-1: X-Y plot of chlorine concentrations

The indoor concentration is affected by the ventilation rate of the building, which was assumed to be 0.5 air changes per hour (Casal, 2008). As given by the explanation of Casal (2008), ventilation rate depends on the building type. Fresh air enters through joints and seams due to the wind and the temperature difference between the outside and inside. For a tightly sealed building, the ventilation rate according to Regulatory Guide 1.78 (U.S. Atomic Energy

Commission (AEC), 1974), should be around 0.016 air per hour. However, the NEI 99-03 document (Nuclear Energy Institute, 2001) has provided enough historical evidence that the in-leakage rates at nuclear power plants have been grossly underestimated. This resulted in significant modifications and capital expenditure to the control room for the utility to fulfil the requirements of Criterion GDC 19.

Figure 5-1 illustrates that the area of concern is within 323 m from the source as the chlorine concentration is around 50 ppm. All individuals need to be evacuated from this area instantaneously. It can be seen that the concentration decreases with distance, and the concentration of 2.8 ppm of chlorine is determined up to 2 100 m away from the source. However, this lower concentration could still produce respiratory irritation (Branscomb et al, 2010). In such areas, respiratory protection gear ought to be worn. In Figure 5-1, it can be seen that chlorine concentration of 0.5 ppm goes as far as 4900 m.

Based on the estimated chlorine concentrations within and outside the control room (24.7 ppm), the operators will not be able to work or function under such a high chlorine concentration. Such a condition would render the entire site inhabitable up to 4.9 km or at least until the vapour cloud has drifted beyond the nuclear site. According to Table 5-1, any outside personnel within a radius of 323 m of the source would be killed within a few minutes. It will also affect people inside dwellings that have a high renewal rate for air, as was the case in Bhopal. Should people attempt to escape and they inadvertently do so in the direction in which the chlorine cloud moves, they will remain inside the cloud. As such, their elevated breathing and heart rate will result in their consuming an even greater amount of chlorine (Casal, 2008).

Inside a building in which the ventilation rate is reduced, the concentration will be significantly lower, thus providing greater protection. Reducing the ventilation rate even further, for example by turning off the ventilation and plugging gaps, and acquiring protection by sheltering can be decisive in the case of relatively short-duration emergencies (Casal, 2008).

The probit equation (3.7) in Chapter 3 can be employed for calculating lethal levels for a given exposure. The values for chlorine are given in Table 5-1.

Table 5-1: Probit values for chlorine (Casal, 2008)

ALOHA® zone	Distance (m)	Concentration (ppm)	Probit value	Fatalities (%)
Red	323	50	1.03	0
Orange	2100	2.8	-0.04	0
Yellow	4900	0.5	-7.45	0
Control room	100	24.7	-0.27	0

Table 5-1 quantifies that there would be zero fatalities to personnel exposed to chlorine for around ten minutes. It would be unlikely for any worker to be exposed for more than tec minutes as the person would have attempted to either escape or find shelter.

The SLAB® results in Table 5-2 compares relatively well with the ALOHA® results.

Table 5-2: SLAB® results for chlorine

Distance(m)	SLAB® (ppm)	ALOHA® (ppm)
100	211	313
323	51	50
2100	5	2.8
4900	2	0.5

There are variances, and this could be due to the SLAB® software being a non-source-term model. The diameter of the rupture opening was established by utilising the source term model of ALOHA®. By assuming that the cylinder has emptied its entire contents in ten minutes, the rupture opening diameter had to be estimated. Nonetheless, the chlorine concentrations do not differ significantly and may suffice for assessing the hazard or for emergency planning.

Finally, the results from both ALOHA® and SLAB® show that no off-site impact is expected from the above chlorine scenario.

The following data provides detailed information pertaining to the chlorine worst-case scenario. It considers chemical data, atmospheric data, the source strength and the threat zone, as well as the threat at point.

CHLORINE WORST CASE SCENARIO

SITE DATA

Location:	CAPE TOWN, SOUTH AFRICA
Building air exchanges per hour:	0.50 (enclosed office)
Time:	11 October 2019 18:47 hours ST (using computer's clock)

CHEMICAL DATA

Chemical name:	CHLORINE
CAS number: 7782-50-5	Molecular Weight: 70.91 g/mol
AEGL-1 (60 min):	0.5 ppm
AEGL-2 (60 min):	2 ppm
AEGL-3 (60 min):	20 ppm
IDLH:	10 ppm
Ambient boiling point:	-34.0°C
Vapour pressure at ambient temperature:	Greater than 1 atm.
Ambient saturation concentration:	1 000 000 ppm or 100.0%

ATMOSPHERIC DATA (MANUAL INPUT OF DATA)

Wind:	1.5 metres/second from NE at 6 metres
Ground roughness:	100 centimetres
Cloud cover:	5 tenths
Air temperature:	29°C
Stability class:	F
No inversion height	Relative humidity: 48%

SOURCE STRENGTH

Direct source:	0.15 kilograms/sec
Source height:	0
Release duration:	10 minutes
Release rate:	9 kilogram/min

Total amount released: 90.0 kilograms

Note: This chemical may flash boil or result in two-phase flow.

THREAT ZONE

Model run: **Heavy Gas**

Red: 323 metres (50 ppm)

Orange: 2.1 kilometres (2.8 ppm)

Yellow: 4.9 kilometres (0.5 ppm)

THREAT AT POINT

Concentration estimates at the point:

Downwind: 100 metres control room distance

Max. concentration: outdoor: 313 ppm

Max. concentration indoor: 24.7 ppm

5.2 SCENARIO 2: AMMONIA

This dispersion analysis assumes that an equal chance that the ammonia vapour cloud might disperse in any direction. Thus, the model results in Figure 5-2 show the predicted ammonia concentration around the source for the most significant area of impact. For the ammonia scenario, the SLAB® software was not used to compare results with ALOHA® since the built-in chemical library of SLAB® does not account for solutions, such as aqueous ammonia.

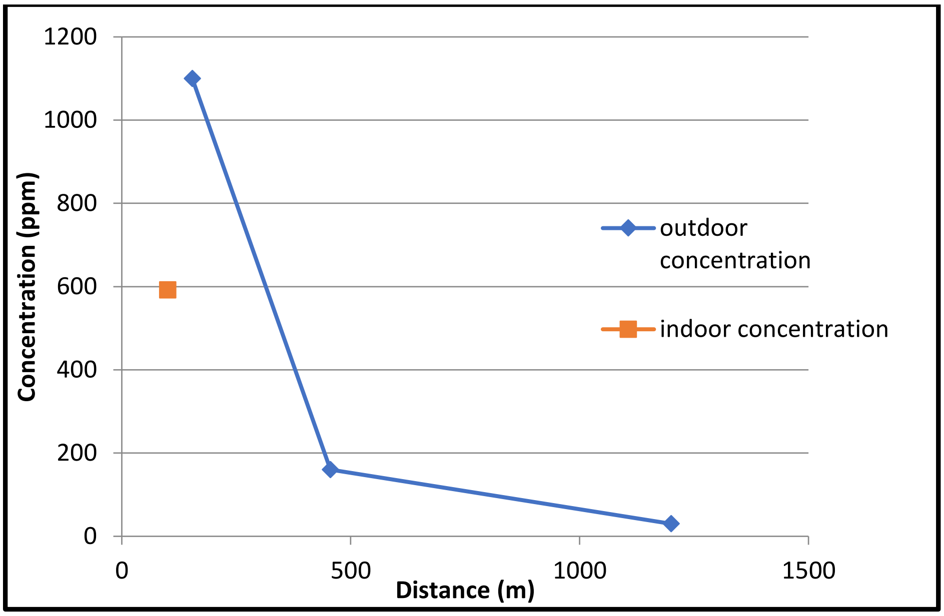


Figure 5-2: X-Y plot of ammonia concentrations

Table 5-3 summarises the AEGL distances for ammonia from the source of release, as well as the probit values associated with the concentrations. The distance between the storage tank and the control room was hypothetically assumed to be 100 m.

