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MASTER'S FINAL PROJECT
MASTER OF ENVIRONMENTAL ENGINEERING

Accident simulations of toxic gaseous emissions, fires and explosions in industrial facilities and their effect on a nearby hospital

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It was hard!!!

Abstract

CCSS is a public entity in charge of providing health and social security services for all the people of Costa Rica (anyone). A hospital, that is planned to be developed in the future, is located close to an industrial and residential zone, where there are companies that manage hazardous chemical substances. This situation represents a risk for hospital users and general habitants in case of industrial accidents like toxic gaseous emissions to the atmosphere, fires and blasts.

As part of a preliminary investigation and academic exercise, three sites that store this type of chemical compounds near the hospital's property were defined and designated as Sites A, B and C. At Site A, ammonium hydroxide is stored in 30% (w/w) solution; at Site B, nitric acid is preserved in solution at 70% (w/w) and Site C contains liquefied highly flammable dimethylamine within a pressurized tank. Therefore, considering flammability and storage conditions with the objective of analyzing eventual consequences, seven scenarios of accidents were planned to study and simulate. For this analysis, ALOHA software was applied, using meteorological data from Costa Rica and comparing the results with the corresponding Spanish legislation ("Real Decreto 1196/2003"), due to the lack of this kind of Costa Rican regulations. From the point of view of the hospital's property, the following results were obtained:

- At scenario 1 (Site A), a spill of aqueous ammonia that forms a pool was defined. It produces a toxic area of vapor cloud that reaches AEGL-1 (alert zone), which represents an impact extension on 4,100 m^2.
- At scenario 2 (Site B), a spill of nitric acid that forms a pool was defined. It produces a toxic area of vapor cloud that reaches AEGL-1 (alert zone), which represents an impact extension on 11,500 m^2.
- At scenario 3 (Site C), a not burning leaking tank of dimethylamine was defined. It produces a toxic area of vapor cloud which does not impact the hospital.
- At scenario 4 (Site C), an ignition of dimethylamine's toxic vapor cloud was defined. It produces a flash fire which does not impact the hospital.
- At scenario 5 (Site C), a blast from the flash fire of dimethylamine was defined. It produces an overpressure which does not impact the hospital.
- At scenario 6 (Site C), a jet fire from a leaking tank of dimethylamine was defined. It produces thermal radiation area which does not impact the hospital.

- At scenario 7 (Site C), a BLEVE and fireball/pool fire from a leaking tank of dimethylamine was defined. It produces thermal radiation area that reaches more than 5 psi (intervention zone), which represents an impact extension on 33,914 m^2.

Variations in wind direction could change the distribution of the consequences on the hospital's property (for all the simulated scenarios). Because of this, it is for sure that the obtained results are not static or definitive. So, considering hospital patients as a critical population group and according to the "Real Decreto 1196/2003", it is not advisable to unify industrial production areas where hazardous chemicals are managed, with residences and hospitals in the same alert zone. Therefore, they must not coexist.

It is important to take into account that a hospital can never stop working and must also be solvent in dealing with emergency situations. Therefore, any impact to human health of people outside the hospital's property (in any of the scenarios) will indirectly affect this facility, as these people will attend to it for medical care and will saturate its services. This means that as part of the operations and organization of the hospital, it is necessary to plan and anticipate what to do in such case. If the hospital does not have sufficient response capacity to care for those affected, it will have to refer them to other health centers, consuming resources and valuable time that would put the people at greater risk.

Because the CCSS is not subject to the regulations of the "Real Decreto 1196/2003", it should consider the results of this project, in order to promote a teamwork group with agrochemical industry companies that surround the hospital for evaluating the risk of toxic, radiative or overpressure pollution about accidents related with spills, leaks, fires and explosions. Also, given that the hospital has not been designed yet, the CCSS should incorporate in the construction plans, solutions in infrastructure and resistance of materials to the fire, suitable electromechanical connections and many other aspects that mitigate the impact of the accidents considered in this MFP.

The agrochemical companies at Sites A, B and C, in order to promote the safety of the infrastructure, their occupants and neighbors, should also update their facilities considering the recommendations in the "Manual de Disposiciones Técnicas Generales Sobre Seguridad Humana y Protección Contra Incendios". And finally, it would be important to generate a plan so that preventive and corrective actions could be taken into account to reinforce primary control systems through operational tasks or projects.

Index

1. Introduction

CCSS is a public entity in charge of providing health and social security services for all the people of Costa Rica (anyone). The insurance covers all the country, for which it has more than 1,300 healthcare centers that sums more than 1,200,000 square meters in infrastructure.

