STUDY OF THE INFLUENCE OF THE MAIN INPUT PARAMETERS ON TOXIC CONSEQUENCE CALCULATION FOR A FORMALDEHYDE RELEASE

A Thesis

by

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ABSTRACT

Formaldehyde is widely used in the chemical industries as a raw material for resins, plastics, fertilizers, and polymers as a solvent, and a preservative. Due to its high reactivity, and acute toxicity, determining the possible consequences of accidental releases of formaldehyde in industries is critical for safety. Despite that, only limited risk analysis work has been done.

In this work, we simulated the consequences of formaldehyde release for an industrial facility. The simulation were performed for two release scenarios, one of which was the worst-case scenario described in the Risk Management Plan (RMP) regulated by the Environmental Protection Agency (EPA), and the other was defined to account for a more probable situation in the industrial facility. The cloud dispersion of three different mixture of formaldehyde was simulated using PHAST, a software for consequence analysis. The consequences were assessed for different atmospheric conditions, wind velocities and hole diameters.

The results show that, for the worst- case scenario, the largest downwind and crosswind distance is represented by stability class F and wind velocity 1.5 m/s. The behavior of the formaldehyde cloud confirms the positive influence of wind velocity on diluting effect.

The effect of direct influence of wind velocity and hole diameter were simulated for more probable scenarios. Simulations reveal that high wind velocities generally result in shorter impact distances. Except for the class D, where the wind velocity promotes the mass transfer of the liquid in the pool and the dispersion depends on pool dynamics, the downwind and crosswind distances increase when wind velocities are increased from 1.5m/s to 5m/s.

The sensitivity analysis for the effect of hole diameter shows that the size of the hole compared to wind and stability class plays a more significant role on the dispersion of the formaldehyde.

DEDICATION

To my parents: Maria Helena Ramirez and Rafael Amaya for their constant love, support, company and encouragement. They made this possible.

To my sister: Martha Lucia Amaya for her love and for always supporting, helping and standing by my side in good and difficult times. She has colored my life with joy.

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NOMENCLATURE

ATSDR	Agency for Toxic Substances and Disease Registry
CAA	Clean Air Act
CFR	Code of Federal Regulations
DNV	Det Norske Veritas
EPA	Environmental Protection Agency
ERPG	Emergency Response Planning Guidelines
FDA	Food and Drug Administration
IARC	International Agency for Research on Cancer
IDLH	Immediate Damage to Life and Health
MKOPSC	Mary Kay O’Connor Process Safety Center
NAICS	North American Industry Classification System
NIOSH	National Institute for Occupational Safety and Health
OSHA	Occupational Safety and Health Administration
PEL	Permissible Exposure Limit
PHAST	Process Hazard Analysis Software Tool
PSM	Process Safety Management
RMP	Risk Management Plan
STEL	Short-Term Exposure Limit
TWA	Time Weighted Average
UDM	Unified Dispersion Model

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1. INTRODUCTION

1.1 Formaldehyde background

Formaldehyde is a colorless and strongly odorous substance. Commercially it is available as a mixture of water, formaldehyde, and alcohol (methanol). The commercial mixture contains 37% wt formaldehyde. A small percentage of low molecular weight alcohol (7-15%) is used to improve the solubility of the formaldehyde and to avoid polymers precipitation under transportation and storage conditions. However, some industry applications require solutions containing less than or equal to 1% of methanol and should kept warm to prevent formation of polymers [6].

Formaldehyde is a versatile chemical that is used as an intermediate compound in the chemical industries. It is widely used in the production of resins, polymers, adhesives and plastics. It is an organic compound with a terminal carbonyl group that makes its structure unique. It has a high level of reactivity and good thermal stability [8, 9]. Some physical properties of formaldehyde are shown in Table 1.

Table 1 Formaldehyde physical properties

PROPERTY	**FORMALDEHYDE**
Chemical formula	CH_2O
Molecular weight	30.03 g/mol
Melting point	-92 °C
Boiling point @ 1 atm	-19 °C
Lower explosion limit	7 %
Upper explosion limit	73 %

1.2 Production methods

Despite the fact that different methods were used, only two processes are prominently used for formaldehyde production: the metal oxide (formox) and the silver process.

The first process is metal oxide is oxidation of methanol in excess air over a mixture of an iron oxide with molybdenum and vanadium [1]. Methanol and oxygen are reacted in a multitubular reactor with a bed temperature ranging from 300 to 400 °C at atmospheric pressure according to the following reaction [2].

$$2\ CH_3OH + O_2 \rightarrow 2\ CH_2O + 2\ H_2O$$

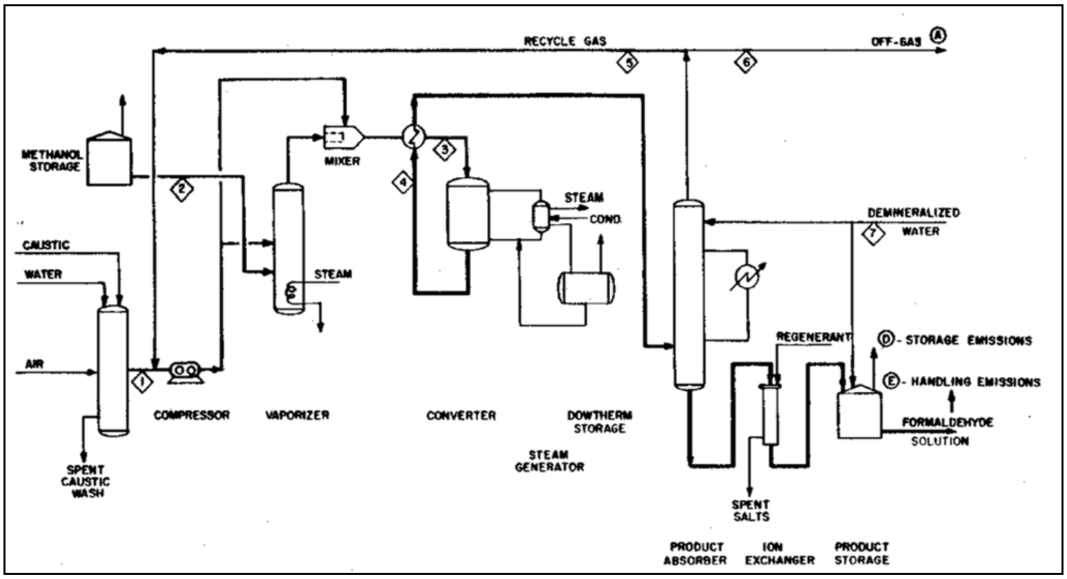

Figure 1 Metal oxide process [3]

The concentration of the formaldehyde in this process is essentially controlled by the quantity of water at the top of the absorption unit. The product stream passes through the ion exchange to decrease formic acid formation. Then the product is sent to storage with a concentration around 50wt% formaldehyde. The overall process yield is estimated between 88 and 91%; however, the methanol conversion is from 98 to 99% [4].

In addition to the high yield, the formox process offers lower temperatures and a longer life for the catalyst compared with the silver-based catalytic method. Also, due to the lower temperatures, fewer by-products are formed, which result in a reduction in the time of residence of the methanol in the whole process, which means a decreasing in risk of fire and explosion[4].

The silver-based process accounts for the significant percentage of the world's capacity, approximately 30 to 50%. The synthesis is performed using silver catalyst in a fixed bed, under lean air conditions. The silver catalyst route is operated at a high temperature between 600 and 700 °C, where two parallel chemical reactions take place to produce formaldehyde. The product becomes a mixture of methanol and air [2]. The first reaction is the methanol oxidation, which is where 50% or more of the formaldehyde is produced. The second reaction is a methanol dehydrogenation.

$$2\ CH_3OH + O_2 \rightarrow 2\ CH_2O + 2\ H_2O$$

$$CH_3OH \rightarrow H_2CO + H_2$$

The key variables of this process are the temperature of the reactor, the water entering with the methanol as a feed of the process and the methanol to oxygen ratio[4]. In terms of advantages of the silver based process, it has stable production conditions, but the plant operates with air deficiencies above the upper explosion limit, which makes this process riskier [1].

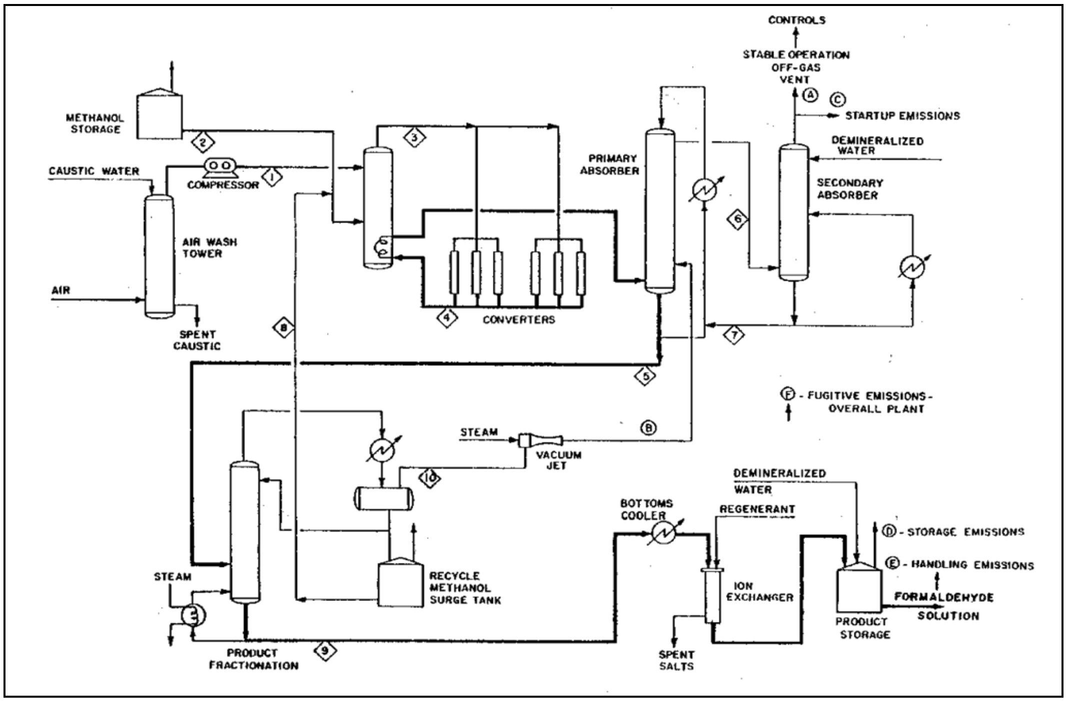

Figure 2 Silver catalyst process [3]

1.3 Potential health hazards

Formaldehyde is considered as an adverse substance for human health. Formaldehyde could affect eyes, skin, respiratory and immune system when an acute or a chronic exposure occurs. The effects of exposure depend on the dose, the duration of exposure, type of exposure, and the presence of other substances [5].

When a release occurs either from a small container or from a large tank, the primary route of exposure is by breathing air containing formaldehyde, which mainly affects the upper respiratory tract. Some of the common symptoms in acute exposure are irritation of the nose, throat, eyes and skin as well as nausea and discomfort. In some cases the exposure could exacerbate symptoms of respiratory illnesses such as asthma [6, 7].