Table 5-3: Ammonia concentration distances and percentage fatalities

ALOHA® zones	Concentrations (ppm)	Distance (m)	Probit values	% Fatalities
Red	1100	154	-5.73	0
Orange	160	456	-12.86	0
Yellow	30	1200	-19.06	0
Control room	592	100	-8.02	0

For the ammonia scenario, the exposure period was 60 min, with no fatalities expected. Figure 5-2 indicates that the control room operators will experience a concentration of 592 ppm ammonia, which is above the IDHL of 300 ppm. Operators will, therefore, have to use breathing apparatus should they need to remain in the control room to continue their functions.

ALOHA® RESULTS FOR AMMONIA WORST CASE SCENARIO

A.1 SITE DATA

Location: CAPE TOWN, SOUTH AFRICA

Building air exchanges per hour: 0.50 (enclosed office)

Time: 11 October 2019, 19:00 hours ST (using computer's clock)

A.2 CHEMICAL DATA

Chemical name: AQUEOUS AMMONIA

Solution strength: 25% (by weight)

Ambient boiling point: 36.4°C

Partial pressure at ambient temperature: 0.72 atm

Ambient saturation concentration: 716,275 ppm or 71.6%

Hazardous component: AMMONIA

CAS number: 7664-41-7 Molecular Weight: 17.03 g/mol

AEGL-1 (60 min): 30 ppm AEGL-2 (60 min): 160 ppm AEGL-3 (60 min): 1 100 ppm

IDLH: 300 ppm LEL: 150 000 ppm UEL: 280 000 ppm

A.3 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)

Wind: 1.5 metres/second from NE at 6 metres

Ground roughness: 100 centimetres Cloud Cover: 5 tenths

Air temperature: 29°C Stability Class: F

No inversion height relative humidity: 48%

A.4 SOURCE STRENGTH

Evaporating puddle (Note: The chemical is flammable.)

Puddle area: 40 square metres

Puddle Volume: 6 000 gallons (22 712 litres)

Ground type: Concrete ground temperature: 29°C

Initial puddle temperature:	Ground temperature
Release duration:	ALOHA® limited the duration to 1 hour
Max average sustained release rate:	9.99 kilograms/min (averaged over a minute or more)
Total amount hazardous component released:	417 kilograms

A.5 THREAT ZONE

Model Run:	**Gaussian**
Red:	154 metres (1 100 ppm = AEGL-3 [60 min])
Orange:	456 metres (160 ppm = AEGL-2 [60 min])
Yellow:	1.2 kilometres (30 ppm = AEGL-1 [60 min])

A.6 THREAT AT POINT

Concentration estimates at the point:

Downwind:	100 metres control room distance

Max. concentration:

Outdoor:	2 260 ppm
Indoor:	592 ppm

5.3 Scenario 3: Natural Gas

The natural gas concentration 1 000 m from the control room is an estimated 55 200 ppm. As natural gas is generally not toxic, the control room occupants may be slightly drowsy for a few minutes but they could manage the ventilation by closing the ventilation dampers, further reducing the concentration (Burger, 2016).

A jet will form if natural gas is released under pressure, being carried along and blending with ambient air. A jet fire will occur if the gas is at a flammable concentration and it meets an ignition source. Because the release from the underground pipeline has significant momentum, the soil cover will be blown away and the resultant fires will be vertical, with lower hazard ranges than a horizontal fire (Burger, 2016).

From the ALOHA® calculations, the red zone shows that a 10 kW/m^2 thermal radiation threat zone covers a total distance of 324 m, while the orange zone shows a 5 kW/m^2 heat at 452 m. The yellow zone shows a 2 kW/m^2 heat spread to a distance of 243 m. Any person in the red zone could be killed within 20 seconds by the jet fire, which is unlikely to affect on-site personnel. However, the orange threat zone could potentially have an impact on the entry and exit points of the nuclear site since an underground gas pipeline could be within a distance of

500 m. In Table 5-4, the ALOHA® thermal radiation zones results are compared with manually calculated results. The calculated results are shown in A.35, A.36, and A.37 (Appendix F).

Table 5-4: Thermal radiation results

Thermal radiation	ALOHA® distances (m)	Empirical distances (m)
2 kW/m^2	700	842
5 kW/m^2	452	543
10 kW/m^2	324	389

In the ALOHA® estimate, a maximum peak overpressure of 5 000 Pa up to 1.4 km occurs. Thus, the RMP overpressure of 6 895 Pa (1 psi) is never exceeded, and hence no structural damage to SSC or buildings is expected. Generally, a peak overpressure of 5 000 Pa causes minor damages to houses, such as windows shattering. However, on-site personnel might be sensitive to that pressure, especially pressure-sensitive organs, such as the eardrums and the lungs. The distance from the point of release where the flammable gas has expanded to concentration levels under the lower flammability limit (5 000 ppm) is estimated to be 3.4 km using a dispersion analysis software program. Therefore, it can be deduced that flame pockets within flammable limits could drift over the site placing emergency equipment and on-site personnel at risk

The trajectories of debris fragments projected by a shock wave and the adverse effects on human health are not predicted by ALOHA®.

Primarily, a rupture or large leak leads to a gas pipeline accidental release. A leak only causes injury or damage in the event of an ignition leading to a fire or explosion involving these factors (Burger, 2016):

- Failure causing a large release must occur. Several potential causes of failure exist, but a guillotine break would most likely be caused by an earthquake exceeding the gas pipeline's design limits.
- The released substance has to come into contact with an igniting source, which could be heat or sparks produced by mechanical damage.
- Depending on the conditions of the release, which includes the mass of material and when ignition occurs, the consequences could be a localised fire (for instance a jet fire) or a flash fire. When the pipeline goes across open areas, it is highly unlikely that the vapour cloud formed during the release would explode.
- Lastly, individuals who are within the range of harm (consequence distance) of the fire or explosion are at risk. The degree of injury, even fatality, can be established by considering the distance from the release.

ALOHA® Results for methane worst case scenario

SITE DATA

Location: CAPE TOWN, SOUTH AFRICA

Building air exchanges per hour: 0.50 (enclosed office)

Time: 11 October 2019; 19:26 hours ST (using computer's clock)

CHEMICAL DATA

Chemical name: METHANE

CAS number: 74-82-8 Molecular Weight: 16.04 g/mol

PAC-1: 65 000 ppm PAC-2: 230 000 ppm PAC-3: 400 000 ppm

LEL: 50 000 ppm UEL: 150 000 ppm

Ambient boiling point: -161.5°C

Vapour pressure at ambient temperature: greater than 1 atm

Ambient saturation concentration: 1 000 000 ppm or 100.0%

ATMOSPHERIC DATA (MANUAL INPUT OF DATA)

Wind: 1.5 metres/second from NE at 6 metres

Ground roughness: 100 centimetres Cloud Cover: 5 tenths

Air temperature: 29°C Stability Class: F

No inversion height relative humidity: 48%

SOURCE STRENGTH

Flammable gas is burning as it escapes from pipe

Pipe diameter: 30-inch pipe length: 1 000 metres

Unbroken end of the pipe is closed off.

Pipe roughness: smooth hole area: 707 square inch

Pipe press: 257 atmospheres

Pipe temperature: 29°C

Max flame length: 88 metres

Burn duration: 1 minute

Max burn rate: 1 180 000 kilograms/min

Total amount burned: 75 543 kilograms

THREAT ZONE (GAUSSIAN SELECTED)

Model run: Gaussian

Red: 1.0 kilometres (50 000 ppm)

THREAT AT POINT

Concentration estimates at the point:

Max. concentration:

Threat zone:

Downwind: 1 000 metres control room distance

Outdoor: 55 200 ppm

Indoor: 2 650 ppm

Threat modelled: Thermal radiation from jet fire

Red: 324 metres (10.0 kW/(sq m) = potentially lethal within 60 sec)

Orange: 452 metres (5.0 kW/(sq m) = 2nd degree burns within 60 sec)

Yellow: 700 metres (2.0 kW/(sq m) = pain within 60 sec)

THREAT ZONE (GAUSSIAN SELECTED)

Threat modelled: Flammable area of vapour cloud

Model run: Gaussian

Red: 1.7 kilometres (30 000 ppm = 60% LEL = flame pockets)

Yellow: 3.4 kilometres (5 000 ppm = 10% LEL)

THREAT ZONE (GAUSSIAN SELECTED)

Threat modelled: Overpressure (blast force) from vapour cloud explosion

Type of ignition: Ignited by spark or flame

Level of congestion: Uncongested

Model run: Gaussian

Red: LOC was never exceeded (8 000 pascal)

Orange: LOC was never exceeded (7 000 pascal)

Yellow: 1.4 kilometres (5 000 pascal)

CHAPTER 6 : CONCLUSION AND RECOMMENDATIONS

6.1 CONCLUSION

Nuclear power plants are potentially high-risk facilities since the consequence of a severe chemical accident at a nuclear power plant can be significant, as is shown in this study through hypothetical examples. The safety of nuclear power plants and their respective facilities can be increased by adequate characterisation of hazards to cope with the effects of these hazards. An assessment was made of a chemical release and the impact thereof on the control room and outside environment. Inleakage into a control room of contaminated air during accidental (or deliberate) releases of hazardous materials can represent a significant health and safety issue for operators of both nuclear power plants and chemical process plants. The assessment focused on the most extensively used hazardous chemical products, being ammonia and chlorine. The explosion assessment considered off-site sources of potential explosion and the resulting blast and projectile damage.