Since its distribution is so widespread in the territory, its facilities are often close to multiple types of buildings, according to the municipal land use and urban regulations. Thus, it is not atypical to find a healthcare center located into a mixed urban zone (industrial and residential). In this case, a hospital will be built relatively close to a zone, where hazardous chemicals are managed, mainly for agricultural use. Obviously, this situation represents a risk for hospital users (internal staff, patients -whose normal physiological capacity is diminished- and clients in general) and habitants, in case of emission accidents of toxic substances to the atmosphere or events related with fires or blasts.

In the present study, it is assumed from an academic point of view, that, around the mentioned hospital, there are three agrochemical companies handling dangerous substances, in which industrial accidents may occur. Taking this into account and according to the weather conditions of the zone, it is necessary to determine the consequences to human health in the event of such accidents according to the related regulations and also, establish if hospital and this kind of industries can coexist closely in the same zone.

In any case, the study is important for the general population because, if an accident of this type occurs and even though the immission might not reach the hospital's property, the affected people do will need medical support in the same hospital and could saturate the resolutive capacity of it. Therefore, to avoid this chaotic situation, a planned response is necessary.

The study has as a significant restriction to access the actual information about types and amounts of chemical substances that are produced and / or stored in the mentioned sites, as well as the variability of the processes and lines of production that are developed there. This means that the quantities and compounds to be analyzed may differ according to the modifications of their inventories or the chemical and industrial processes they apply. So the present MFP cannot be considered as a formal and official public document, it is an academic and hypothetical exercise.

Therefore, it is proposed that according to the results and trends obtained in this MFP, it will be coordinated with these private companies to jointly study the situation considering much more facts and data to integrate a global response that also could involve other public and private organizations for the proper management of emergencies.

1.1. Location of the hospital in relation to the agrochemical industry and existence of hazardous chemicals

The location of the hospital was defined as a ground surface or area of coverage, which will contemplate the infrastructure of the hospital (includes buildings, parking lots, engine room, internal streets, and any related facility). It has not been designed yet.

Once the future hospital was located, a review of the surrounding area was carried out to determine the number of existing agrochemical companies. Each one was consulted via telephone or e-mail about the dangerous chemicals and process conditions they manage and how are stored, whether pressurized or not. Those industries that only handled granulated agrochemicals (most of them) were discarded, due to the stability of the final product to melt and evaporate at ambient temperature.

Once the information was collected, a visit was made to the chosen organizations to get a better idea of the management they carry out with the dangerous compounds and the safety measures applied. About the specific manufacturing processes, the companies were more hermetic when providing information. Also, due to aspects of market competition, they did not want to explain in detail how much they produce monthly, just how much dangerous substances are usually stored (information on inventory management was not provided).

It is emphasized that despite having received the collaboration of these private companies, they wish not to be mentioned their name in the present work, even though they showed openness in teaching the facilities. So, most of the obtained data was taken as a result of the visit and interviews carried out, that is to say, there are no official reports, trades or documents that support the collection of the data.

So, if the results of the present study show that the hospital is at risk of being affected in the event of accidents in the surrounding agrochemical industry, companies are willing to collaborate more openly, provided there is an official request between the competent authority of the government and private organizations. This is because this industry has many years to exist and, as part of their operating permissions, they have never been asked for a similar analysis to this one, so because of the hospital is the one who has just arrived in the neighborhood, it needs to evaluate the existing risk conditions around it.

1.2. Types of accidents in the agrochemical industry near the hospital

Based on the technical assessment of the storage conditions of hazardous compounds in the agrochemical industry near the hospital, two fundamental aspects were determined. First, it was important to define the type of accident that could occur and second, to estimate the effects these accidents could generate. Thus, for the stored liquid chemicals that are related with this work (because there are many types of chemical accidents), the following events may occur (Nolan, 2011 and ALOHA, 2016):

1) Accidents with toxic substances:
   a) *Evaporating pool.*
   b) *Leaking tank (not burning).*
2) Accidents with flammable and toxic substances:
   a) *Flash fire.*
   b) *Blast.*
   c) *Jet fire.*
   d) *BLEVE and fireball.*
   e) *Pool fire.*

For more details of each accident, see Attachment 1.

1.3. Analytical models for described type of accidents, description, and simulation

The mathematical models that form part of the analytical (but not exclusive) basis of most specialized commercial software to determine the dispersion of air pollutants, overpressures and thermal radiation are described below shortly.