Additionally, allergic contact dermatitis is produced as a result of dermal exposure. These reactions are characterized by redness, rashes, blisters, swelling and dry skin, which can be intensified by humidity, heat and friction. In some cases, allergic contact dermatitis could have an effect on the immune system [8].

In terms of chronic exposure to formaldehyde, various studies have been done since the early 1980's for government agencies and industry entities. These assessments have focused on formaldehyde carcinogenicity potential in humans[9]. Based on epidemiological studies, the International Agency for Research on Cancer (IARC) classifies formaldehyde as a substance carcinogenic to humans and links it to leukemia [7]

1.4 Regulations and exposure

To reduce work exposure for employees and the general public, government agencies have issued a series of standards regulating formaldehyde airborne concentration. The Food and Drug Administration (FDA), the Agency for Toxic Substances and Disease Registry (ATSDR) and the National Institute for Occupational Safety and Health among other agencies have developed regulations and guidelines for toxic substances in which formaldehyde is included [5].

In addition, the Occupational Safety and Health Administration (OSHA) regulates work exposures through the OSHA formaldehyde standard 29 CFR 1910.1048.

The purpose of this standard is to protect employee’s occupational exposure from formaldehyde gas, aqueous solution or any material that releases formaldehyde.

The Occupational Safety and Health Administration (OSHA) has established thresholds for formaldehyde in the workplace. The permissible exposure limit, or PEL, is 0.75ppm. The PEL measure is based on an 8 hours time weighted average exposure (TWA). Moreover, OSHA sets a short-term exposure limit called STEL. The formaldehyde STEL is 2ppm, which is the maximum concentration allowed during a 15 minute period. Finally the action level is 0.5ppm calculated as an 8 hours time weighted average exposure (TWA)[10].

In addition, the National Institute for Occupational Safety and Health (NIOSH) has defined the Immediate Damage to Life and Health (IDLH) as 30ppm, which is the maximum concentration of formaldehyde one could escape in 30 minutes without symptoms or any irreversible health effects.

Furthermore, Environmental Protection Agency (EPA) has the Risk Management Plan for industrial facilities aiming to prevent serious potential damage to human health and environment as well as to mitigate the consequence of those accidents. According to 48 CFR part 68, the threshold quantity for accidental release prevention for formaldehyde is 15,000lb and a toxic endpoint of 0.012 mg/L [11].

Table 2 Occupational exposure limits in US for formaldehyde [7].
(Ca^{d}: substance is carcinogenic, A2b: Suspected human carcinogenic, Sen: sensitizer)

	Concentration [ppm]	**Interpretation**	**Carcinogen Classification**
OSHA	0.75	TWA	Ca^{d}
	2.0	STEL	
NIOSH	0.016	TWA	Ca^{d}
	0.1	Ceiling	
ACGIH	0.3	Ceiling	A2^{b}, Sen

2. OFFSITE CONSEQUENCE ANALYSIS

2.1 Introduction

According to the rule “Chemical Accident Prevention Provision” issued by the U.S. Environmental Protection Agency (EPA) the development, implementation and updating of Risk Management Program (RMP) is required for those facilities that handle, process, manufacture or store flammable and toxic materials in an amount above the threshold quantity for a regulated substance in a process. Being subjected to the rule implies performing an offsite consequence analysis which in turn involves the consideration of the worst-case release scenario and the alternative release scenarios, and the selection of the parameters for modeling a release [11].

2.2 Risk management program

The main objective of the RMP is the prevention and mitigation of releases that can cause injuries to the community and damage to the environment. The program comprises three main parts, the five-year accident records, a study of potential offsite consequences considering a worst-case accidental release, and a prevention program and emergency plan for an accidental release. The Code of Federal Regulations (CFR) in the part 68 covers any facility that process large quantities of hazardous materials above the threshold. The rule also applies to any individual, corporation, state, agency or department belonging to government as well as private business that owns or operates a stationary source[11].

A stationary source is defined under Clean Air Act (CAA) as any equipment, structures, installations, buildings, or substance emitting stationary activities that is owned by the same industrial group, which are located on one or more contiguous properties, which are under control of the same person or persons under common control and from which any accidental release may occur. Nevertheless, if there are multiple operations under the same owner but they are not connected or they are connected by pipelines, those are considered as separate stationary sources. Transportation is not covered by the definition of stationary source; however the concept includes transportation containers used for storage[11].

The CFR in the part 68 of Title 40 lists the substances and amounts established as a threshold in order to determine the applicability of the Risk Management Program (40 CFR 68.130). The list includes 63 flammable substances (gases and volatile liquids) that have the capacity to produce fire and explosions, and 77 toxic chemicals that have the potential to cause health effects or deaths. The rule applies as well to flammable mixtures (above 1 percent concentration) that meet the standard for the National Fire Protection Association (NFPA).

The rule covers any process with a threshold quantity of a regulated substance. A process can be any storage, on-site movement, use or manufacturing activity. The complexity of a process can be as simple as a single storage vessel or as difficult as a system of interconnected vessels. If there is a single vessel connected that contains regulated substance above the threshold quantity, this vessel is considered as the single covered process. If there are more than one vessel connected through piping that in total (tanks, piping and hoses) hold more than a threshold amount of any regulated substance, the whole arrangement is considered as the single covered process; finally, if there are multiple vessels separately located that contain the same regulated substance and they could be involved in a potential release, it is necessary to sum up each quantity, determine if the total amount of the substance exceeds the threshold, and consider that set as a single covered process. The amount of the substance using for threshold comparison is the maximum quantity at any time in each vessel instead of the maximum capacity of the vessel. The approach to identify processes subjected to Part 68 of the CFR is shown in figure 3[11].

Once covered processes are identified it is necessary to define the actions to take in order to comply with the rule. Those actions are outlined in three programs based on the risk and the level of effort necessary to prevent the accident. Each process is eligible for only one program even if a process consists of different operating units where the highest program level is assigned to all parts.

The Program 1 comprises processes that would not affect public receptors when a worst-case release occurs. A worst-case release is understood as the release of the largest amount of a regulated substance from a process that results in the greatest distance to an end point or distance before the vapor cloud, fire or explosion is dissipated and injuries from exposures will not occur. Therefore, public receptors refer to residences, institutions, buildings and recreational areas beyond the property boundaries or with unrestricted access by the public at any time, where individuals are exposed to an accidental release. Furthermore, to be qualified for Program 1 a process must have no accidents for the past five years due to a regulated substance where the exposition, reaction products, overpressure and radiant heat led to offsite injuries, deaths, or response and restoration actions for an environmental area [11].

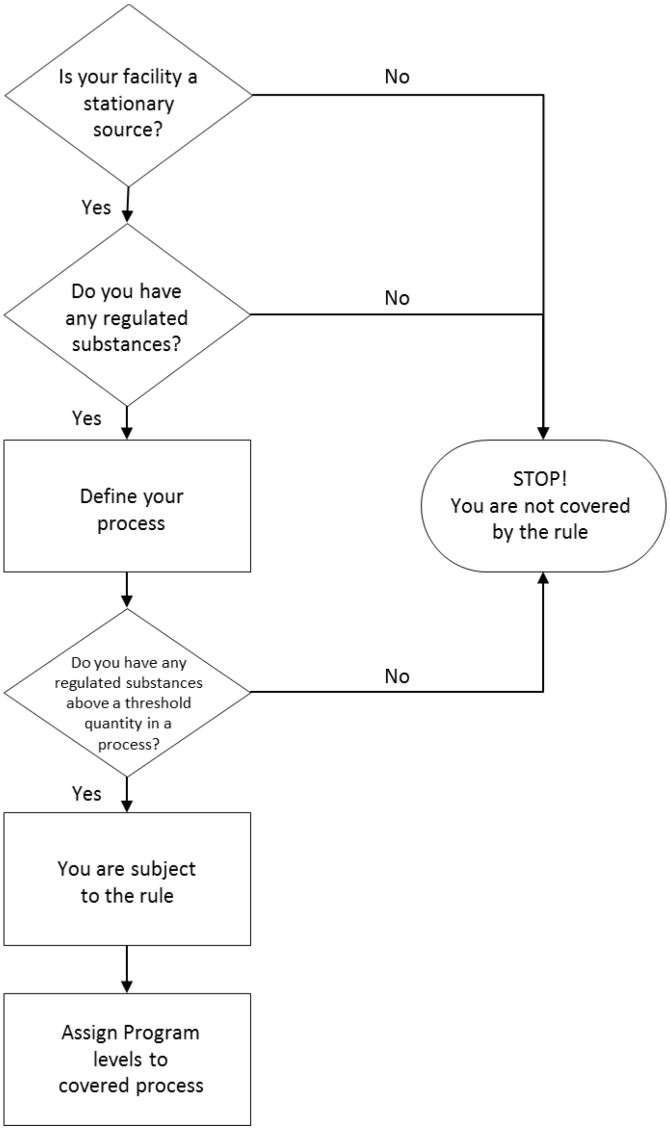

Figure 3 Approach to identify covered processes

A process that is not eligible for Program Level 1 that is subjected to OSHA PSM or belonging to manufacturing NAICS codes, is classified into the Program Level 3. The OSHA Process Safety Management Standard intends to protect the health and safety of the workers in case of accidental releases and covers facilities that have more than a threshold amount of a regulated substance in their processes. On the other hand, NAICS codes represent the activities that have reported a significant number of releases. Finally, the process that is not categorized both in Program Level 1 or 3 is automatically assigned to Program Level 2. The methodology to evaluate the program level and the requirements to develop a RMP according to each program is described in figure 4 [11].

2.3 Five-year accident history

The five-year accident history is a report of the five years previous to the submission or the update on the Risk Management Program which includes the accidental releases caused by the regulated substances from covered processes. The five-year accident history includes only the releases from all covered processes where a regulated substance is held above the threshold quantity, thus, a release of a regulated substance below the threshold is not required to be detailed in the accident history. Moreover, the accident history covers only the releases that cause at least on-site injuries, deaths or important property damage, or offsite injuries, deaths, property damage, environmental destruction or evacuation. Having an accidental release recorded does not mean that the process has to be excluded from Program Level 1, unless it has caused offsite impacts [11].