Three accident scenarios were developed to postulate a hazardous gas release from each scenario; these are:

- on-site ammonia release (storage tank rupture);
- on-site chlorine release (continuous release); and
- off-site methane release (pipeline rupture).

Dense gas (for example, DEGADIS, SLAB® or ALOHA®) or neutrally buoyant gas models (for example, AFTOX or ALOHA®) model accidental toxic chemical releases from industrial storage tanks or pipelines.

Table 6-1: Summary of dispersion codes

Code Name and Acronym	Application	Limitation	Special Features
ALOHA®	ALOHA® applies two types of models to calculate the downwind movement and concentration levels of gaseous dispersion: Gaussian and heavy gas dispersion model. ALOHA® was also designed with first responders in mind.	ALOHA® models do not account for terrain steering or changes in wind speed and horizontal direction.	ALOHA® has been designed to reduce operator error during high-stress information accident response in the following ways: It does extensive input checking using a rule-based formulation, which prevents many common user errors. It includes an extensive on-line help system and extensive chemical library.
DEGADIS	Atmospheric dispersion of dense gas releases.	No provision for high-velocity releases.	None.
SLAB®	Denser-than-air dispersion.	Cannot be used for chemical solutions.	Use FORTRAN language.
AFTOX	AFTOX provides estimates of toxic chemical concentrations and hazard distances.	The Gaussian equation model calculates average distances for given concentration values.	None.
HABIT Code	Calculation of chemical concentration and exposure.	Only available in the USA.	Endorsed by USNRC.

Chemical gas releases were modelled using ALOHA® based on conservative assumptions. The model was furthermore used to simulate a flammable gas release resulting from a pipe rupture nearby the nuclear site.

The research has met its primary objectives as set in the research methodology:

- Analysis of toxic chemical safety from the perspective of satisfying a licensing requirement, evaluating the risk focused on enhancing safety (hardware or software / procedures). This would entail a comprehensive re-evaluation of inventory, evaluation of the validity of previous calculations and the associated assumption.
- Analysis of worst-case scenario's using ALOHA® as the computational tool.
- Analysis for the release of a flammable gas. It provided guidance on steps which should be taken, how likely is an explosion and who will be affected. The inputs are short and straightforward, and the results understandable to a non-specialist engineer.

Appropriately modelling dispersion for accidental release scenarios may not be straightforward, but it is critical. One case study showed that while more than one model could be applied, different models may yield different results because each model is associated with inherent assumptions and limitations.

A deterministic consequence analysis based on conservative assumptions was performed. Overall, ALOHA® is a useful and straightforward simulation tool to help a nuclear power utility to assess potential hazards for chemical substances stored on-site or being transported near to a nuclear facility. This novel approach allows the analysis to be simple such as in the cases presented in this study or as complicated as the theory section describes. The real challenge is to account for all uncertainty around the input parameters as some of it will either be based on historical data or engineering judgements and assumptions. A more complex model does not necessarily lead to more accurate predictions. As the number of input variables goes up in the advanced models, the room for input data error increases. Also, the level of user understanding must increase to make proper use of the model.

Despite the shortcomings of the ALOHA® program, it is a powerful and useful tool for utilities that do have access to some of the models mentioned in Table 6.1. Furthermore, it may also be used as a basis for notifying nearby residents to take the necessary safety precautions to ensure their own safety and that of their properties.

In this study, a conservative approach to assessing the effects of thermal radiation explosion were followed. A guillotine break of a natural gas pipeline near a nuclear power plant was postulated as the initiating event. Again, ALOHA®, as well as the point source method, was used for this assessment. Even though many of the assumptions in this study were conservative, the results show that the risk associated with the gas pipeline break is very low. It was found that the control room will not experience an overpressure from any source to the point where sever damage is expected. Still, any entrance or exit roads in the vicinity of the jet fire could be affected, which could ultimately have an adverse effect on emergency evacuation or restrict authorities from entering the site. Finally, for there to be risk, people must be present within the harmful range (consequences distance) of the fire or explosion. How close the people are will determine whether any injuries or fatalities result.

Based on the IDHL exposure limits for ammonia and chlorine and the toxic equations incorporated in the ALOHA® software, the consequences modelling dispersion results shows that ammonia and chlorine gases disperses to large distances with significant levels of toxic concentrations before the process of dilution to a less harmful concentration. Thus, control room operators and emergency personal onsite will be subjected to high concentration of both ammonia and chlorine. Sensitivity analysis should be carried out on the study to identify the impacts of atmospheric conditions on both ammonia and chlorine gas dispersions.

The basic conclusion is that the application of dispersion models for consequences analysis will be useful for taking appropriate measures to reduce any material/human loss due to accidental release. The final risk can then be determined by multiplying these consequences by the frequencies of the accidents over time. In essence, it is defined as a quantitative risk analysis, which is a powerful approach to help improve safety in the nuclear industry.

6.2 RECOMMENDATIONS

The following recommendations should be considered by nuclear utilities and in future dispersion studies:

- It may be useful to compile and tabulate the inventory and application of each chemical substance stored and transported regularly on or to nuclear power plants. Compiling such an inventory was not undertaken in this study, as each nuclear power plant should be reviewed on a case-by-case basis.
    - ∗ 10 CFR 50.34 from the US NRC requires that “changes” to the licensing basis of the plant be evaluated. These changes include any change in hazardous chemicals inventory. South African and European plants have periodic safety reviews (National Nuclear Regulator, 2001). These should be mandated to reconsider the changes in inventory of toxic materials and flammable gases since the last review or since establishing the plant’s license basis. If the licensing basis is satisfactory, one can assure a safe condition by looking at plant changes.
- In real accidents, responders rarely have all the necessary information required to run a gas dispersion model. Reasonable assumptions must be made. One of the significant unknowns is the release rate to the atmosphere. Sensitivity analysis should be carried out in future studies to determine the impact of various atmospheric conditions on toxic gas dispersions.
- Particle chemical release prevention is the more desirable release mitigation, especially in the case of induced releases as efforts by station personnel to mitigate the other effects of the initiating hazard could be seriously hampered. However, as it is not possible to identify all potential sources of chemical release, a mitigation response strategy is also considered important.
- To prevent the compounding complication of a toxic chemical release being induced by an external hazard, it is considered prudent to make all efforts to prevent a large induced chemical spill. This could be achieved by limiting or ensuring adequate resilience of the chemical storage facilities against external hazards, such as earthquakes, flooding, tornadoes and extreme winds.
- It can be concluded that a PSA could better serve the optimisation of safety improvements from an as-low-as-reasonably achievable perspective. The PSA should screen the core damage frequency risk due to chemical releases, using the PSA screening criteria. If necessary, the PSA should be expanded to include a chemical release model. The PSA can then be used as a notification model to the local council or municipality in the event of a toxic chemical release or spill that occurs within the risk radius of the nuclear site.
- The HABIT code is generally available from the US NRC but only to utilities in the USA. It is, therefore recommended, that the NNR enquire from the US NRC whether a copy of the code could be made available to them.

- Plant procedures typically address beyond-design-basis accidents. If the release of a toxic gas is a beyond-design-basis accident, it is appropriate that a more in-depth analysis be performed, taking credit for existing preventive and mitigative measures. If the consequence of an accident is still unacceptable, the implementation of additional measures should be considered.
- Emergency response procedures should address these types of accidents. One peripheral benefit of this would be that, to prepare a procedure, one would have to address the consequences of the accident and the measures in place to prevent or mitigate the accident.