1.3.1. The Gaussian air pollutant dispersion model

The atmospheric dispersion models are also known as atmospheric diffusion models, air dispersion models, air quality models, and air pollution dispersion models. This modeling is the mathematical simulation of how air pollutants disperse in the atmosphere. It is performed with computer programs that solve the mathematical equations and algorithms which simulate the pollutant dispersion. The dispersion models are used to estimate or to predict the downwind concentration of air pollutants emitted from sources such as industrial plants, vehicular traffic, or accidental chemical releases. The results of dispersion modeling, using worst case accidental releases and meteorological conditions, can provide estimated locations of impacted areas, and be used to determine appropriate protective actions.

The dispersion models vary depending on the assumptions used to develop the model, but all require the input of data that may include:

- Meteorological conditions such as wind speed and direction, the amount of atmospheric turbulence (as characterized by what is called the "stability class"), the ambient air temperature, the height to the bottom of any inversion aloft that may be present, cloud cover and solar radiation.
- The emission parameters such the type of source, the mass flow rate, the source location and height, the source exit velocity, and the source exit temperature.
- Terrain elevations at the source location and at receptor locations, such as nearby homes, schools, businesses, and hospitals.
- The location, height, and width of any obstructions (such as buildings or other structures) in the path of the emitted gaseous plume as well as the terrain surface roughness.

Many of the modern, advanced dispersion modeling programs include a pre-processor module for the input of meteorological and other data, and many also include a post-processor module for graphing the output data and/or plotting the area impacted by the air pollutants on maps. The plots of areas impacted usually include isopleths showing areas of pollutant concentrations that define areas of the highest health risk. The isopleths plots are useful in determining protective actions for the public and first responders. (Arzate, 2004).

1.3.2. The heavy gas model and the models to analyze blasts and fires (flash fires, jet fires, BLEVEs and pool fires)

Industrial gases are globally produced, processed, transported, and stored in considerable quantities. A significant portion of these gases are heavier than air due to their high molecular weight and/or the low temperatures associated with some accidental release scenarios. The most commonly used gases include flammable gases (liquefied petroleum gas and liquefied natural gas) as well as the toxic heavy gases (chlorine and ammonia).

While light gases, due to densities lower than air, rise up and can be analyzed by the Gaussian model, the heavy gases sink to the ground, where they can spread and flow through uneven terrain. They can remain below ground for long periods of time potentially representing a danger to humans and environment and generally, can involve longer distances than light gases. (Dong et al, 2017)

That is why the Gaussian model does not apply for analyzing the behavior of heavy gases. In this case, several adjustments must be made to develop a significant study. For the present work, and as will be explained further, the software ALOHA was chosen to make predictions. It is very clear about the internal logic that uses when applying the Gaussian model, which is the most used all over the world by the scientific community, commercial computational programs, and teaching centers.

Nevertheless, in relation with heavy gases, ALOHA will automatically determine -based on the storage conditions, accident characteristics, the physical properties of the leaking compound and the meteorological conditions-, if it is more appropriate to use the heavy gases model instead of the Gauss model. Also, the results obtained are mainly graphs, so there is no tabulated data or calculation memory (formulas and process of calculus) to corroborate the estimates made. This is not atypical for this type of programs since most of them do not show the user the internal logic and the characteristics of each model, including the scientific basis of them.

Similar to blasts and fires models, ALOHA does not clarify the type of equations and calculus that are applied for the analysis. In this sense, the interpretation value of the obtained results is emphasized over the process of its internal estimation. For a more detailed analysis, it is recommended to use specific software or models for blasts and fires, like for example, Bevi (RIVM, 2009) and “Yellow Book” (CPR, 2005).

1.4. Reference limits for gaseous concentrations of pollutants, overpressure and thermal radiation

The results of applying each of the analytical models mentioned would not make sense without reference limits to compare them with. These ranges are explained below.

1.4.1. Gaseous concentrations of pollutants

In the case of the Gaussian and heavy gas models for sizing the affected areas according to the displacement of the toxic cloud and its concentrations, several LOCs of gaseous pollutants can be used, which are public exposure guidelines. Due to the lack of this kind of regulations in Costa Rica, this MFP was designed according to "Real Decreto 1196/2003" (which is actually very restrictive) and the most common reference limits which are AEGLs, ERPGs, and TEELs, in that same order of priority. These concentrations limits were applied for emissions of 60 minutes, which is the maxima default lapse of time analysis used by ALOHA. For more details about LOCs, see Attachment 2.

1.4.2. Explosive limits for flammable substances (flash fires)

In addition to the aforementioned limits, for the case of the evaporation of flammable substances and in order to determine the displacement of the toxic cloud that can be burned if it is found with an ignition source, the concentrations defined by LEL and UEL are used. They both refer to the mixture's proportion of a gaseous compound in the air. If the mixture of the gas is between LEL and UEL with a proper ignition source, it will burn. (Nolan, 2011 and ALOHA, 2016).