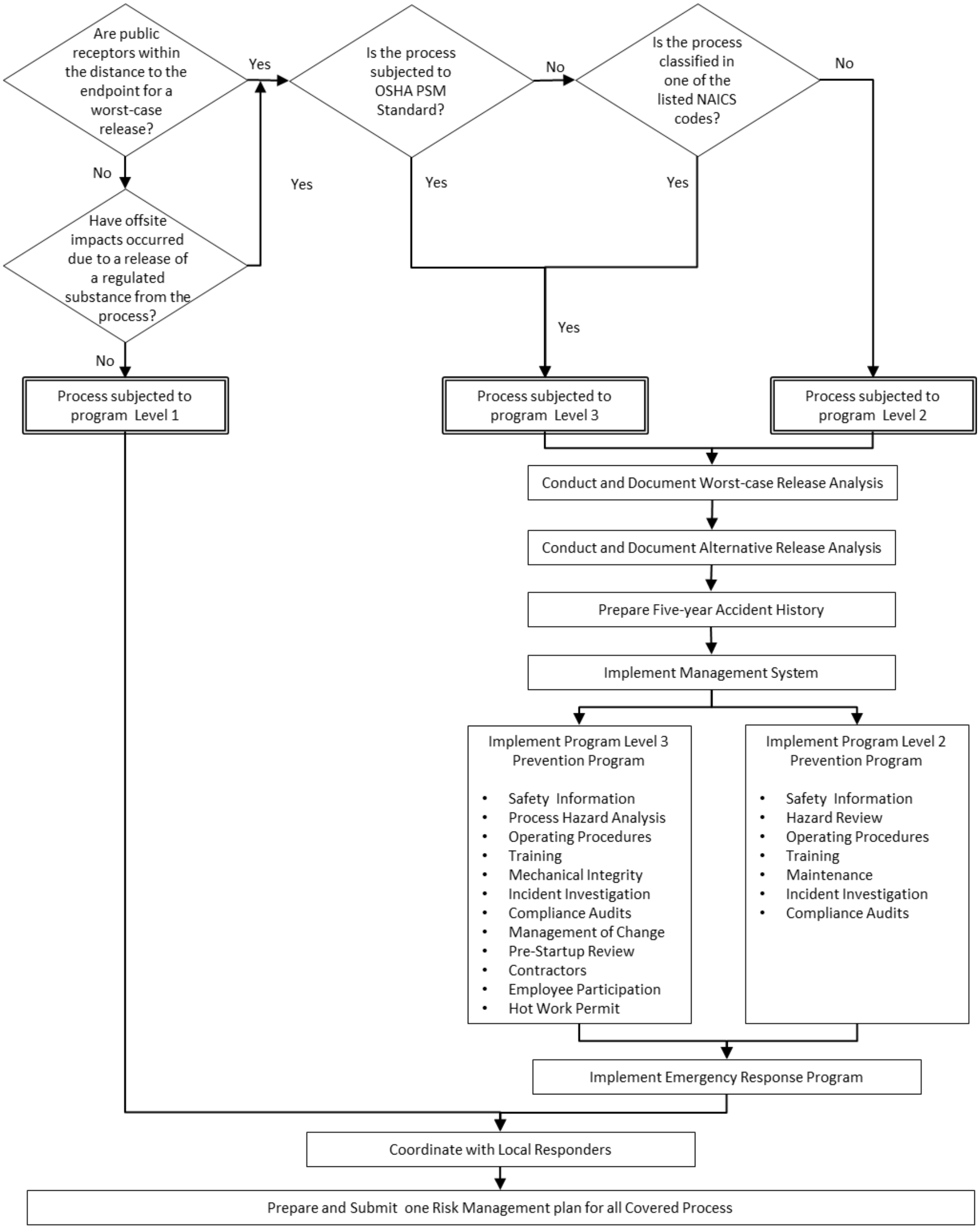

Figure 4 Program levels and requirement for covered process

Every report should include the date and time on which the accidental release started and the duration of the release. It contains the name of the chemical according to the CFR part 68 or the name of the primary regulated substance for a mixture, the amount of each substance release and the events that produce the release such as gas release, liquid spill, evaporation, fire, explosion or runaway reaction. Furthermore, it requires the detection of release sources as storage vessel, process vessel, piping, transfer hose, valve, pump, join, among others, and the identification of weather conditions at time of event including wind speed and direction, temperature, stability class and precipitations[11].

Accurate reporting entails the evaluation of on-site and offsite effects attributed to the accident or mitigation activities, the investigation of the initiating event and the factors that contribute to the accident taking into account equipment failure, human error, improper procedures, overpressurization, upset condition, by-pass condition, maintenance, process design, weather conditions and management error to avoid the failures. Lastly, the report should also show if offsite response agencies were notified and all measures taken by the facility to prevent the repetition of the accident such as upgraded equipment, revised maintenance, improved training, reviewed procedures, executed new mitigation program, updated emergency response plan, changed process, reduced inventory or no actions were implemented [11].

2.4 Offsite consequence analysis

The offsite consequence analysis covers two main parts: the worst-case release scenario analysis and alternative release scenario analysis. The purpose of the first one is to figure out the potential impact and the effects on the population, geographical areas and public receptor of a hypothetical worst-case accidental release. The worst-case release is defined by EPA as the release of the greatest amount of a regulated substance from a stationary source that reaches the largest distance from the place where the release happened to a defined endpoint, beyond which serious damage is not estimated to occur [11].

The classification of a process in a Program Level 1 depends on the results of the worst-case release analysis for all flammable and toxic regulated substances above the threshold and it must be conducted for each process that may qualify for Program 1. So, if the distance to any public receptor is greater than the distance to the specified endpoint the process is eligible for Program 1, otherwise it will be categorized in Program 2 or 3. For processes belonging to Program Level 2 or 3 one worst-case analysis must be done for the regulated flammable substances and one for the toxic regulated substances above the threshold in a process. Since the release with the largest distance to the endpoint has the capacity to affect the largest number of people and geographical area, it is considered the only release to report in the RMP[11].

Modeling the worst-case release for a toxic substance implies taking into account the properties of the substance, selecting a dispersion model and assuming some conditions as shown in table 3. The endpoints used for the model are listed in the CFR in the part 68 and represent the concentrations below which all individuals may be exposed to the substance for less than one hour without health consequences. On the other hand, modeling the worst-case release for a flammable substance assumes that the amount of flammable substance produces a vapor cloud formation and subsequent explosion. The distance to an endpoint is calculated to an overpressure of 1 psi from the explosion point and the release of the total amount of the substance is assumed in most of the circumstances. The greatest distance to an endpoint mainly depends on the amount of the flammable substance, following a proportional relationship[11].

Alternative scenarios are required for Program level 2 and 3 and are intended to evaluate the potential consequences of hypothetical releases having more realistic conditions. There are two main features for an alternative scenario. First, it should be more probable to occur in comparison to the worst-case scenario and second, it should get an endpoint offsite. However, if the endpoint for the alternative scenario does not reach the fence line, it must be reported. For different processes or facilities that handle the same substance above the threshold only one scenario must be examined. For toxic substances at least one scenario must be studied for each substance above the threshold in programs 2 or 3, and for flammable substances one scenario should be considered for all regulated substances[11].

Selecting an alternative release scenario should contemplate releases from events such as uncoupling at transfer hoses, malfunctioning at valves, failure at joints or welds for piping, cracks in pumps, drains, overfill and spill in vessels. Furthermore, the analysis implies the consideration of active mitigation systems as pressure relieving mechanisms, fire water systems and shutdown systems, passive systems, five-year accident history and other possible scenarios. Parameters required for modeling alternative release scenarios are shown in table 3[11].

2.5 Emergency response program

Emergency response is stated by OSHA as the actions taken by the employees and other selected responders outside the release area to an event that results in, or has the potential to produce, an uncontrolled release of a regulated substance. The definition does not cover responses to releases where the substance can be controlled at the time of the release by the workers in the surrounding area or by maintenance personnel. Part 68 of CFR requires the implementation of the Emergency Response program for processes that belong to Program 2 or 3 when the employees are prepared to respond to releases of regulated substances[11].

If the facility intends to respond to the release with the employees, the emergency response program must include an emergency response plan, emergency response equipment procedures, employee training and procedures to keep the program updated. Under certain circumstances it may be inappropriate for workers to perform response operations. However, the facility must guarantee effective emergency response to any release through the cooperation of local response agencies, which implies the facility has to take part in developing the community emergency response plan, and the facility has to determine that the local fire department or local responders have the capability to handle a release in terms of equipment and training[11].

The response plan defines the actions regarding first aid and medical assistance to treat affected individuals; the procedures to notify the community and agencies about the incident; and the actions to be followed by employees on-site over the course of the release, such as interpretation of signals, activation of alarms systems, safe evacuation, and mitigation and decontamination activities after the incident. The emergency equipment plan explains the actions to use and maintain the equipment relevant to an emergency response including detection devices, and communications systems. The training program outlines the procedures that personal and contractor should learn and follow in case of a release, such as evacuation actions, activation of alarm systems and the location and use of emergency equipment[11].

Table 3 Parameter for modeling release scenarios

Parameter	**Worst-case release scenario**	**Alternative release scenario**
Endpoints	• Toxic substances: 40 CFR, Part 68, Appendix A. • Flammable substances: overpressure of 1 psi for vapor cloud explosion.	• Toxic substances: 40 CFR, Part 68, Appendix A. • Flammable substances: overpressure of 1 psi for vapor cloud explosion, radian heat of 5kW/m^2 for firewalls or pool fires and Lower flammability limits LFL for vapor cloud fires.
Wind Speed	Wind speed 1.5 m/sec or higher speed demonstrated during the 3 previous years.	Wind speed 3 m/s (EPA) or usual meteorological conditions at the site.

Table 3 Continued

Stability	Stability class F or less stable atmosphere demonstrated during the 3 previous years.	Stability class D (EPA) or Usual meteorological conditions at the site.
Ambient temperature	Highest daily maximum temperature along the last 3 years or 25 C.	Average temperature for the site or 25 C.
Humidity	Average humidity for the site or 50 percent humidity.	Average humidity for the site 50 percent humidity.
Height of release	Ground level release for toxic substances.	Determined by the release scenario.
Topography	Urban or rural.	Urban or rural.
Gas density	Tables or models used for dispersion of regulated substances.	Tables or models used for dispersion of regulated substances.
Temperature	• Liquids: highest daily maximum temperature along the last 3 years • Gases liquefied: boiling points.	Process or ambient temperature appropriate for each scenario.

3. OVERVIEW OF CONSEQUENCE MODELING

3.1 Source term models

Modeling the source phenomena is critical for any consequence modeling methodology. The source term depends on the type of rupture and spill emission situation such as, pipe rupture, hole in a tank and fragmenting jet. The model provides information related to the total quantity discharged, the rate of discharged and the state of it. The units used to define the source emission are mass per unit time [12]. The four basic steps reported in the literature to determine a source emission rate:

- Determining the time dependence of release scenario
- Identifying the most applicable source-term model
- Gathering specific input data and physical properties necessary for modeling.
- Calculating the source emission rate.

Figure 5 will depict the important steps mentioned above and any source term modeling procedure will have to follow these guidelines for a systematic approach[13].