To conclude, although this study is conservative, its findings would suggest that future research should attempt to include sensitivity analysis and QRAs. The goal of the sensitivity analysis and QRAs is to assess the risk and the influence of the variability of parameters on concentration results.

The findings from the PSA and QRA could assist by clarifying the following:

- The design basis assumptions will not be significant challenged;
- Procedures for mitigating the consequences of hazards such as chemical release need to be improved;
- Equipment qualification needs to be reassessed;
- Modifications are required to improve mitigation of the consequences of hazards, for example, seismic resilience storage tanks;
- Additional monitoring for toxic gases; and
- Updates of the final safety analysis report are necessary.

CHAPTER 7 : BIBLIOGRAPHY

[1] American Industrial Hygiene Association. 1991. *Emergency response planning guidelines*. https://www.aiha.org/get-involved/aiha-guideline-foundation/erpgs. Accessed 14 June 2020.

[2] Belke, J.C. 2001. Chemical accident risks in U.S. industry—A preliminary analysis of accident risk data from US hazardous chemical facilities. In: Pasman, H.J., Fredholm, O. & Jacobsson, A., eds. *Proceedings of the 10th International Symposium on Loss Prevention and Safety Promotion in the Process Industries*, Stockholm, Sweden. pp. 1275-1314.

[3] Britter R.E. & McQuaid, J. 1988. *Workshop on the dispersion of dense gases. HSE contract report 17/1988*. https://www.hse.gov.uk/research/crr_pdf/1988/crr88017.pdf. Accessed 7 June 2020.

[4] Branscomb, L.M., Fagan, M., Auerswald, P., Ellis, R. N., & Barcham, R. 2010. *Rail transportation of toxic inhalation hazards. Regulatory Policy Program Working Paper: RPP-2010-01*. https://www.hks.harvard.edu/sites/default/files/centers/taubman/files/Fagan_UTC20_working_paper_2010.pdf. Accessed 19 March 2020.

[5] Burger, L.W. 2016. *Quantitative Risk Assessment of the proposed Ibhubesi Gas Project*. Report No. R/15/SE-01 Rev 0.3. https://sahris.sahra.org.za/sites/default/files/additionaldocs/Appendix%2014%20-%20Risk.pdf. Accessed 20 June 2020.

[6] Cameo Chemicals. n.d. *Cameo chemicals*. https://cameochemicals.noaa.gov. Accessed 20 June 2020.

[7] Casal, J. 2008. *Evaluation of the effects and consequences of major accidents in industrial plants*. 2nd ed. Amsterdam: Elsevier.

[8] Center for Chemical Process Safety. 1994. *Guidelines for evaluating the characteristics of vapor cloud explosions, flash fires, and bleves*. New York: American Institute of Chemical Engineers.

[9] Center for Chemical Process Safety. 1995. *Guidelines for consequences analysis of chemical releases*. New York: American Institute of Chemical Engineers.

[10] Center for Chemical Process Safety. 1996. *Guidelines for evaluating process plant buildings for external explosions and fires*. New York: American Institute of Chemical Engineers.

[11] Chang, Y.S., & Samsa, M.E. 2007. *Probabilistic Consequences Model of accidental chemical release*, US Department of Energy.

https://publications.anl.gov/anlpubs/2008/61981.pdf. Accessed 19 July 2020.

[12] Crowl, D.A., & Louvar, J.F. 2011. *Chemical Process Safety: Fundamentals with applications*. 3rd ed. New York: Prentice Hall.

[13] Dai, W. 2004. *Applying proper dispersion models for industrial accident releases*. Dallas, Texas: Trinity Consultants.

[14] Department of Labour (South Africa). 2001. Occupational Health and Safety Act, 1993: Major mazard installation regulations (Notice 22506). *Government Gazette*, 7122: 433, 30 July 2001.

[15] Ermak, D.L. 1990. *User's manual for SLAB: An atmospheric dispersion model for denser-than-air releases*. California: Lawrence Livermore National Laboratory.

[16] Federal Agency for Nuclear Control. 2012. *National progress report on the stress tests of nuclear power plants*.

[17] Havens, J., & Spicer, T. 1989. *User's guide for the DEGADIS 2.1 dense gas dispersion model*. N.C: U.S. Environmental Protection Agency.

[18] Health Partners. n.d. Health Partners. http://www.healthpartners.com. Accessed 01 July 2020.

[19] International Atomic Energy Agency (IAEA). 1989. *On-site habitability in the event of an accident at a nuclear facility*. Vienna: International Atomic Energy Agency.

https://gnssn.iaea.org/Superseded%20Safety%20Standards/Safety_Series_098_1989_Pub812e_web.pdf. Accessed 12 February 2020.

[20] Jones, R., Lehr, W., Simecek-Beatty, D., & Reynolds, R. M. 1989. *ALOHA® (Areal Locations of Hazardous Atmospheres) 5.4.4 Technical documentation*. Seattle, Washington: Department of Commerce, NOAA, National Ocean Service, Office of Response and Restoration.

[21] Khan, F. I., & Abbasi, S. A. 1999. The world's worst industry accident of 1990s what happened and what might have been: A quantitative study. *Process Safety Progress*, 18(3), 135-145.

[22] Kimura, C.Y, & Budnitz, R.J. 1987. Evaluation of external hazards to nuclear power plants in the United States. Livermore CA: Lawrence Livermore National Laboratory.

[23] Kleindorfer, P. R., Belke, J. C., Elliott, M. R., & Lee, K., Lowe, R.A., & Fieldman, H.I. 2003. Accident epidemiology and the US chemical industry: accident history and worst-case data from RMP*info. *Risk Analysis*, 23(5), 865-881.

[24] Konersmann, R., Christiane. K., & Ludwig, J. 2009. *On the risks of transporting liquid and gaseous fuels in pipelines*. Berlin: BMA Federal Institute for Materials Research and Testing.

[25] Lobo, A.G. 2016. Estimations of toxic vapour concentrations, by atmospheric dispersion calculations, in a nuclear power plant control room, following an offsite accidental release in the frame of probabilistic safety assessment. https://upcommons.upc.edu/bitstream/handle/2117/102001/Main_Report_AGL.pdf. Accessed 12 April 2020.

[26] Madhusoodan, O., & Dhiman, A. K. 2010. Problem failure and safety analysis of ammonia plant: A review. *International Review of Chemical Engineering*, 2(6), 631-646.

[27] Mannan, S. 2004. *Lee's loss prevention in process industries: Hazard identification, assessment and control, Volume 3*. 3rd ed. Oxford: Butterworth-Heinemann.

[28] Nilsson K. 2009. *Preliminary analysis of the natural gas delivery pipeline between Young and Bomen NSW*. Document Number: APAGRO\08-B196. Revision B.

[29] Nuclear Regulatory Commission. 2001. Evaluating the habitability of a nuclear power plant control room during a postulated hazardous chemical release. RG-1.78. https://www.nrc.gov/docs/ML0131/ML013100014.pdf. Accessed 22 March 2020.

[30] Nuclear Regulatory Commission. 2003. Demonstrating control room envelope integrity at nuclear power reactors. RG-1.197. https://www.nrc.gov/docs/ML0314/ML031490664.pdf. Accessed 19 July 2020.

[31] National Nuclear Regulator. 2019. *Interim Regulatory Guide: Periodic safety review of nuclear power plants RG-0028*. https://nnr.co.za/wp-content/uploads/2020/10/RG-0028-Interim-Guide_final_red-block-1.pdf. Accessed 07 June 2020.

[32] National Transport Safety Board (NTSB). 2003. *Pipeline accident report: Natural gas pipeline rupture and fire near Carlsbad, New Mexico*. https://www.ntsb.gov/investigations/AccidentReports/Reports/PAR0301.pdf. Accessed 14 April 2020.

[33] NIOSH. 1994. *NIOSH pocket guide to chemicals hazards*. Washington DC: US Department of Health and Human Services.

[34] NSC (US). 1996. Areal location of hazardous atmospheres (ALOHA) user's manual. Washington DC: National Safety Council.