1.4.3. Overpressures limits for blasts

Due to the lack of this kind of regulations in Costa Rica, this MFP was designed according to the overpressure values, indicated in "Real Decreto 1196/2003" that can be checked in Attachment 4.

1.4.3. Thermal radiation limits for jet fires, pool fires and BLEVEs

Due to the lack of this kind of regulations in Costa Rica, this MFP was designed according to the thermal radiation values for 30 seconds (time period available for both, intervention and alert zones), indicated in "Real Decreto 1196/2003" that can be checked in Attachment 5.

1.5. ALOHA: the software chosen for analysis

Following the procedure, the USEPA's and NOOA's freeware ALOHA was chosen as the computer tool that making use of the mentioned mathematical models and depending on the introduced data, carries out the dispersion analysis of pollutants and the determination of overpressures and thermal radiation. ALOHA was designed to respond to emergency situations by estimating hazard zones associated with the emission of hazardous compounds. (ALOHA, 2016).

ALOHA is used primarily for emergency response or planning situations, where the goal is to assess the threat posed to the general public by a chemical release. For toxic releases, ALOHA uses public exposure guidelines preferentially for the default toxic level of concerns (LOCs), because these guidelines are specifically designed to predict how the general public will respond to a short-term, one-time release.

ALOHA's results can be unreliable when the following conditions exist: very low wind speeds, very stable atmospheric conditions, concentration patchiness -particularly near the release source- and wind shifts and terrain steering effects.

ALOHA does not account for the effects of: byproducts from fires, explosions, or chemical reactions; particulates, chemical mixtures, terrain and hazardous fragments. The technical reasons for choosing ALOHA for this MFP are related to the criteria of the "Comisión Técnica de Prevención y Reparación de Daños Medioambientales del MAGRAMA", see Attachment 3.

2. Objectives

The main objective of this study is to determine if a hospital can be reached by the toxic effects, overpressure or radiation associated to accidents in the surrounding agrochemical industry. In order to accomplish this objective, the following goals are proposed:

- To define the scenarios of accidents in the agrochemical industry near the hospital related to emission of contaminants, blasts and fires.
- To determine the concentrations of gaseous pollutants, overpressures and radiation on the hospital ground level against the corresponding exposure levels defined by legislation.
- To set if the hospital's property is at risk when being located close to this industry.

3. Results and discussions

3.1. Location of the hospital and the agrochemical industry around it, as well as weather and geographical conditions of the zone

As mentioned, the study area is the future hospital's property, which is the site where the effects of dispersion of gaseous pollutants, overpressures and thermal radiation produced by accidents in the surrounding agrochemical industry will be analyzed. Three sites were found to store hazardous chemicals, which were designated by privacy policies as Site A, Site B and Site C, whose location with respect to the hospital is shown in the following diagram:

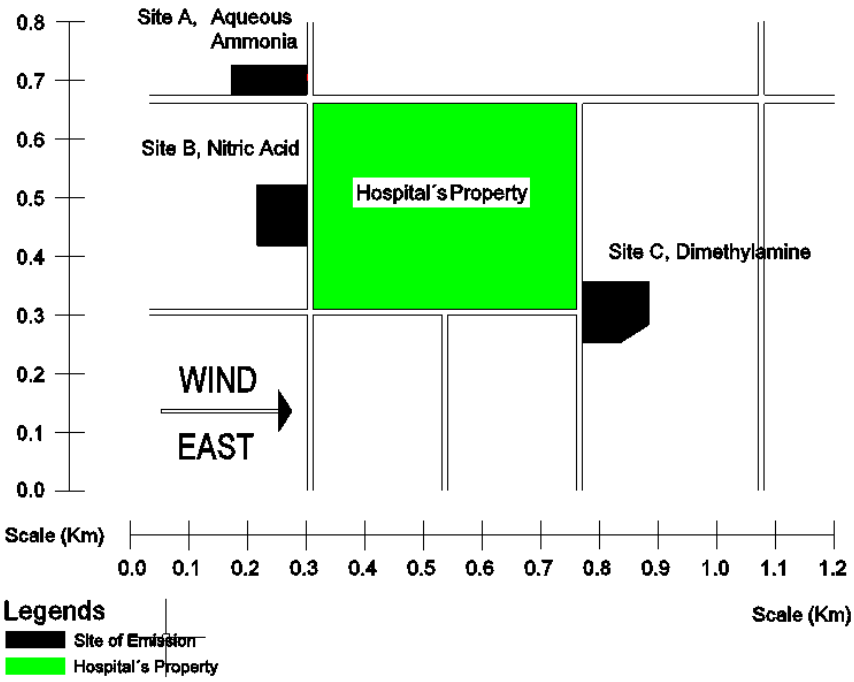

Figure 1. Location of hospital and surrounding sites where industrial accidents could happen.