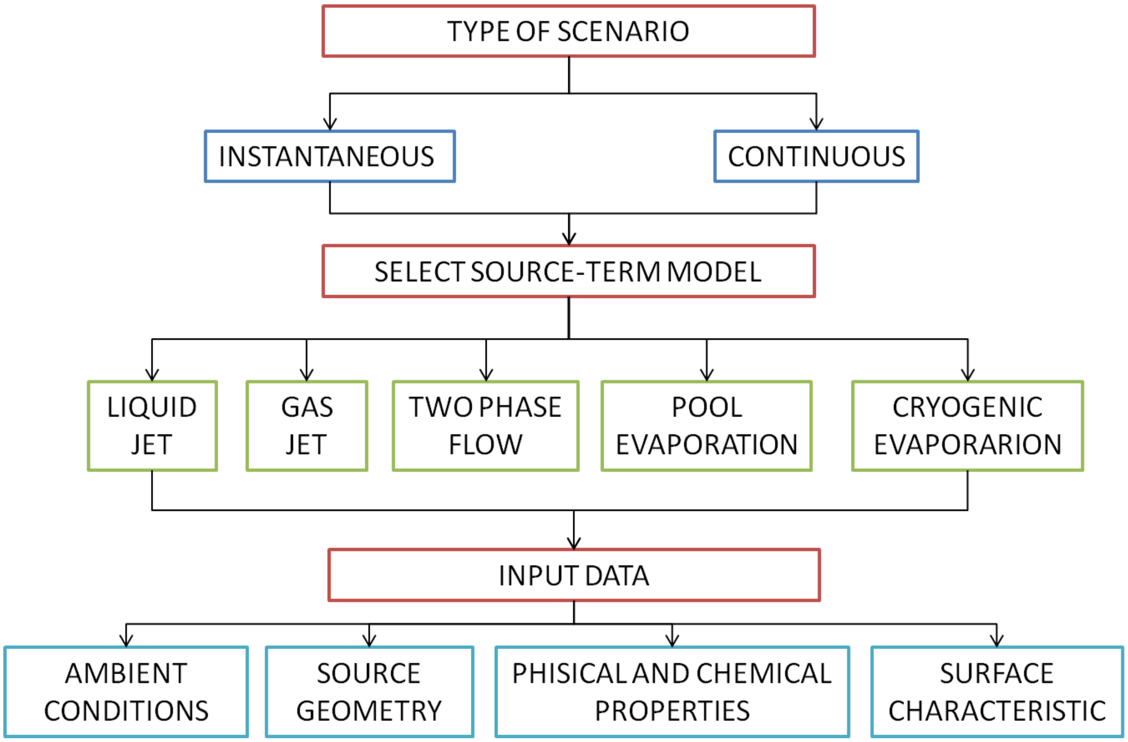

Figure 5 Source-term modeling procedure

3.2 Dispersion models

Primary interest of dispersion model techniques is to describe how the formaldehyde is transported downwind, calculate the distance to reach certain endpoint concentration level and plot contour of those concentrations. The type of dispersion has been categorized as passive and dense depending on gas behavior[13].

Mathematical models are essential tools to evaluate the consequences of the accidental release of hazardous materials. Modeling a toxic gas release to the air might give different outcomes depending on type of resulting dispersion, the basic mathematical formulation and the set of data used to calibrate them. The behavior of a gas release is characterized by the diffusivity equation [14]

$$\frac{d\chi}{dt} + u\frac{d\chi}{dx} + v\frac{d\chi}{dy} + w\frac{d\chi}{dz} = K_x\frac{d^2\chi}{dx^2} + K_y\frac{d^2\chi}{dy^2} + K_z\frac{d^2\chi}{dz^2}$$

Where (x,y,z) are rectangular coordinates, (u, v,w) are the mean wind speed for each coordinate, (Kx, Ky, Kz) are exchange/ diffusion coefficients for the respective direction, t is the time, and χ is the concentration.

Approaches to model dispersion include different models such as gradient transfer, statistical, similarity, and top hat, box and slab. Gradient transfer models known as well as K models intend to solve the diffusion equation through the use of the correlation between each individual exchange coefficient and the wind speed. Statistical models assume that the concentration profiles follow a Gaussian shape, proposing standard deviation as characterization parameters for the concentration. Similarity models are applied specially for buoyant plumes and consist in an equation obtained from dimensional analysis for the rate of growth of any specific dimension of the cloud. This model does not offer information about the concentration; however it is used to find the dispersion coefficient in statistical models. The top hat, box and slab models are part of family models. The top hat model assumes a flat top where the mixing happens, the box model is considered as a cylinder with uniform concentration at a given time, while slab model the concentration depends on the distance. Both box and slab models are mainly applied for dispersion of dense gases, nevertheless the box model is used to model passive dispersion for a defined area [14].

A resulting dispersion can be treated as passive dispersion or dense gas dispersion. Passive dispersion is known as the dispersion of gases with neutral buoyancy. It is appropriate for small releases or for large releases if the density of the gas and the chemical temperature is close to the surrounding air. Studies conducted in passive gas dispersion that are of industrial significance involve continuous release from elevated source, releases in urban areas and instantaneous and continuous point source releases at the ground level. An important feature to take into consideration for ground level releases is that the cross section of a concentration profile has a Gaussian type (bell shape); however this type of dispersion is also characterized by the increasing in the spread of the concentration as the time passes, and by the variation in the concentration downwind determined in turn by the strength of the source.

Different models have been developed to represent the passive dispersion. Roberts Model (1923) gave the solutions for the diffusion equation using the Fickian diffusion coefficient K. However, the model showed that the concentrations obtained were not similar to those gotten from experimentation. The model was not suitable to represent dispersion in the atmosphere, but it established a baseline for subsequent studies on passive dispersion. Sutton Model (1953) is based on modifications of Robert Model. It considers meteorological constants such as index n and diffusion parameters Cx, Cy, Cz that depend on stability conditions. Pasquill Model (1961) uses the equation for a continuous elevated point source presented by Sutton to derivate an equation for a continuous point source at ground level. The model provides formulations to calculate meteorological parameters such as vertical spread h and lateral spread θ of a toxic substance based on turbulence measurements. The model offered as well a set of curves to determine those parameters when measures are not available. The set of curves are tagged from A that indicates high turbulence and high diffusion, through F that implies low turbulence and low diffusion. Thereafter, in Pasquill-Gifford Model (1962) the Pasquill method for calculating vertical and horizontal was reformulated to obtain dispersion coefficients $\sigma_x, \sigma_y, \sigma_z$ as a standard deviations[14, 15]

3.3 PHAST tool

PHAST (Process Hazard Analysis Software Tool) is a package developed by DNV (Det Norske Veritas) and today it is one of the most used packages in the chemical and oil and gas industries for assessing accident consequences. PHAST software allows studying the consequence of an accident from the release to the dispersion and/or explosion of the chemical[16].

PHAST interconnects different event models for predicting behavior and calculating consequences. PHAST is able to simulate an accident release from the release point, and also includes models to simulate rainout, pool vaporization and evaporation, as well as energy release from fire or explosion. Source terms models such as leaks, line ruptures, tank collapses, and long pipes could be simulated in combination with the Unified Dispersion Model (UDM) to study the consequence of material release[17, 18].

A specific event is modeled using PHAST base on the conditions of the process or equipment as temperature, pressure, composition, material properties and atmospheric conditions. Moreover, PHAST requires short time to complete calculations once the inputs are fulfilled; the results are suitable and broadly used for risk assessment in industry safety analysis. Also, one of the PHAST advantages is the inclusion of more source terms models even for dense clouds [16, 19].

The Unified Dispersion Model (UDM) is an integral model, which is a group of differential equations, that describes the behavior of the cloud as a function of time or distance. The set of equations covers all the phases of the dispersion of the cloud, jet, dense and passive dispersion. The UDM is able to simulate the development of the cloud resulting from the release through all the phases without the problems associated with the interfacing of each model phase and the discontinuous transitions between them. The UDM model applies the same formulation for both instantaneous and continuous release [16, 17].

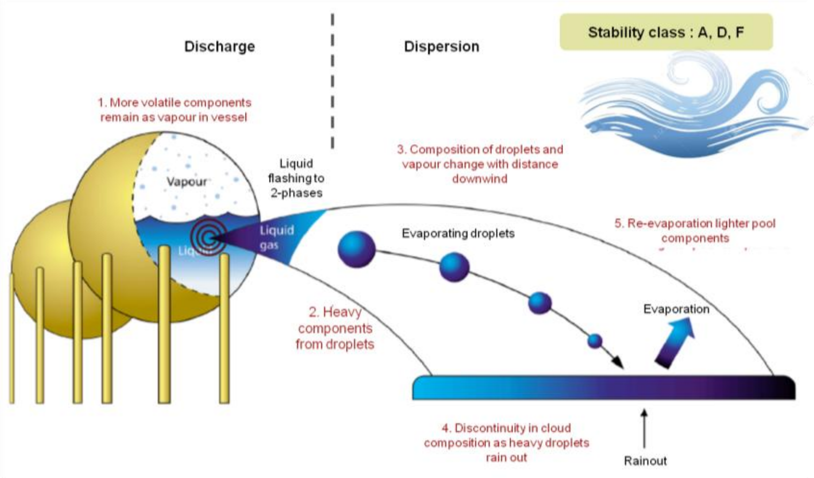

Figure 6 Development of a toxic release.
Figure adapted from [18]

The UMD model infers that after the touchdown the dispersion is over a flat terrain with constant ambient conditions and uniform roughness. It does not take into account the effect of obstacles and congestion[18].

4. PROBLEM STATEMENT

4.1 Motivation

Catastrophic incidents in the chemical process industry such as the Flixborough disaster and the Bhopal disaster have intensified government and industry efforts to identify and manage risk. For that reason, Environmental Protection Agency (EPA) and Occupational Safety and Health Administration (OSHA) promulgated the Risk Management Plan (RMP) and the Process Safety Management (PSM) program, respectively, for hazardous substances. Consequence analysis of an accidental release of toxic chemicals is one of the key elements in such programs. One of the main objectives of consequence analysis is to have a better understanding of how a facility should be sited or installed and designed, in order to avoid any negative impact on the environment and the population in case a hazardous situation takes place.

Previous works had focused on several substances such as chlorine and ammonia [17, 20, 21]; however, it is interesting that formaldehyde has not yet been part of such studies despite that the fact both production and consumption of formaldehyde have ascended.

In 2000, Annual US formaldehyde production was reported greater than 4.6 million tons and it was raised during the last years due to the expansion of resins and plastics based on formaldehyde mainly in China and United States. [6, 22]. As a result, in 2011 the profit by global formaldehyde market was USD 10,886.7 million and is expected to reach USD 18,061.4 million by 2018. Products as urea formaldehyde resins accounted the main share of the formaldehyde market with 39.2% share in total volume consumption in 2012 [1, 23].

Since OSHA has estimated that about 2.1 million people were exposed to formaldehyde in the workplace in 1995 in the United states [6] and also formaldehyde is categorized as highly toxic, and a carcinogen, consequence analysis on that is strongly recommended.

4.2 Objective

The purpose of this research is to perform a consequence analysis of formaldehyde release. The objectives of this study are:

1) To consider an accidental release of formaldehyde at three different concentrations (pure formaldehyde, 50% formaldehyde solution and 37% formaldehyde solution)and carry out the corresponding consequences calculation.

2) To simulate two scenarios for each mixture and assess the effect of the variability of the main input parameters on the impact areas (wind, stability class and hole size).

5. METHODOLOGY

The methodology flowchart is provided in the Figure 7. In order to perform the consequence analysis of formaldehyde release, a literature review was done. The next step is analyzing the consequence using two different scenarios. Finally, a sensitivity analysis will be executed.