[35] Nuclear Energy Institute (NEI). 2001. *NEI 99-03 Control room habitability assessment guidance*. https://www.nrc.gov/docs/ML0206/ML020600236.pdf. Accessed 20 June 2020.

[36] Office of Response and Restoration, 2013.

https://response.restoration.noaa.gov/oil-and-chemical-spills/chemical-spills/resources/thermal-radiation-levels-concern.html. Accessed 04 February 2023.

[37] Ramsdell. J.V., & Simonen, C.A. 1997. Atmospheric relative concentrations in building wakes. Richland: Pacific Northwest National Laboratory.

[38] Ramsdell, J.V., & Stage, S. A. 1998. *Computer codes for evaluation of control room habitability (HABIT V1.1)*. Richland: Pacific Northwest National Laboratory.

[39] Schleder, A.M. 2015. Quantitative dispersion analysis of leakage of flammable and /or toxic substance on environments with barriers or semi-confined. https://upcommons.upc.edu/bitstream/handle/2117/95767/TAMS1de1.pdf?sequence=1&isAllowed=y. Accessed 21 April 2020.

[40] Shunxiang, H., Feng, L., Qingcun, Z., Fei, H., Jiang, Z. & Zifa, W. 2015. Modeling and optimal control of atmospheric pollution hazard in nuclear and chemical disasters. *Procedia IUTAM*, 17, 79-90.

[41] Simmons, J. A., Erdmann, R. C., & Naft, B. N. 1974. *Risk of catastrophic spills of toxic chemicals*. Los Angeles: School of Engineering and Applied Science, California University (Technical report).

[42] Tseng, J. M., Su, T. S., & Kuo, C. Y. 2012. Consequences evaluation of toxic chemical release by ALOHA. *Procedia Engineering*, 45, 384-389.

[43] Uijt de Haag, P. A. M., & Ale, B. J. M. 1999. *Guidelines for quantitative risk assessment (Purple book)*. Delft: PGS.

[44] U.S. Atomic Energy Commission (AEC). 1974. *Regulatory Guide 1.78 Assumptions for evaluating the habitability of a nuclear power plant control room during a postulated hazardous chemical release*. https://www.nrc.gov/docs/ML0037/ML003740298.pdf. Accessed 08 August 2020.

[45] U.S. Environmental Protection Agency (EPA). 1996. Accidental release prevention requirements: Risk management programs under Clean Air Act section 112(r)(7). *Federal Register*, 61(120), 31668-31730.

[46] U.S. Environmental Protection Agency (EPA). 2009. *Risk management program guidance for offsite consequence analysis*. https://www.epa.gov/sites/default/files/2013-11/documents/oca-chps.pdf. Accessed 21 August 2020.

[47] U.S. Environmental Protection Agency (EPA). 2019a. *Air quality dispersion modelling - Alternative models*. https://www.epa.gov/scram/air-quality-dispersion-modeling-alternative-models. Accessed 30 July 2020.

[48] U.S. Environmental Protection Agency (EPA). 2019b. *Emergency response*. https://www.epa.gov/emergency-response. Accessed 30 July 2020.

[49] U.S. Environmental Protection Agency (EPA). 2019c. *Chemicals under the Toxic Substances Control Act (TSCA)*. https://www.epa.gov/chemicals-under-tsca. Accessed 30 July 2020.

[50] U.S. Environment Protection Agency (EPA). 2019d. *Computer-aided management of emergency operations (CAMEO)*. https://www.epa.gov/cameo. Accessed 30 July 2020.

[51] U.S. Nuclear Regulatory Commission (NRC). 1977. *Regulatory Guide 1.95 Protection of nuclear power plant control room operators against an accidental chlorine release*. https://www.nrc.gov/docs/ML0037/ML003740310.pdf. Accessed 20 August 2020.

[52] U.S. Nuclear Regulatory Commission (NRC). 1983. *Information notice no. 83-62: Failure of redundant toxic gas detectors positioned at control room ventilation air intakes*. https://www.nrc.gov/reading-rm/doc-collections/gen-comm/info-notices/1983/in83062.html. Accessed 24 August 2020.

[53] U.S. Nuclear Regulatory Commission (NRC). 2013. *Regulatory guide 1.91 Evaluations of explosions postulated to occur at nearby facilities and on transportation routes near*

nuclear power plants. https://www.nrc.gov/docs/ML1217/ML12170A980.pdf. Accessed 18 April 2020.

[54] Van den Bosch, C. J. H., & Weterings, R.A.P.M., eds. 1997. *Methods for the calculation of physical effects (Yellow book)*. 3rd ed. Delft: PGS.

[55] Wing, J. 1979. *NUREG-0570 Toxic vapour concentrations in the control room following a postulated accidental release*. Washington DC: Nuclear Regulatory Commission.

[56] Peter, S., & Winokur, P. 2011. *Review of the hazards and controls associated with anhydrous ammonia system*. Washington DC: Defense Nuclear Facilities Safety Board.

[57] Wheatley, S, Sovacool, B.K., & Sornette, D. 2016. *Reassessing the safety of nuclear power*. Energy Research & Social Science. Elsevier. https://ethz.ch/content/dam/ethz/special-interest/mtec/chair-of-entrepreneurial-risks-dam/documents/publications/elsevier.pdf. Accessed 04 July 2019.

APPENDIX A
CHEMICAL THRESHOLD QUANTITY
(LISTED UNDER THE US RISK MANAGEMENT PLAN)

UNO ID No.	Substance	Threshold Quantity (tons)
1001	Acetylene (dissolved)	2
1005	Ammonia	20
1010	Butadiene	25
1031	Carbon disulphide	20
1017	Chlorine	10
1154	Diethylamine	20
1155	Diethyl ether	20
1033	Dimethyl ether	20
1032	Dimethylamine (anhydrous)	20
1160	Dimethylamine (solution)	20
1035	Ethane (compressed)	15
1961	Ethane (refrigerated liquid)	15
1962	Ethylene (compressed)	15
1038	Ethylene (refrigerated liquid)	15
1036	Ethylamine	25
1040	Ethylene oxide	5
1050	Hydrogen chloride (anhydrous)	10
1051	Hydrogen cyanide (anhydrous)	10
1052	Hydrogen fluoride (anhydrous)	10
1969	ISO – Butane	25
1055	ISO –Butylene (Isobutene)	25
1075	LPG (liquid petroleum gas)	25
1971	Methane (compressed)	15
1011	n-Butane	25
1012	n-Butylene (butene)	25
1076	Phosgene	2
1978	Propane	25
1077	Propylene	25
1079	Sulphur dioxide (liquefied)	15
1829	Sulphur trioxide (liquefied)	15
1083	Trimethylamine (anhydrous)	25
1086	Vinyl chloride	25

APPENDIX B
HEALTH HAZARDS CHARACTERISTICS OF AMMONIA

A.7 IDENTIFICATION

Chemical name: Ammonia

Synonyms: Ammonia gas, anhydrous ammonia

Molecular formula: NH_3

A.8 CHEMICAL AND PHYSICAL PROPERTIES

Physical state and Appearance: Colourless gas

Odour description: Sharp, irritating, pungent

Molecular weight: 17

Conversion factors: 1 mg/m^3 – 1.44 ppm

Vapour density: 0.59 relative to air

Reactivity: Forms ammonium hydroxide on contact with water

Solubility in water: Extremely soluble

Toxicity inhalation-rat LC_{L0} = 2 000 ppm/4 h

A.9 CURRENT EXPOSURE GUIDELINES

IDHL = 300 ppm

NRC-2 min = 100 ppm

Recommended Two-Minutes Exposure Limit = 300 ppm

A.10 GENERAL BIOLOGICAL PROPERTIES

Ammonia is a potentially hazardous substance, although it occurs naturally as a result of many biological processes. It can produce acute effects on humans and animals. Ammonia has strong alkaline and hygroscopic properties that cause irritation or corrosion to damp tissue surfaces such as the eyes, the respiratory system, and the skin. Ammonia has a pungent odour; the odour threshold of ammonia is in the region of 5 ppm. Concentrations between 20 and 50 ppm are detectable by most people. Its pungent odour provides an adequate warning of its presence well below the hazardous concentration levels.