From the above figure, Site A is located at the northwest of the future hospital's property. Site B is located at the east of this same zone and Site C at the southeast. It is noted that all of them, are single storied building type and that their surroundings are sheltered, by other facilities and natural elements.

The prevailing weather conditions required to conduct the analysis of the gaseous emissions behavior were obtained from the Meteorological Institute of Costa Rica (IMCR), based on several measurements made since the last century. The table below shows monthly data on wind speed, ambient temperature and relative humidity.

Table 1. Weather conditions and ground roughness at Sites A, B and C.

Month	*Wind speed (m/s)*[1]	*Air temperature (°C)*[2]	*Humidity (%)*[3]
January	14.9	17.9	83.5
February	14.4	18.3	81.9
March	14.1	18.9	81.3
April	13.0	19.6	82.4
May	9.4	20.0	85.5
June	8.9	19.9	86.1
July	10.6	19.6	86.2
August	9.3	19.7	86.1
September	7.4	19.7	86.2
October	7.8	19.7	86.9
November	10.2	19.0	87.5
December	13.2	18.3	85.7
Average	**11.1**	**19.2**	**84.9**

Thus, for all sites A, B and C, as well as for the location of the hospital, average annual wind velocity is 11.1 m/s; the ambient temperature is 19.2°C and the relative humidity is 84.9%.

In addition, according to the same data source, it is important to highlight the following geographic and meteorological aspects that are needed for the analysis of gaseous pollutants, overpressures and thermal radiation through ALOHA:

- Elevation (above mean sea level): 1,396 m.
- Offset from local standard time to GMT: +6 hours.
- Measurement height above ground of the weather station: 10 m.
- Ground roughness: urban.
- Wind direction: west-east.
- Cloud cover (nubosity): partly cloudy.
- Stability class: D (neutral).
- No inversion considered.

[1] Data collected since 1997 to 2015, IMCR.
[2] Data collected since 1951 to 2014, IMCR.
[3] Data collected since 1993 to 2014, IMCR.

3.2. Hazardous chemicals stored at Sites A, B and C and types of accidents

At Site A, ammonium hydroxide is stored in 30% (w/w) solution; at Site B, nitric acid is preserved in solution at 70% (w/w) and Site C contains liquefied dimethylamine within a pressurized tank. Based on the analysis that is intended to be performed by ALOHA and the data it requires as inputs, the most important properties of the commented substances are shown below:

Table 2. Properties of chemicals involved in accidents at Sites A, B and C.

Characteristic	*Site A's chemical, aqueous ammonia,*	*Site B's chemical, nitric acid,*	*Site C's chemical, dimethylamine*
Chemical formula	NH_4OH	HNO_3	$(CH_3)_2NH$
Physical state	Liquid solution, 30% w/w	Liquid solution, 70% w/w	Liquified gas
Molecular weight	17.03 g/mol	63.01 g/mol	45.08 g/mol
AEGL-1 (1 hour)	30 ppm	0.16 ppm	10 ppm
AEGL-2 (1 hour)	160 ppm	24 ppm	66 ppm
AEGL-3 (1 hour)	1,100 ppm	92 ppm	250 ppm
Ambient boiling point	21.6˚C	117.3˚C	3,1˚C
IDLH	300 ppm	25 ppm	300 ppm
LEL	150,000 ppm	Nonflammable	28,000 ppm
UEL	280,000 ppm	Nonflammable	144,000 ppm
Vapor pressure	---	---	>1 atm
Partial pressure at ambient temperature:	0.75 atm	0.0038 atm	---
Ambient saturation concentration (ppm)	88,500	4,441	1,000,000

It should be noted that there are evidently in these sites many more chemicals stored but these are the most representative of each, according to the queries made regarding their hazard and stored amount. Also, as an important fact, note that only the nitric acid compound is nonflammable and the only one stored in a pressurized tank is the dimethylamine, which is not a solution, as the others are.