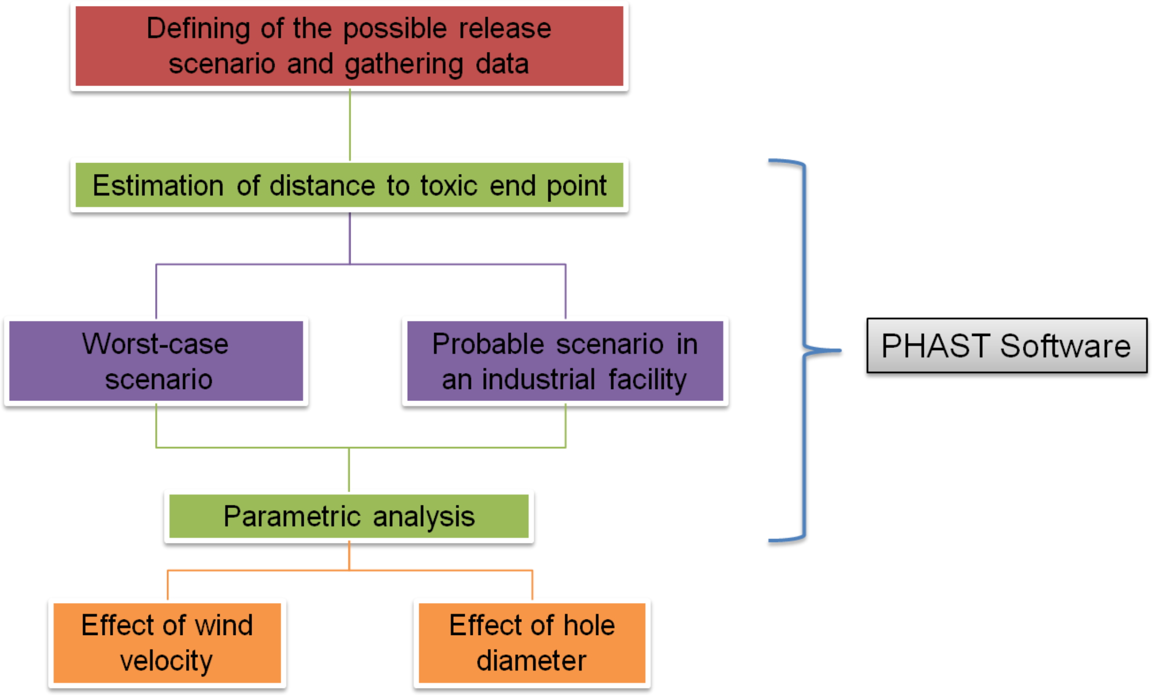

Figure 7 Proposed research methodology

The formaldehyde release was modeled in PHAST taking into account all the basic assumptions mentioned in RMP for industries and a more probable scenario as is described in table 4. The RMP regulation considers the worst-case scenario where the largest quantity of a regulated substance is released which results in the greatest distance to the toxic endpoint. Consequence parameters proposed such as 1.5 m/s wind speed and class F atmosphere stability at ground level should were considered [11].

Table 4 Scenarios details

WORST- CASE SCENARIO	REALISTIC CASE SCENARIO
✓ Tank volume = 200m^3 ✓ Release of the whole inventory of the tank over a short period of time. ✓ Release time 10min. ✓ Liquid state at 25°C ✓ Ground level ✓ Three mixtures of formaldehyde (pure formaldehyde, 50 wt % formaldehyde and 37 wt% formaldehyde) ✓ Four different ambient conditions (1.5/A, 5/D, 6/D and 1.5/F). ✓ Concentration of interest ERPG-2 (10ppm) and IDLH (30ppm)	✓ Tank volume = 200m^3 ✓ Release through a hole on a storage tank ✓ Liquid state at 25°C ✓ Leak on the bottom of the tank ✓ Three mixtures of formaldehyde (pure formaldehyde, 50 wt % formaldehyde and 37 wt% formaldehyde) ✓ Three atmospheric condition classes (A, D and F) ✓ Three different diameters (10mm, 30mm and 50mm) ✓ Concentration of interest ERPG-2 (10ppm) and IDLH (30ppm)

Three mixtures of formaldehyde were chosen: pure formaldehyde, a 50 wt % formaldehyde solution and 37 wt% formaldehyde solutions; being the last two the commercial concentrations for aqueous formaldehyde. Table 5 shows composition for each mixture.

Table 5 Composition of mixtures simulated

	Pure formaldehyde	**50% solution**	**37% solution**
Formaldehyde (w %)	100	50	37
Methanol (w %)	0	10	10
Water (w %)	0	40	53

Finally, a parametric analysis was carried out by varying one parameter at a time while the all the other parameters were kept constant. The influence of wind, atmospheric stability and hole diameter were studied.

6. RESULTS AND DISCUSSION

This section presents the results of the simulation performed using PHAST software for both the worst-case scenario and a realistic release incident scenario previously described in the methodology section. The first run of simulations was conducted in the PHAST software for the worst-case which assumes a release of the whole inventory of the tank over a short period of time of 10min. Then, a release through a hole on the bottom of a storage tank where the formaldehyde is contained was simulated.

The parametric analysis was carried out by varying one parameter at a time while the all the other parameters were kept constant. It is important to highlight that it was not the aim of this work to validate the accuracy of the PHAST's Unified Dispersion model (UDM); the main goal was to study the effect of the variation of input parameters.

6.1 Worst-case scenario

Three mixtures of formaldehyde were chosen: pure formaldehyde, 50 wt % formaldehyde and 37 wt% formaldehyde. The calculation of the impact areas was estimated for each mixture for the toxic levels ERPG-2 (10ppm) and IDLH (30ppm). The inventory of material discharged was based on process conditions [3] and representative atmospheric conditions were assumed base on previous studies[20]. Release time was selected 10min in accordance with RMP guidelines and the American Institute of Chemical Engineers[11].

PHAST software allows making release and dispersion calculations together avoiding the possible error due to data handling. Also, the software itself is able to identify whether or not the initial dispersion phase requires a dense gas dispersion model as well as the occurrence of a transition phase to low density.

Figure 8 shows a typical graph of the maximum concentration footprint of the cloud from PHAST, in this case it was generated by a mixture of 50% formaldehyde. The concentration of interest for this simulation is 10ppm with an averaging time of 10 min. The cloud was simulated at four different ambient conditions.

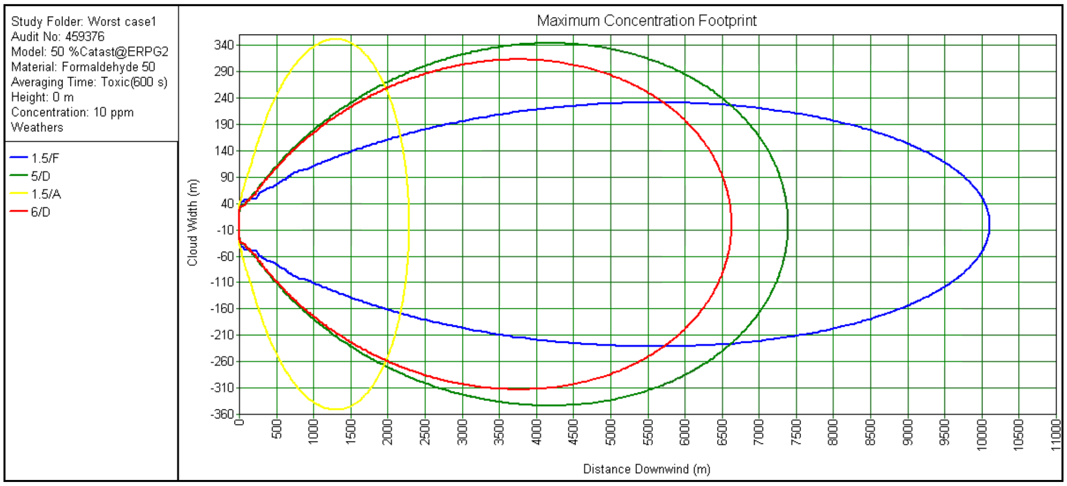

Figure 8 Dispersion of a 50 (w/w) % formaldehyde solution at different weather conditions with an averaging time 10 min.

The downwind distance and the crosswind distance calculated with PHAST for the sixteen possible scenarios are summarized in table 6. It can be observed that the largest distance is reached by stability class F and velocity 1.5m/s for all the three solutions which are in agreement with the results reported in the literature for other substances [20].

The reason for the longer distance lies in the effect of stability class on the turbulence and the speed of dispersion. Although the wind speed is low the high stability level of atmosphere inhibits mechanical turbulence and thus increases the speed of the dispersion of the cloud. With reference to the extremely unstable class A, the downwind distance values are lower than the ones for class D. However, higher crosswind distances were obtained for class D than that for the class A. Additionally, a difference from 9 to 11% can be found for class D at different wind velocity

Table 6 Result summary for worst-case scenario

			ERPG-2 (10ppm)		**IDLH (30ppm)**	
Mixture	**Wind velocity (m/s)**	**Stability class**	**Downwind distance (m)**	**Crosswind distance (m)**	**Downwind distance (m)**	**Crosswind distance (m)**
Pure Formaldehyde	1.5	A	10238	3055	4950	1984
	6.0	D	24126	1967	11387	1110
	5.0	D	27145	2185	12642	1232
	1.5	F	49428	7048	49286	4793
50% solution	1.5	A	2290	703	1133	376
	6.0	D	6630	625	3442	354
	5.0	D	7393	687	3811	387
	1.5	F	10108	463	5129	263
37% solution	1.5	A	1625	522	791	273
	6.0	D	4748	469	2504	267
	5.0	D	5259	513	2752	292
	1.5	F	9742	447	4932	254

Pure formaldehyde disperses over the largest areas in terms of toxicity. Once the methanol and water are added to the solution, the behavior under the same conditions is different for both downwind distance and crosswind distance. However, the difference of the downwind distance between class A and D remains within the range of 55 to 65 % for the three solutions for both concentrations of interest, ERPG-2 and IDHL.

The calculated downwind distances using PHAST were correlated by a linear regression in order to compare the dependence of the results on the solution concentrations. As can be seen in table 7 and figure 9 and 10, the atmospheric condition 1.5/F has the highest downwind and crosswind distance and also it is characterized by the highest slope for the three solutions. Finally, the wind velocity has a positive impact on the dispersion of the cloud; however, in the case of pure formaldehyde the dependence on wind velocity is strong.