Gaseous ammonia affects the mucous membranes and the respiratory tract and severely irritates the eyes. Inhaling high concentrations may cause pulmonary oedema. High gas concentrations in the air may also cause blisters and chemical burns on the skin. The effects of exposure to various vapour concentrations are summarised in Table C.1.

Table C.1: Effect of exposure to ammonia (NIOSH, 1994)

Vapour Concentration (ppm)	General Effect	Exposure Period
5	Odour detectable by some people.	–
25	–	Occupational exposure standard long-term, 8 hours.
35		Occupational exposure short-term, 15 minutes.
50-100	Irritation detectable by most people.	Tolerable for people unaccustomed to exposure for up to 2 hours. People accustomed to exposure can tolerate higher concentration over the same period.
400-700	Immediate eye, nose, and throat irritation.	30-minute to 1-hour exposure causes no serious damage although upper respiratory tract irritation may persist for 24 hours following a 30-minute exposure. Aggravation of existing respiratory problems could occur.
1000-2000	Severe coughing, severe eye, nose, and throat irritation.	Damage to eyes and respiratory system could result in death in minutes if not treated quickly. 30-minute exposure could produce severe effects in people predisposed to severe respiratory problems.
3000-4000	Severe coughing, severe eye, nose, and throat irritation.	Could be fatal within 30 minutes. Estimated LC_{50} (derived from animal data) for 2-hour exposure in this region.
5000-12000	Respiratory spasm. Rapid asphyxia.	Fatal within minutes. Estimated LC_{50} (derived from animal data) for 30-minute exposure in this region.

APPENDIX C
HEALTH HAZARDS CHARACTERISTICS OF CHLORINE

A.11 IDENTIFICATION OF CHLORINE

Chemical name:	Chlorine
Molecular formula:	Cl_2

A.12 CHEMICAL AND PHYSICAL PROPERTIES

Physical state and Appearance:	Yellowish gas
Odour description:	Irritating and pungent (bleach)
Molecular weight:	70.91
Conversion factors:	1 mg/m^3 – 0.3 ppm
Vapour density:	2.5 relative to air
Reactivity:	Highly oxidising
Solubility in water:	5.7 g/ℓ at 300°C
Toxicity: inhalation-rats LC50 – (1 h)	= 293 ppm

A.13 CURRENT EXPOSURE GUIDELINES

IDHL	= 25 ppm
NRC-2 min	= 15 ppm
Recommended two-minute exposure limit	= 30 ppm

A.14 GENERAL BIOLOGICAL PROPERTIES

Because chlorine has many applications, much data exists on its health effects (Table D.1 below). Chlorine exposure occurs through inhalation or skin or eye contact. Inhalation irritates the mucous membranes of the nose, throat, and lungs. Direct skin contact with gaseous or liquid chlorine may result in chemical burns.

Table D.1: Health effects of chlorine inhalation (NIOSH, 1994)

Concentration (ppm)	Health Effects
1–3	Mild mucous membrane irritation
5–15	Moderate irritation of upper respiratory tract
30	Immediate chest pain, vomiting, and coughing
40–60	Toxic pneumonitis and pulmonary oedema
430	Death within 30 minutes
1000	Death within a few minutes

APPENDIX D
CHLORINE WORST CASE SCENARIO (WCS)

A.15 SITE DATA

Location:	CAPE TOWN, SOUTH AFRICA
Building air exchanges per hour:	0.50 (enclosed office)
Time:	11 October 2019 18:47 hours ST (using computer’s clock)

A.16 CHEMICAL DATA

Chemical name:	CHLORINE
CAS number: 7782-50-5	Molecular Weight: 70.91 g/mol
AEGL-1 (60 min):	0.5 ppm
AEGL-2 (60 min):	2 ppm
AEGL-3 (60 min):	20 ppm
IDLH:	10 ppm
Ambient boiling point:	-34.0°C
Vapour pressure at ambient temperature:	Greater than 1 atm.
Ambient saturation concentration:	1 000 000 ppm or 100.0%

A.17 ATMOSPHERIC DATA (MANUAL INPUT OF DATA)

Wind:	1.5 metres/second from NE at 6 metres
Ground roughness:	100 centimetres
Cloud cover:	5 tenths
Air temperature:	29°C
Stability class:	F
No inversion height	Relative humidity: 48%

A.18 SOURCE STRENGTH

Direct source:	0.15 kilograms/sec
Source height:	0
Release duration:	10 minutes

Release rate: 9 kilogram/min

Total amount released: 90.0 kilograms

Note: This chemical may flash boil or result in two-phase flow.

A.19 THREAT ZONE

Model run: **Heavy Gas**

Red: 323 metres (50 ppm)

Orange: 2.1 kilometres (2.8 ppm)

Yellow: 4.9 kilometres (0.5 ppm)

A.20 THREAT AT POINT

Concentration estimates at the point:

Downwind: 100 metres control room distance

Max. concentration: outdoor: 313 ppm

Max. concentration indoor: 24.7 ppm

APPENDIX E
ALOHA® RESULTS FOR AMMONIA (WCS)

A.21 SITE DATA

Location: CAPE TOWN, SOUTH AFRICA

Building air exchanges per hour: 0.50 (enclosed office)

Time: 11 October 2019, 19:00 hours ST (using computer’s clock)

A.22 CHEMICAL DATA

Chemical name: AQUEOUS AMMONIA

Solution strength: 25% (by weight)

Ambient boiling point: 36.4°C

Partial pressure at ambient temperature: 0.72 atm

Ambient saturation concentration: 716,275 ppm or 71.6%

Hazardous component: AMMONIA

CAS number: 7664-41-7 Molecular Weight: 17.03 g/mol

AEGL-1 (60 min): 30 ppm AEGL-2 (60 min): 160 ppm AEGL-3 (60 min): 1 100 ppm

IDLH: 300 ppm LEL: 150 000 ppm UEL: 280 000 ppm

A.23 ATMOSPHERIC DATA: (MANUAL INPUT OF DATA)

Wind: 1.5 metres/second from NE at 6 metres

Ground roughness: 100 centimetres Cloud Cover: 5 tenths

Air temperature: 29°C Stability Class: F

No inversion height relative humidity: 48%

A.24 SOURCE STRENGTH

Evaporating puddle (Note: The chemical is flammable.)

Puddle area: 40 square metres

Puddle Volume: 6 000 gallons (22 712 litres)

Ground type: Concrete ground temperature: 29°C

Initial puddle temperature: Ground temperature

Release duration: ALOHA® limited the duration to 1 hour

Max average sustained release rate: 9.99 kilograms/min (averaged over a minute or more)

Total amount hazardous component released: 417 kilograms

A.25 THREAT ZONE

Model Run: **Gaussian**

- Red: 154 metres (1 100 ppm = AEGL-3 [60 min])
- Orange: 456 metres (160 ppm = AEGL-2 [60 min])
- Yellow: 1.2 kilometres (30 ppm = AEGL-1 [60 min])

A.26 THREAT AT POINT

Concentration estimates at the point:

- Downwind: 100 metres control room distance

Max. concentration:

- Outdoor: 2 260 ppm
- Indoor: 592 ppm

APPENDIX F
ALOHA® RESULTS FOR METHANE (WCS)

A.27 ITE DATA

Location: CAPE TOWN, SOUTH AFRICA

Building air exchanges per hour: 0.50 (enclosed office)

Time: 11 October 2019; 19:26 hours ST (using computer's clock)

A.28 CHEMICAL DATA

Chemical name: METHANE

CAS number: 74-82-8 Molecular Weight: 16.04 g/mol

PAC-1: 65 000 ppm PAC-2: 230 000 ppm PAC-3: 400 000 ppm

LEL: 50 000 ppm UEL: 150 000 ppm

Ambient boiling point: -161.5°C

Vapour pressure at ambient temperature: greater than 1 atm

Ambient saturation concentration: 1 000 000 ppm or 100.0%

A.29 ATMOSPHERIC DATA (MANUAL INPUT OF DATA)

Wind: 1.5 metres/second from NE at 6 metres

Ground roughness: 100 centimetres Cloud Cover: 5 tenths

Air temperature: 29°C Stability Class: F

No inversion height relative humidity: 48%

A.30 SOURCE STRENGTH

Flammable gas is burning as it escapes from pipe

Pipe diameter: 30-inch pipe length: 1 000 metres

Unbroken end of the pipe is closed off.