Taking these properties as guides (flammability and storage) and with the objective of categorizing the analysis, a hierarchical diagram was made to determine the possible accidents that can happen, which is shown below:

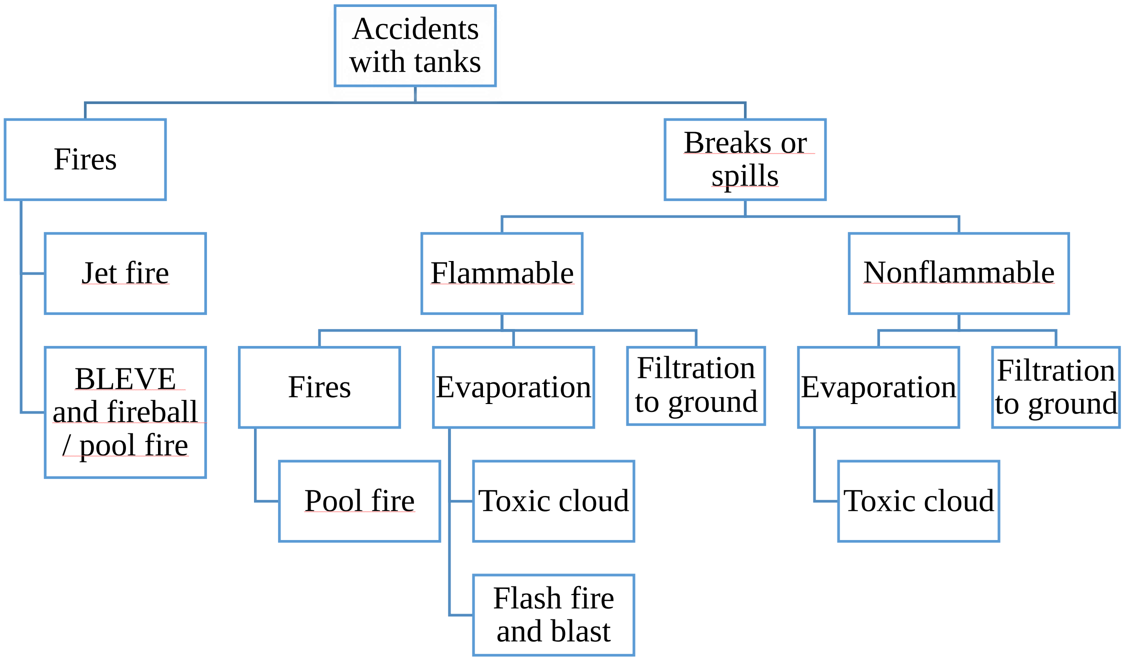

Figure 2. Possible accidents according to flammability and storage conditions.

As it can be observed from the above diagram, all accidents happen from failures related with tanks and from internal or external events. In case of fires, a jet fire can occur if the chemical escapes from the tank and immediately encounters a source of ignition (spark or flame). Also, a BLEVE can happen if an external source boils the tank up and makes it explode, which causes a fire ball. Eventually, a pool fire is also possible.

On the other hand, the containing of the tanks can spill due to a hole (break) or failure in a valve, forming pools which can evaporate, burn or filtrate to the ground. If the chemical is flammable and the pool makes contact with an ignition source, it can generate a pool fire. If not, it can evaporate at its particular rate according with its chemical and physical properties. Thus, it can produce a toxic cloud that if encounters a source of ignition and the concentration of it is between the explosive limits, a flash fire could happen and maybe a blast, too. At any case, the chemical solution could infiltrate to the ground. If the chemical of the pool is nonflammable, it just can evaporate (forming a toxic cloud) or infiltrate to the ground.

In summary, the following table defines the possible accidents that can occur in Sites A, B and C and their consequences, taking into account the alternatives of analysis given by ALOHA. It includes the model to be applied for each case and the type of parameter it will measure, according to the related legislation (Spain, 2003):

Table 3. Scenarios of accidents at Sites A, B and C.[4]

Scenario	**Site and Chemical**	**Type of Accident**	**Consequences**	**Model Run**	**Type of Parameter[5]**
1	Site A, aqueous ammonia, NH_4OH (liquid solution, 30% w/w)	Evaporating pool	Toxic area of vapor cloud	Gaussian	AEGLs
2	Site B, nitric acid, HNO_3 (liquid solution, 70% w/w)	Evaporating pool	Toxic area of vapor cloud	Gaussian	AEGLs
3	Site C, dimethylamine, $(CH_3)_2NH$ (pressurized liquid)	Leaking tank (not burning)	Toxic area of vapor cloud	Heavy gas	AEGLs
4			Flammable area of vapor cloud (flash fire)	Heavy gas	Thermal radiation
5			Blast area of vapor cloud explosion	Heavy gas	Overpressure
6		Leaking tank (jet fire)	Thermal radiation area	Not specified by ALOHA	Thermal radiation
7		BLEVE and fireball/pool fire	Blast and thermal radiation area	Not specified by ALOHA	Overpressure (BLEVE) and thermal radiation (fireball/pool fire)

[4] Other possible scenarios like flash fire and blast of aqueous ammonia (flammable chemical) were not considered in this table, because after running the related models in ALOHA, the results are not significant or negible.
[5] According to "Real Decreto" 1196/2003.