Table 7 Regression parameters for the worst-case scenario

Mixture	**ERPG-2 (10ppm)**		**IDLH (30ppm)**	
	m	**r^2**	**m**	**r^2**
Pure formaldehyde	12059	0.92	13426	0.74
50% solution	2421	0.93	1235.7	0.92
37% solution	2486	0.92	1267.1	0.92

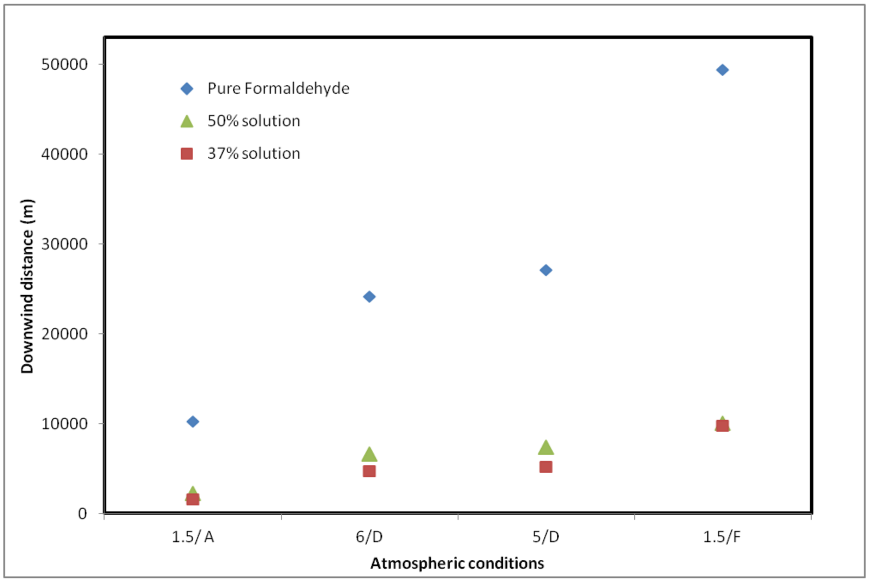

Figure 9 Maximum downwind distance corresponding to ERPG-2 as a function of atmospheric condition

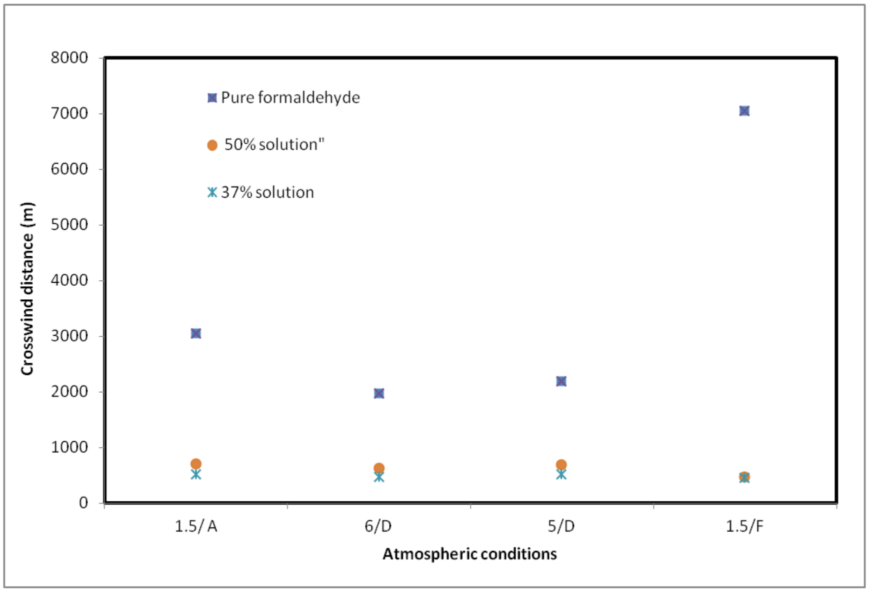

Figure 10 Maximum crosswind distance corresponding to ERPG-2 as a function of atmospheric condition

6.2 Realistic release cases

The release scenarios took into account conditions as close to real accident events. The scenario assumed a release through a hole on a storage tank where a mixture of formaldehyde is contained in the liquid state at 25°C. Tank pressure was fixed atmospheric and the storage tank was considered cylindrical vertical with a total volume of 200 m^3. The simulations were done considering a leak at the bottom of the tank which implies that the release occurs in the liquid phase at the greatest flow rate. In addition, a mitigation time of 600 seconds was adopted after the initial release and a dispersion concentration of interest equal to ERPG-2 (10 ppm) or IDHL (30 ppm) depending on the scenario under study.

6.2.1 Effect of wind velocity

The atmospheric conditions taken into consideration in this work were those representatives for the most likely conditions [16]. Three atmospheric condition classes were adopted: the extremely unstable class A, the neutrally stable D and the very stable F. The aforementioned classes were modeled at different but consistent wind velocities. Maximum impact distances were calculated using PHAST for each climate pair for the three mixtures using a diameter constant of 30mm as is shown in table 8.

Figure 11 shows the maximum concentration of pure formaldehyde simulated at different atmospheric classes and wind velocities using ERPG-2 as a concentration of interest for a hole diameter of 30mm.

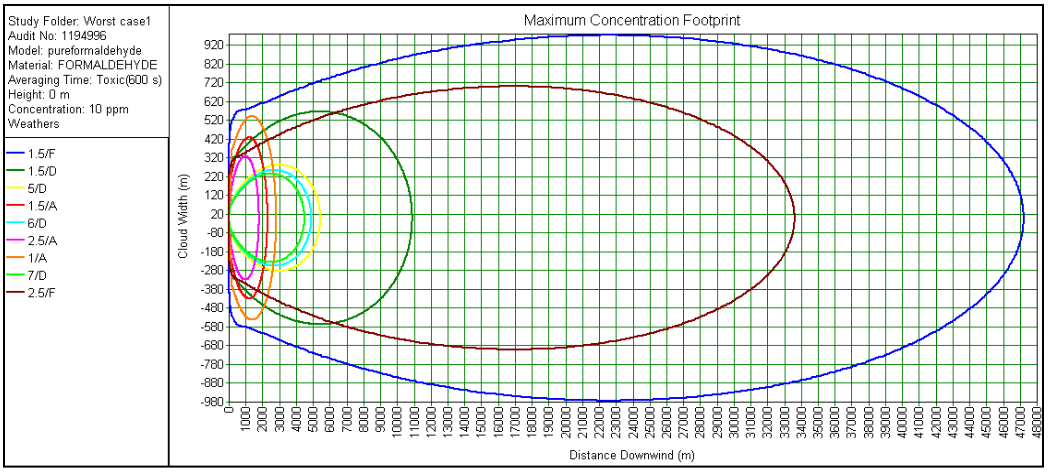
Study Folder: Worst case1
Audit No: 1194996
Model: pureformaldehyde
Material: FORMALDEHYDE
Averaging Time: Toxic(600 s)
Height: 0 m
Concentration: 10 ppm
Weathers

Figure 11 Pure formaldehyde's concentration footprint at different wind velocities

It can be observed that higher wind velocities result in shorter impact distances. Data reported in Table 8 are in good agreement with this affirmation with the exception of one case (downwind and crosswind distance under class D for 37 % solution) where an increasing value of wind velocity from 1.5 m/s to 5 m/s results in an increase on the distances. Class F has the largest distances compared with class A and D due to high stability and low velocity. Additionally, class F shows a strong dependence on the wind velocity as can be confirmed by comparing the slopes for the three mixtures in Table 9. The influence of wind velocity on maximum impact distance is well represented by linear trends; correlation coefficients were close to 0.999 with the exception of a few cases.

Table 8 Result summary for effect of wind velocity

Mixture	**Stability Class**	**Wind velocity (m/s)**	**ERPG-2**		**IDLH**	
			Downwind distance (m)	**Crosswind distance (m)**	**Downwind distance (m)**	**Crosswind distance (m)**
Pure formaldehyde	A	1.0	2809	1083	1506	730
		1.5	2294	857	1263	559
		2.5	1786	657	1010	419
	D	1.5	10891	1133	5244	703
		5.0	5432	564	2817	334
		6.0	4895	510	2556	302
		7.0	4487	470	2360	277
	F	1.0			23538	1961
		1.5	47220	1946	20207	1166
		2.5	33607	1401	15185	821
50% solution	A	1.0	1941	665	1059	397
		1.5	1577	558	871	335
		2.5	1255	461	712	280
	D	1.5	7420	695	3775	390
		5.0	3802	389	2018	223
		6.0	3441	356	1836	205
		7.0	3208	335	1716	192
	F	1.0	39632	1484	17939	812
		1.5	29868	1116	13979	595
		2.5	21483	851	10361	463
37% solution	A	1.0	1241	434	643	240
		1.5	1133	411	612	236
		2.5	937	353	520	207
	D	1.5	3350	316	1465	143
		5.0	2964	313	1586	180
		6.0	2693	287	1449	166
		7.0	2487	267	1343	154
	F	1.0	521	101	393	73
		1.5	260	55	200	56
		2.5			76	18

Taking a closer view to stability class D for the three mixtures, it can be seen that the higher velocities promote a faster dilution of the cloud of the pure formaldehyde and the 50% solution. As the wind velocity increases the downwind distance and crosswind distance decrease. However, for the 37% formaldehyde solution, when the concentration of interest is equal to IDHL (30ppm) an unexpected behavior is revealed, Figure 12 and 13 (red line). This unexpected result is observed because under the stable atmospheric conditions offered by class D, high wind velocity could have two opposite effects; high velocities enhance the dilution of the toxic cloud and promote the mass transfer from the liquid pool by boosting the evaporation rate. Figure14 shows an increase in the total mass of the cloud due to high wind velocity

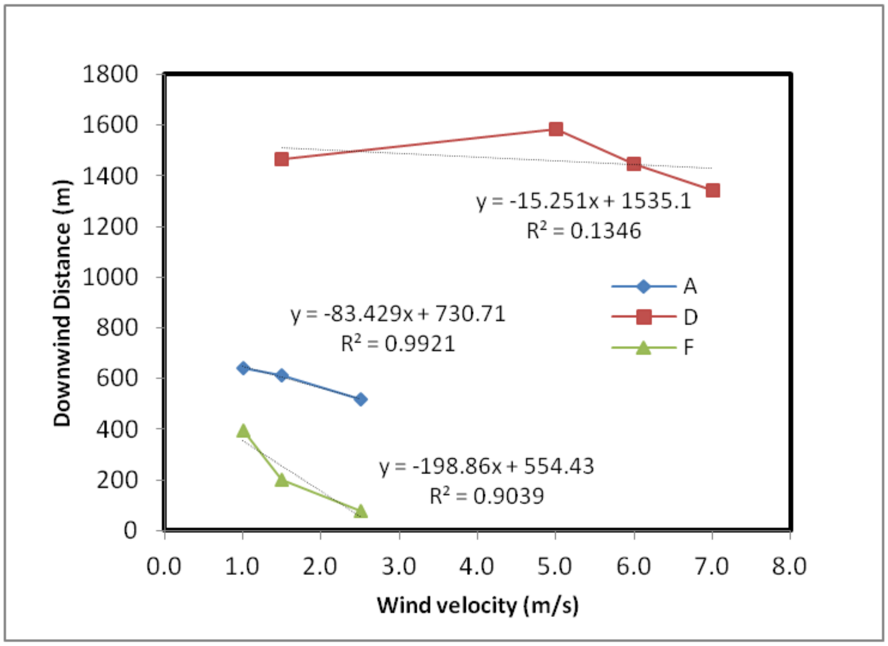

Figure 12 Downwind distance as a function of wind velocity for a 37% formaldehyde solution