- Pipe roughness: smooth hole area: 707 sq in
- Pipe press: 257 atmospheres
- Pipe temperature: 29°C
- Max flame length: 88 metres

Burn duration: 1 minute

Max burn rate: 1 180 000 kilograms/min

Total amount burned: 75 543 kilograms

A.31 THREAT ZONE (GAUSSIAN SELECTED)

Model run: Gaussian

Red: 1.0 kilometres (50 000 ppm)

A.32 THREAT AT POINT

Concentration estimates at the point:

Max. concentration:

Threat zone:

Downwind: 1 000 metres control room distance

Outdoor: 55 200 ppm

Indoor: 2 650 ppm

Threat modelled: Thermal radiation from jet fire

Red: 324 metres (10.0 kW/(sq m) = potentially lethal within 60 sec)

Orange: 452 metres (5.0 kW/(sq m) = 2nd degree burns within 60 sec)

Yellow: 700 metres (2.0 kW/(sq m) = pain within 60 sec)

A.33 THREAT ZONE (GAUSSIAN SELECTED)

Threat modelled: Flammable area of vapour cloud

Model run: Gaussian

Red: 1.7 kilometres (30 000 ppm = 60% LEL = flame pockets)

Yellow: 3.4 kilometres (5 000 ppm = 10% LEL)

A.34 THREAT ZONE (GAUSSIAN SELECTED)

Threat modelled: Overpressure (blast force) from vapour cloud explosion

Type of ignition: Ignited by spark or flame

Level of congestion: Uncongested

Model run: Gaussian

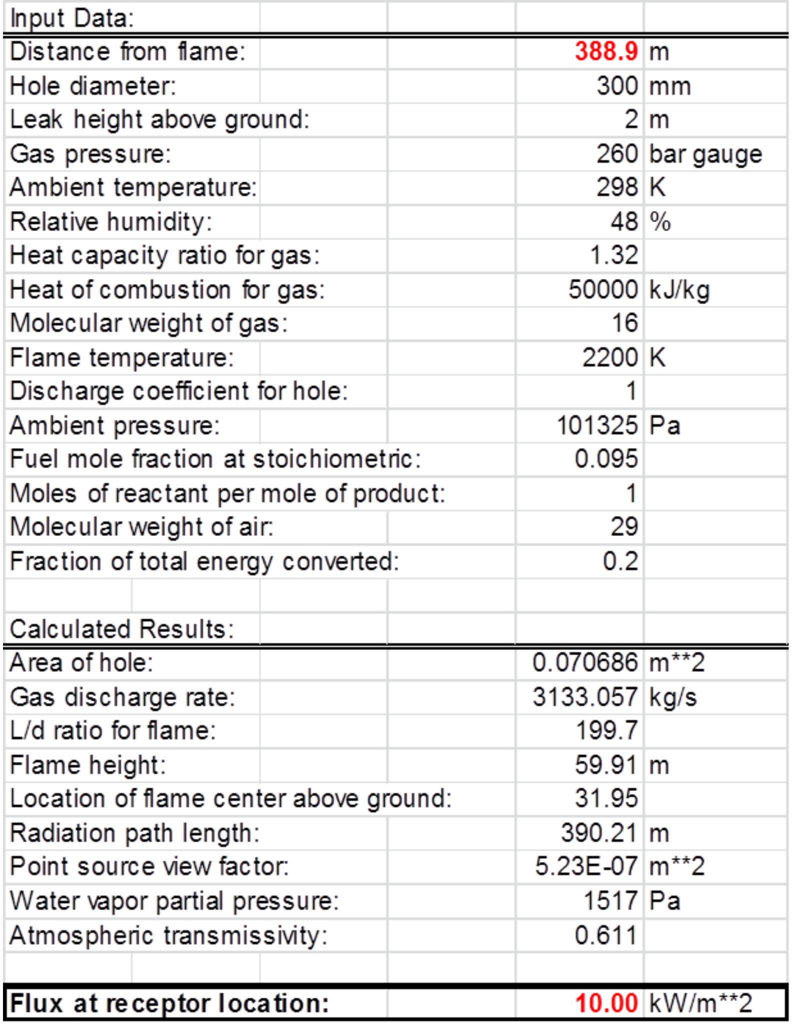
Red: LOC was never exceeded (8 000 pascal)

Orange: LOC was never exceeded (7 000 pascal)

Yellow: 1.4 kilometres (5 000 pascal)

APPENDIX G
CALCULATED THERMAL RADIATION VALUES FOR METHANE

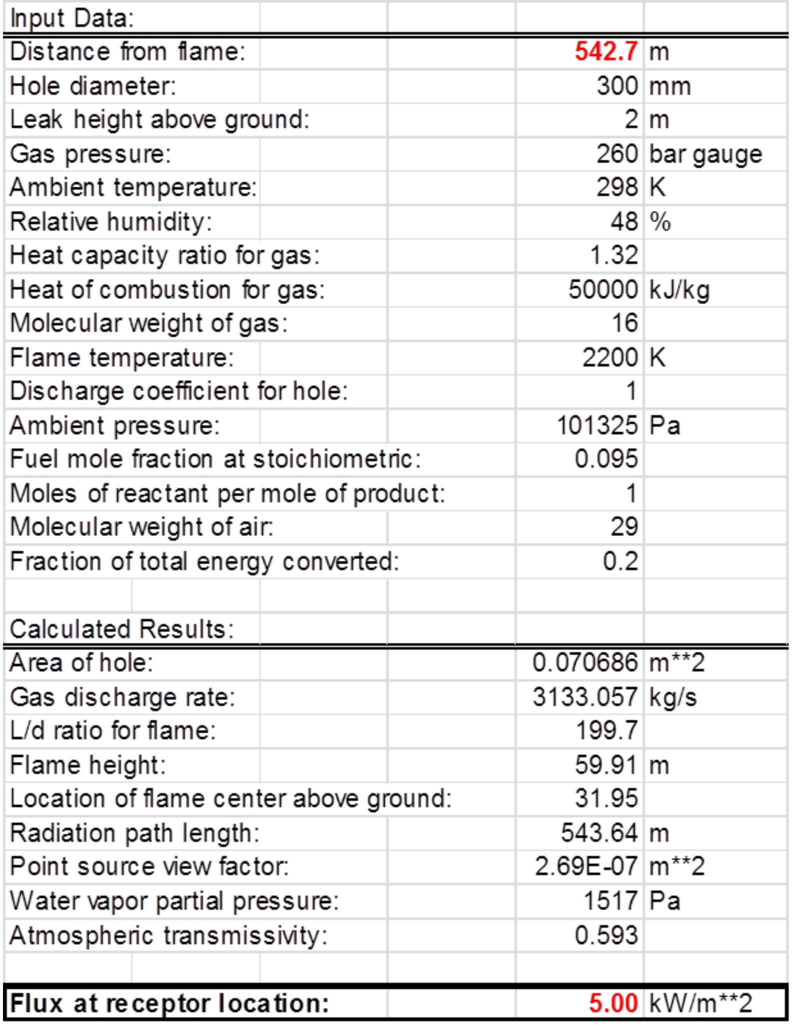
A.35 FOR 10 kW/m^2



Input Data:		
Distance from flame:	388.9	m
Hole diameter:	300	mm
Leak height above ground:	2	m
Gas pressure:	260	bar gauge
Ambient temperature:	298	K
Relative humidity:	48	%
Heat capacity ratio for gas:	1.32	
Heat of combustion for gas:	50000	kJ/kg
Molecular weight of gas:	16	
Flame temperature:	2200	K
Discharge coefficient for hole:	1	
Ambient pressure:	101325	Pa
Fuel mole fraction at stoichiometric:	0.095	
Moles of reactant per mole of product:	1	
Molecular weight of air:	29	
Fraction of total energy converted:	0.2	
Calculated Results:		
Area of hole:	0.070686	m**2
Gas discharge rate:	3133.057	kg/s
L/d ratio for flame:	199.7	
Flame height:	59.91	m
Location of flame center above ground:	31.95	
Radiation path length:	390.21	m
Point source view factor:	5.23E-07	m**2
Water vapor partial pressure:	1517	Pa
Atmospheric transmissivity:	0.611	
Flux at receptor location:	**10.00**	kW/m**2