3.3. Analysis of accidents at Site A

To model the accidents in Site A, it is necessary to define the basic storage and release conditions of aqueous ammonia. These are shown in the following table:

Table 4. Storage conditions and release of aqueous ammonia by accident at Site A.

Chemical	Aqueous Ammonia
Type of accident	Evaporating pool
Area of the pool	200 m²
Volume of the pool	8 m³
Ground type	Concrete
Ground temperature	19.2˚C
Pool temperature	Ground temperature
Realease duration	60 minutes (by default)
Maximun average sustained release rate	207 kg/min, see Figure 3
Total amount hazardous component released	1,508 kg

The evaporation rate of the chemical has the following behavior during the leak:

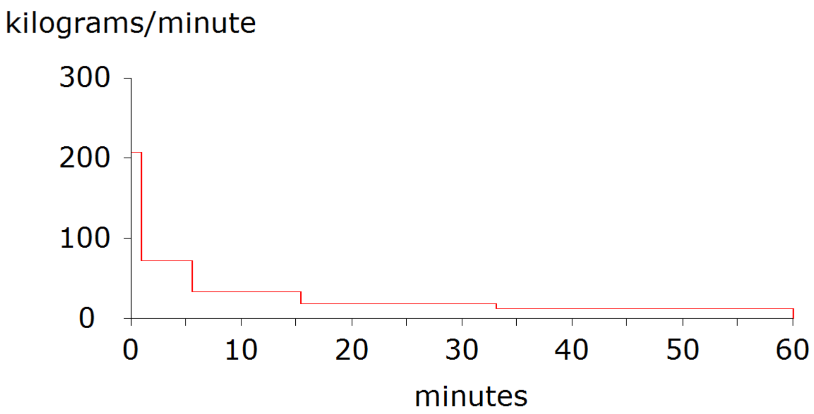

Figure 3. Evaporation rate of aqueous ammonia at Site A (ALOHA, 2016).

From the above, during the first 10 minutes practically 90% of the compound escapes from the pool to the atmosphere. Therefore, following consequences could occur:

3.3.1. Toxic area of vapor cloud, scenario 1

When carrying out the model run (Gaussian), the following dispersion chart of pollutants is generated (Figure 4):

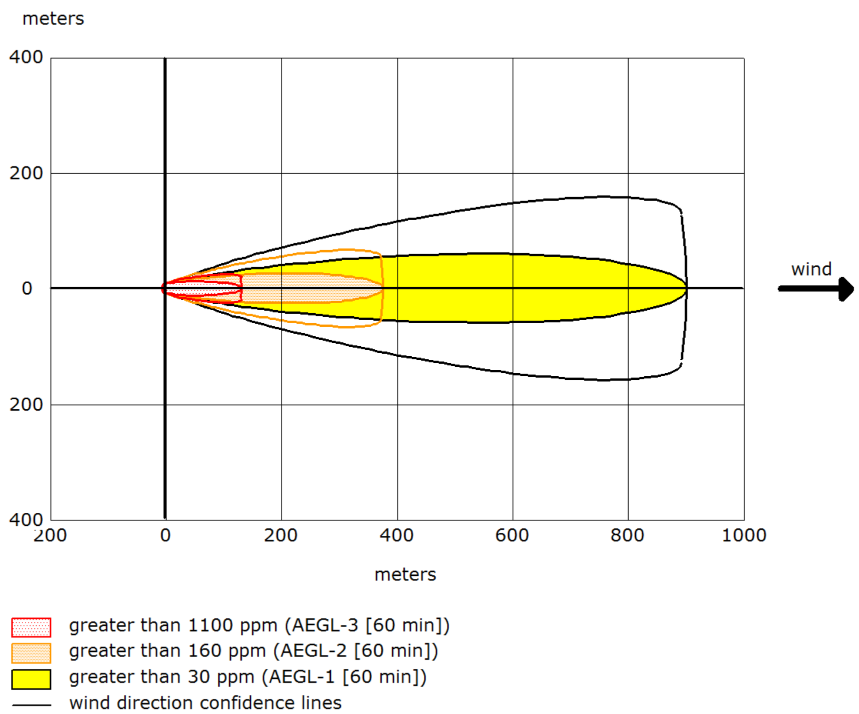

Figure 4. Toxic cloud of aqueous ammonia due to the accident at Site A. (ALOHA, 2016).