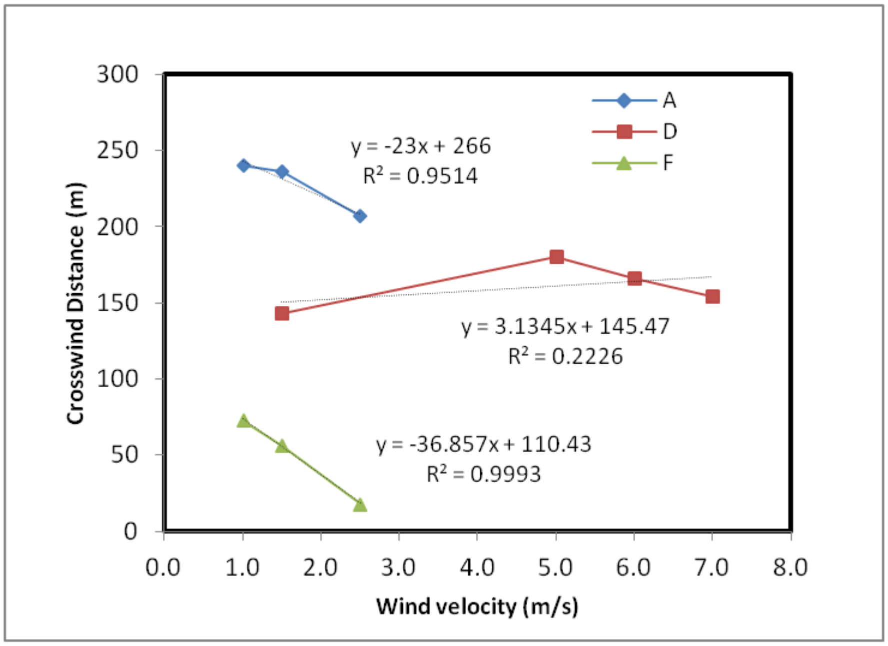

Figure 13 Crosswind distance as a function of wind velocity for a 37% formaldehyde solution

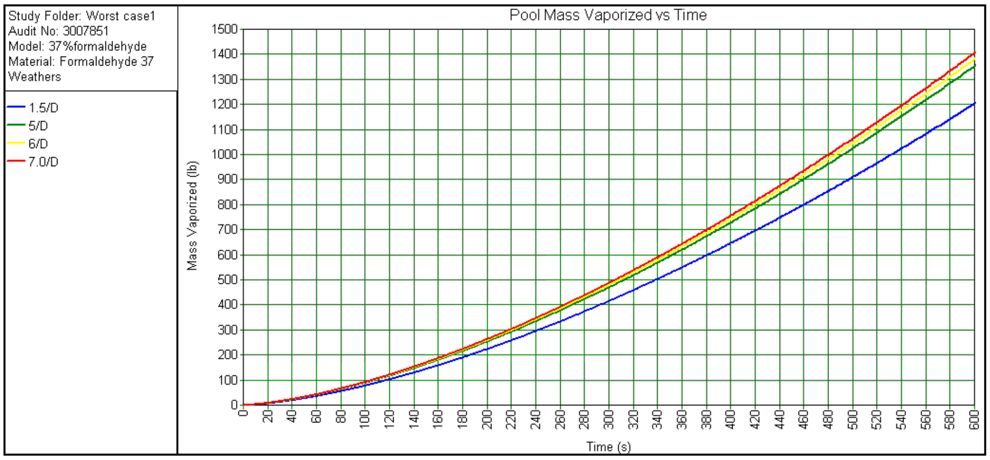

Figure 14 Evaporated mass from the liquid pool of 37% formaldehyde solution as a function of time at different atmospheric conditions

Finally, the worst dispersion condition is a result of a combination of low wind velocity and high stability. From the above results, the sensitivity analysis indicates that for a hole size of 30mm the worst dispersion conditions is 1.5/F for pure formaldehyde, 1/F for a 50% solution of formaldehyde and 1/F for a 37% solution of formaldehyde.

Table 9 Regression lines parameters for the effect of wind velocity

		Stability class A				**Stability class D**				**Stability class F**			
		ERPG-2		**IDLH**		**ERPG-2**		**IDLH**		**ERPG-2**		**IDLH**	
		D	W	D	W	D	W	D	W	D	W	D	W
Pure formaldehyde	m	-657	-272	-319	-197	-1223	-126	-550	-81	-13613	-545	-5490	-700
	r^2	0.96	0.95	0.97	0.94	0.95	0.95	0.96	0.95	1.00	1.00	0.99	0.84
50% solution	m	-438	-130	-221	-74	-801	-68	-394	-37	-11569	-399	-4847	-218
	r^2	0.95	0.95	0.94	0.95	0.95	0.95	0.95	0.96	0.95	0.92	0.95	0.90
37% solution	m	-201	-54	-83	-23	-152	-7	-15	3	-522	-92	-198	-36
	r^2	0.99	0.99	0.99	0.95	0.96	0.67	0.13	0.23	0.99	0.99	0.90	0.99

D = Downwind distance

W = Crosswind distance

6.2.2 Effect of hole diameter

The hole diameter was varied during the study to assess its effect on the maximum distance covered. Three different diameters where selected: 10mm, 30mm and 50mm based on previous studies reported in the literature [17, 20]. Figure 15 shows an example of the results obtained from PHAST software when a mixture of 37% formaldehyde is released through three different sizes of hole in an atmospheric condition 1.5/A.

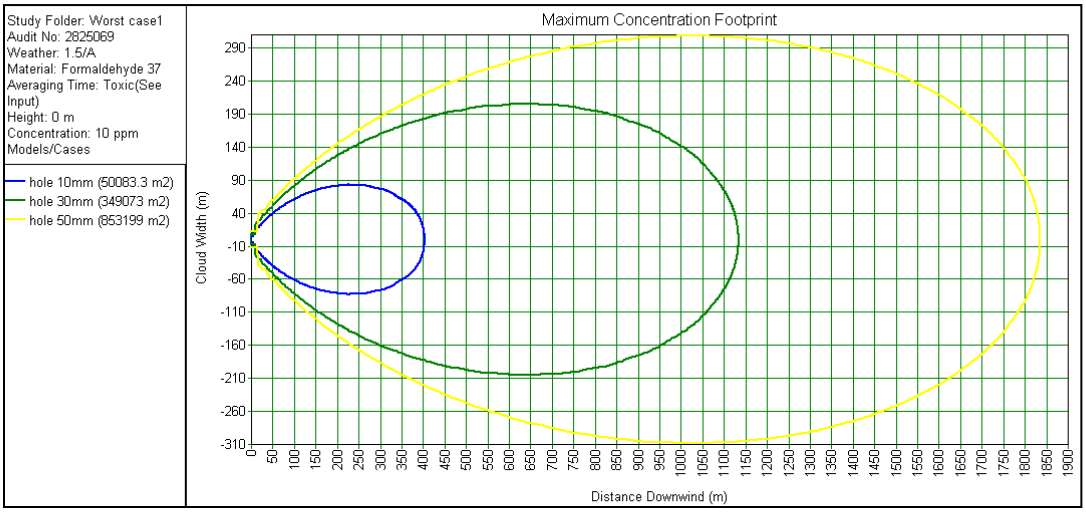
Study Folder: Worst case1
Audit No: 2825069
Weather: 1.5/A
Material: Formaldehyde 37
Averaging Time: Toxic(See Input)
Height: 0 m
Concentration: 10 ppm
Models/Cases

Figure 15 Maximum concentration for a 37% formaldehyde solution at different hole diameters

A total of 144 possible scenarios where simulated in order to see the influence of the hole size at different atmospheric conditions; the summary of the result is reported in Table 10. For this sensitivity analysis four representative atmospheric conditions were selected (1.5/A, 6/D, 5/D and 1.5/F). Each diameter size was varied while other parameters such as atmospheric condition, mitigation time, storage conditions and concentration of interest (ERPG-2 or IDLH) were kept constant. Here the objective was to determine the significant effect of each diameter and their combinations with atmospheric conditions in the dimension of the impact areas.

Table 10 Result summary for effect of hole diameter

		1.5/A				6/D				5/D				1.5/F			
		ERPG-2		IDLH		ERPG-2		IDLH		ERPG-2		IDLH		ERPG-2		IDLH	
	Hole (mm)	Downwind distance (m)	Crosswind distance (m)	Downwind distance (m)	Crosswind distance (m)	Downwind distance (m)	Crosswind distance (m)	Downwind distance (m)	Crosswind distance (m)	Downwind distance (m)	Crosswind distance (m)	Downwind distance (m)	Crosswind distance (m)	Downwind distance (m)	Crosswind distance (m)	Downwind distance (m)	Crosswind distance (m)
Pure formaldehyde	10	748	309	435	197	1419	167	779	100	1562	183	856	110	11017	573	5409	356
	30	2294	857	1263	559	4895	510	2556	302	5432	564	2817	335	47220	1946	20207	1166
	50	3835	1334	2027	872	8641	836	4374	489	9618	923	4823	541	49246	3378	37348	1949
50% solution	10	550	224	316	136	1074	126	595	73	1173	136	651	79	6393	296	3150	159
	30	1578	558	871	335	3441	354	1836	205	3802	389	2018	223	29866	1116	13979	595
	50	2699	880	1456	526	5963	573	3104	325	6604	626	3418	354	49066	1956	25947	1014
37% solution	10	403	165	224	96	858	102	477	59	941	111	525	64	58	14	29	12
	30	1133	411	612	236	2693	287	1449	166	2964	313	1586	180	260	55	200	54
	50	1835	617	963	354	4671	466	2453	265	5154	507	2694	289	478	92	360	78

The data was analyzed and graphed in order to see the maximum variation of the distance over the range of each diameter, wind velocity and atmospheric condition in a general way. For graphs 16, 17 and 18 maximum values obtained for each scenario were considered, which means the worst condition for each mixture.

Generally, it was observed that the size of the hole compared to wind and stability class plays a more significant role on the dispersion (blue bars for the next three graphs). The largest difference in the maximum distances is associated with the hole size. However, a significant influence is associated with the wind velocity in regard to the crosswind distances.