APPENDIX G
CALCULATED THERMAL RADIATION VALUES FOR METHANE

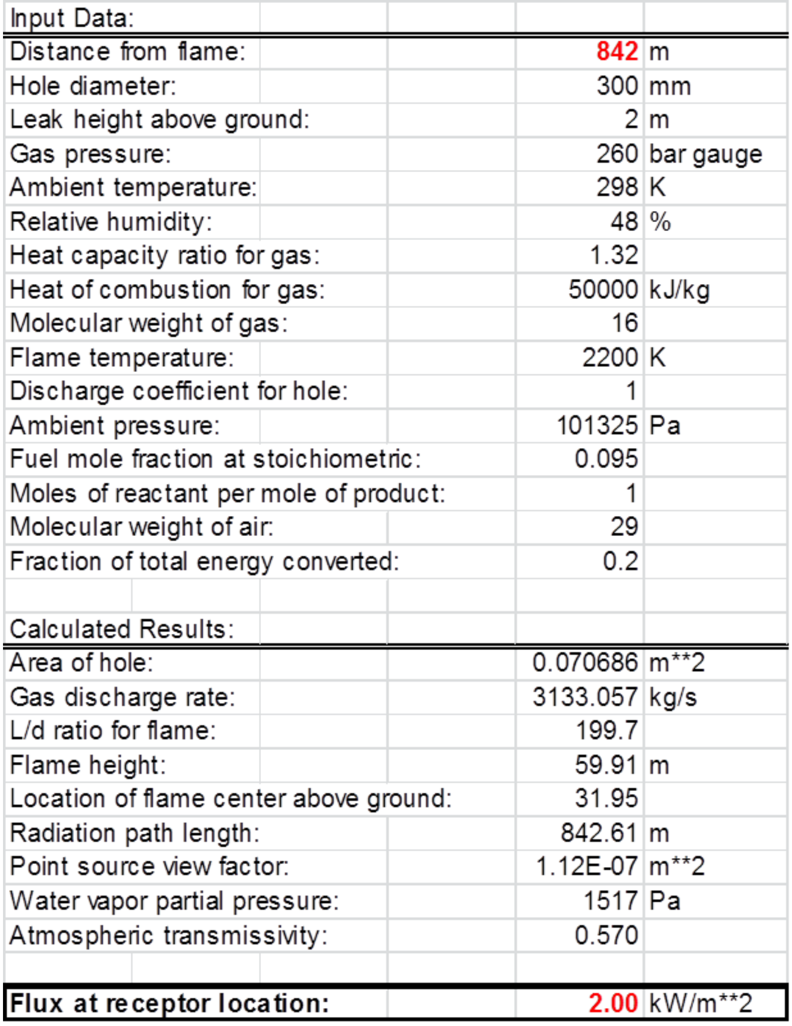
A.36 FOR: 5 kW/m^2



Input Data:		
Distance from flame:	542.7	m
Hole diameter:	300	mm
Leak height above ground:	2	m
Gas pressure:	260	bar gauge
Ambient temperature:	298	K
Relative humidity:	48	%
Heat capacity ratio for gas:	1.32	
Heat of combustion for gas:	50000	kJ/kg
Molecular weight of gas:	16	
Flame temperature:	2200	K
Discharge coefficient for hole:	1	
Ambient pressure:	101325	Pa
Fuel mole fraction at stoichiometric:	0.095	
Moles of reactant per mole of product:	1	
Molecular weight of air:	29	
Fraction of total energy converted:	0.2	
Calculated Results:		
Area of hole:	0.070686	m**2
Gas discharge rate:	3133.057	kg/s
L/d ratio for flame:	199.7	
Flame height:	59.91	m
Location of flame center above ground:	31.95	
Radiation path length:	543.64	m
Point source view factor:	2.69E-07	m**2
Water vapor partial pressure:	1517	Pa
Atmospheric transmissivity:	0.593	
Flux at receptor location:	5.00	kW/m**2

APPENDIX G
CALCULATED THERMAL RADIATION VALUES FOR METHANE

A.37 FOR: 2 kW/m^2



Input Data:		
Distance from flame:	842	m
Hole diameter:	300	mm
Leak height above ground:	2	m
Gas pressure:	260	bar gauge
Ambient temperature:	298	K
Relative humidity:	48	%
Heat capacity ratio for gas:	1.32	
Heat of combustion for gas:	50000	kJ/kg
Molecular weight of gas:	16	
Flame temperature:	2200	K
Discharge coefficient for hole:	1	
Ambient pressure:	101325	Pa
Fuel mole fraction at stoichiometric:	0.095	
Moles of reactant per mole of product:	1	
Molecular weight of air:	29	
Fraction of total energy converted:	0.2	
Calculated Results:		
Area of hole:	0.070686	m**2
Gas discharge rate:	3133.057	kg/s
L/d ratio for flame:	199.7	
Flame height:	59.91	m
Location of flame center above ground:	31.95	
Radiation path length:	842.61	m
Point source view factor:	1.12E-07	m**2
Water vapor partial pressure:	1517	Pa
Atmospheric transmissivity:	0.570	
Flux at receptor location:	**2.00**	kW/m**2

APPENDIX H
3-SAMPLE SLAB INPUT

Chlorine release for release amount of 200 lb and meteorological conditions (release type = two-phase, horizontal jet release; wind direction = north; wind speed = 1.5 m/s; stability class = A)

Line No.	Value	Input Parameter	Input Parameter Description
1	3	IDSPL	Spill source type
2	1	NCALC	Numerical sub-step parameter
3	0.070 906	WMS	Molecular weight of source material (kg)
4	498.1	CPS	Vapour heat capacity at constant pressure (J/kg-K)
5	239.1	TBP	Boiling point temperature (K)
6	0.88	CMEDO	Initial liquid mass fraction
7	287 840.0	DHE	Heat of vaporisation (J/kg)
8	926.3	CPSL	Liquid heat capacity (J/kg-K)
9	1574.0	RHOSL	Liquid density of source material (kg/m^3)
10	1978.34	SPB	SPB saturation pressure constant
11	-27.01	SPC	Saturation pressure constant
12	239.10	TS	Temperature of source material (K)
13	0.15	QS	Mass source rate (kg/s)
14	0.002	AS	Source area (m^2)
15	600.0	TSD	Continuous source duration (s)
16	0.0	QTIS	Instantaneous source mass (kg)
17	1.0	HS	Source height (m)
18	1.0	TAV	Concentration averaging time (s)
19	5 000.0	XFFM	Maximum downwind distance (m)
20	0.0	ZP(1)	1st height of concentration calculation (m)
21	0.0	ZP(2)	2nd height of concentration calculation (m)
22	0.0	ZP(3)	3rd height of concentration calculation (m)
23	0.0	ZP(4)	4th height of concentration calculation (m)
24	1.0	ZO	Surface roughness height (m)
25	10.00	ZA	Ambient measurement height (m)
26	1.50	UA	Ambient wind speed (m/s)
27	302.6	TA	Ambient temperature (K)
28	48	RH	Relative humidity (per cent)
29	6.0	STAB	Stability class values
30	-1.0	TER	Termination indicator

APPENDIX I
SLAB RESULTS FOR CHLORINE

Distance (m)	Downwind concentrations (ppm)
1.04	62300
1.07	48400
1.11	43200
1.15	40200
1.20	38100
1.26	35900
1.33	33800
1.42	31600
1.53	29400
1.65	27000
1.80	24600
1.99	22100
2.20	19600
2.47	17200
2.78	14900
3.16	12800
3.61	11000
4.16	9410
4.82	8090
5.60	6850
6.55	5470
7.69	4490
9.06	3730
10.70	3120
12.70	2610
15.00	2190
17.90	1830
21.30	1530

Distance (m)	Downwind concentrations (ppm)
25.40	1270
30.30	1060
36.30	884
43.40	735
51.90	612
62.20	508
74.50	422
89.40	350
107.00	290
129.00	240
154.00	199
187.00	165
230.00	135
286.00	106
360.00	79.3
456.00	57.5
581.00	40.7
743.00	28.2
951.00	19.3
1220.00	13
1560.00	8.61
2010.00	5.65
2570.00	3.67
3290.00	2.37
4200.00	1.52
5360.00	0.967
6830.00	0.615