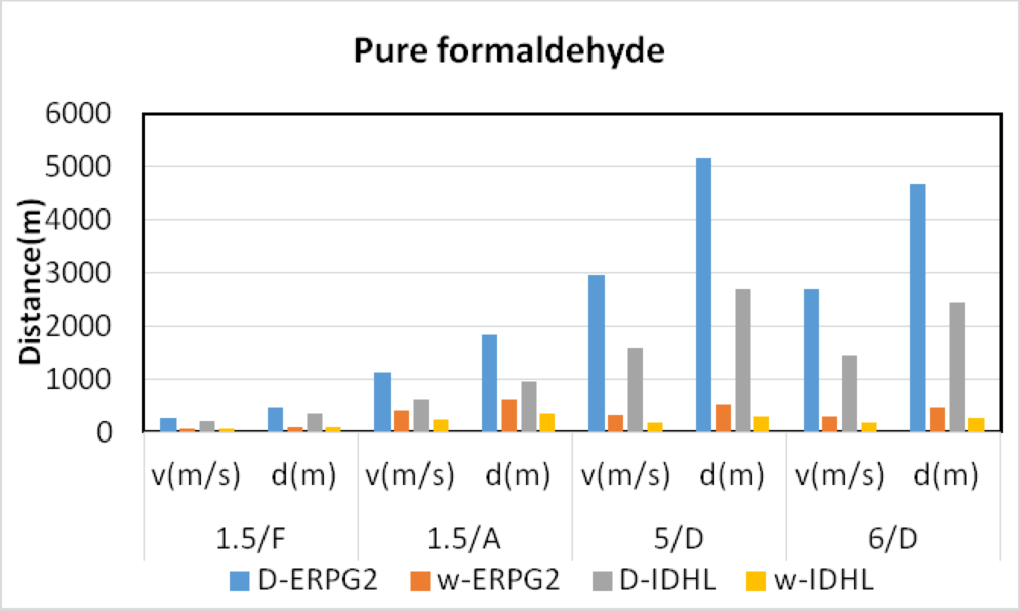

Figure 16 The combined effect distance, wind velocity and hole diameter for pure formaldehyde

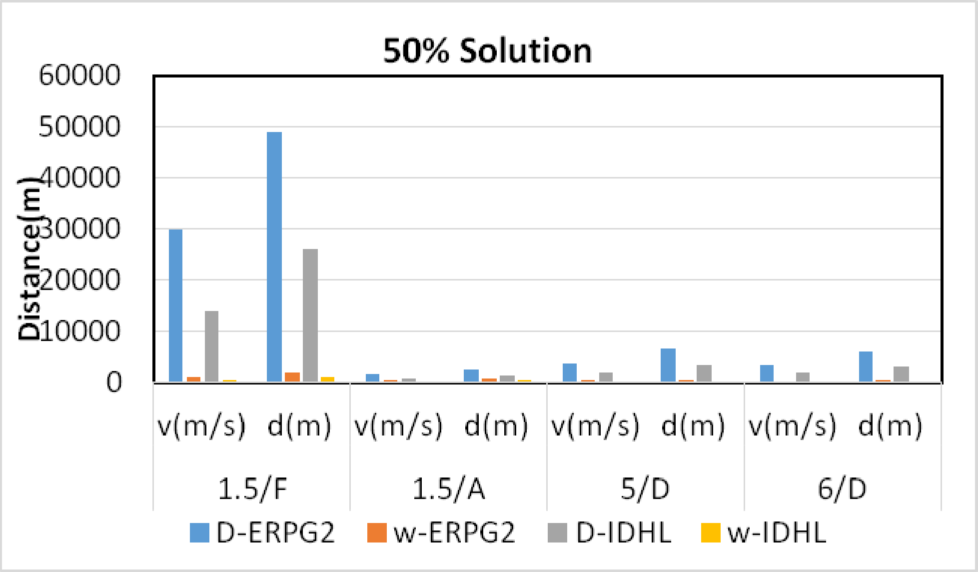

Figure 17 The combined effect distance, wind velocity and hole diameter for a 50% formaldehyde solution

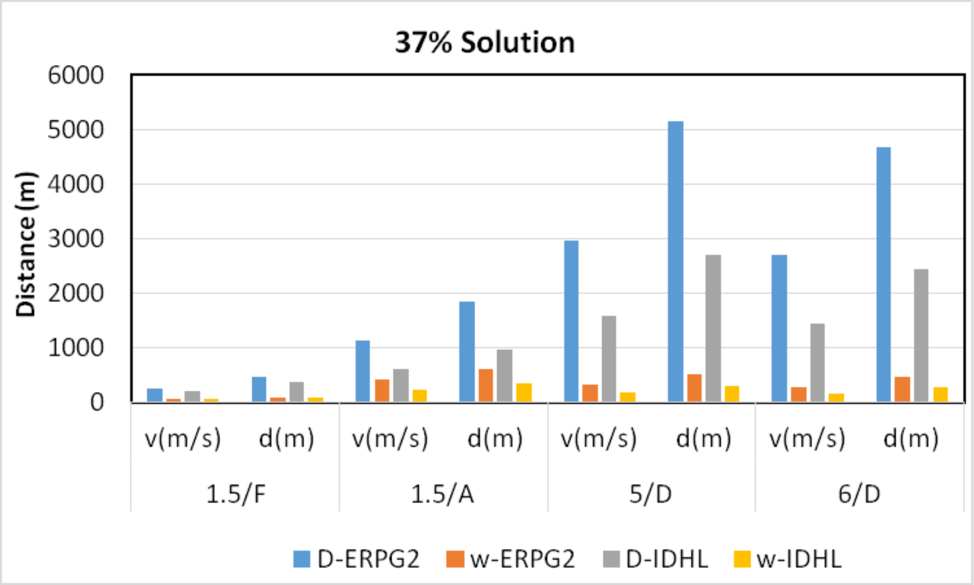

Figure 18 The combined effect distance, wind velocity and hole diameter for pure 37% formaldehyde solution

A detailed analysis was conducted in order to see what the influence of the size of the hole was when it was less than 50mm. It can be seen that the highest value of slope is presented when the diameter changed from 10mm to 30mm for all the weather conditions considered. However, a more significant variation on the slope is observed when the atmospheric condition is 1.5/F which means that is more sensible in terms of change of hole size in the range of 10 to 30mm as figure 16 shows.

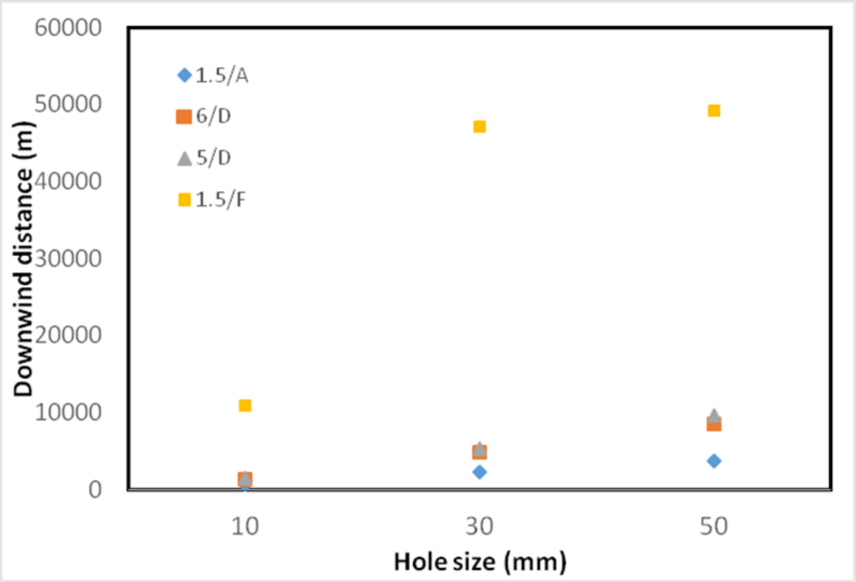

Figure 19 Downwind distance as a function of hole diameter for pure formaldehyde

The data reported in table 10 was ranked from the lowest distance to the highest distances impacted by the toxic cloud for each diameter. The calculated distance was correlated by linear trends to easily compare the dependence of the downwind and crosswind distances among the different hole sizes. As can be seen from table 11, the trend of the downwind distance as a function of hole diameter is quite linear because the regression coefficients are about 0.99.

Table 11 Slope (m) and correlation coefficients (r^2) of the regression lines for downwind distance at different hole diameter

		Pure formaldehyde		**50% Formaldehyde**		**37% Formaldehyde**	
		ERPG2	**IDLH**	**ERPG2**	**IDLH**	**ERPG2**	**IDLH**
1.5/A	m	1543.5	796	1074.5	569.9	716	369.63
	r^2	1.0000	0.9995	0.9994	0.9998	0.9996	0.9992
6/D	m	3611	1797.5	2444	1254.5	1906.5	988
	r^2	0.9995	1.0000	0.9997	1.0000	0.9995	0.9999
5/D	m	4028	1983.5	2715.5	1383.5	2106.5	1084.5
	r^2	0.9995	1.0000	0.9997	1.0000	.9999	0.9998
1.5/F	m	19115	15970	15237	11399	210.05	165.47
	r^2	0.790	0.9982	0.9017	0.9992	0.9996	0.9997

For the pure formaldehyde and the 50% formaldehyde solution, the lowest downwind distance was observed under 1.5/A atmospheric condition. Also, the highest downwind distance for both mixtures is reached under 1.5/F condition. However, differently from 37% formaldehyde solution, the shortest distance is obtained for atmospheric condition 1.5/F and the maximum downwind for 5/D for both concentrations of interest (ERPG-2 or IDLH).

With reference to the downwind distance under the class D, the impact distances for 5/D and 6/D range in the same interval; the change in distance is about 8-10% when the wind velocity changes from 6m/s to 5m/s. For the case of a change in atmospheric stability (A to F) at a constant wind velocity (1.5m/s) the change in distance is between 90 and 95%. It is also important to mention that when the change occurs from 1.5/A to 6/D being the last one of the most probable conditions in a real scenario, the downwind distance of the toxic cloud increases about 45to 60%. Then, the results allow concluding that stability class has a key role in the formaldehyde dispersion.

7. CONCLUSIONS AND FUTURE WORK

7.1 Conclusions

The effect of the main parameters influencing the maximum distances impacted by a toxic cloud of formaldehyde was studied. Three mixtures of formaldehyde (pure formaldehyde, 50% formaldehyde solution and 37% formaldehyde solution) were chosen for the simulation of the release. Two different types of scenarios were analyzed using PHAST software: a worst-case scenario and an alternative release scenario. A parametric sensitivity analysis was carried out varying one parameter at a time.

A wide-ranging rule cannot be drawn for the calculations of consequences for a toxic cloud of formaldehyde. However, some guidelines can be given based on the results of this work. The results show that for a worst-case scenario, the largest downwind and crosswind distance is represented by stability class F and wind velocity of 1.5m/s for the three mixtures. This behavior is aligned with the widely known rule of diluting effect of the wind. Nevertheless, when the percentage of formaldehyde increases, the downwind and crosswind distances are more sensitive in terms of atmospheric class because the vapor pressure and volatility of the mixture chance.

Simulations for a realistic scenario of a hole leak on the bottom of the tank were carried out. The direct influence of wind velocity and hole diameter were studied. For wind velocity effect on the dispersion of the formaldehyde, it was observed that for pure formaldehyde and 50% formaldehyde solution high values of wind velocity result in shorter impact distances. However, for 37% formaldehyde solution under class D, downwind and crosswind distance increase when wind velocity rises from 1.5m/s to 5m/s showing that the wind velocity promotes the mass transfer coefficient of the liquid in the pool, which means that pool dynamics gain more importance. Also, for the effect of hole diameter, it was observed that the size of the hole compared to wind and stability class plays a more significant role on the dispersion of the formaldehyde. A variation in hole size from 10mm to 30mm under atmospheric conditions of 1.5/F result in dramatic change in the impacted distances.

Simulated cloud footprint can provide necessary data to determine exclusion zones and design a facility layout as well as an emergency response plan. Results allow a better understanding of the dispersion phenomena and the PHAST software adjustable parameters.

7.2 Future work

Evaluate the effect of the possible reaction in the mixture on the dispersion of the cloud and validate those results using experimental data for release of formaldehyde, since PHAST software does not include the effect of chemical reactions.

Include the effect of other substances used in the process and how to manage the risk due to increment on the hazardous substance inventory and their interaction.

Study the behavior of mixtures with a composition less than 37% in order to see the influence of the pool dynamics and molecules interaction on the dispersion of the cloud.

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