It is interpreted from the above that the toxic cloud whose concentration exceeds AEGL-1 reaches almost 900 linear meters in the direction of the wind (west-east) from the point of emission and extends from its central axis to both sides up to 60 linear meters; being able to produce in this zone discomfort, irritation, or certain asymptomatic, non-sensory effects over the general population (alert zone).

Also, the toxic cloud whose concentration exceeds AEGL-2 reaches almost 380 linear meters in the direction of the wind (west-east) from the point of emission and extends from its central axis to both sides up to 26 linear meters, being able to produce in this zone irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape (intervention zone).

In addition, the toxic cloud whose concentration exceeds AEGL-3 reaches almost 130 linear meters in the west-east direction from the point of emission and extends from its central axis to both sides up to 11 linear meters. Into this zone, the effects ca be life-threatening health effects or death zone.

If Figure 4 is superimposed on the location of the hospital's property, it results as follows (Figure 5):

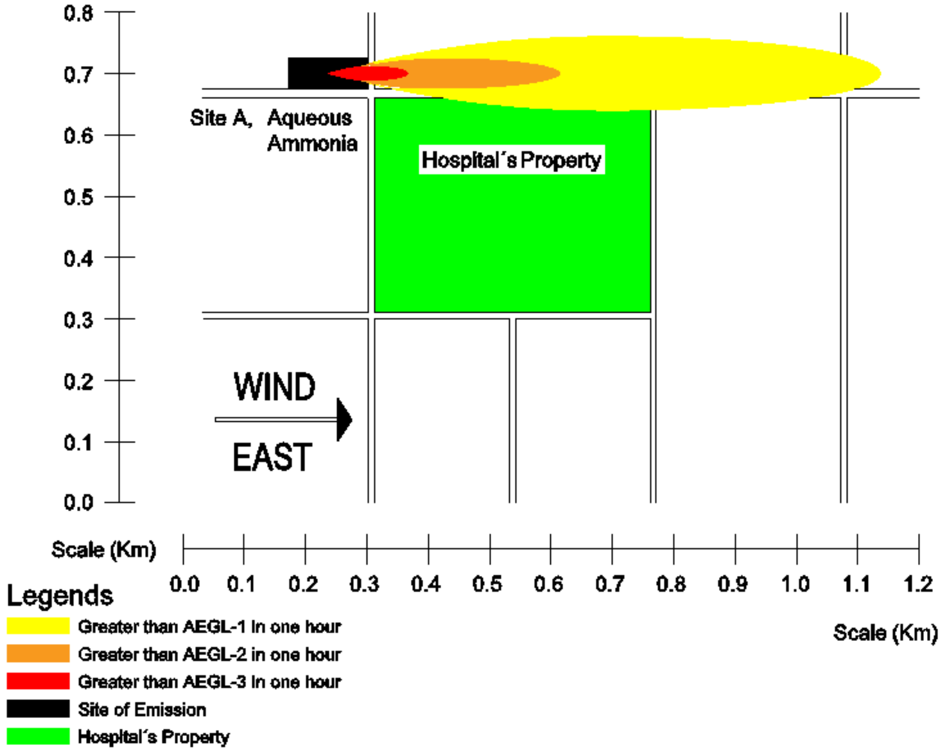

Figure 5. Area of the toxic cloud of aqueous ammonia due to the accident at Site A and its spatial relation with the hospital's property.

Based on the above, the cloud of aqueous ammonia coming from the spill or break of the tank at Site A, would affect the hospital's property, in the northern sector (main accesses), which corresponds to approximately 2.84% of the coverage of the land (4,100 m^2 of 143,932 m^2). This fact, for a concentration that only surpasses AEGL-1 (alert zone).

Evidently, if an accident of this nature happens, even though the toxic cloud would not almost impact the hospital's property, there will be health consequences in those who are reached by the air toxicity (in the rest of the industrial-residential zone), because it will reach AEGL-2 and AEGL-3. These people will probably attend to the hospital and this fact will affect the demand of the healthcare services, so the capacity of response of this infrastructura and its effectiveness will be reduced.

3.4.Analysis of accidents at Site B

To model the accidents in Site B, it is necessary to define the basic storage and release conditions of nitric acid. These aspects are shown in the following table:

Table 5. Storage conditions and release of nitric acid by accident at Site B

Chemical	Nitric acid
Type of accident	Evaporating pool
Area of the pool	135 m²
Volume of the pool	2.25 m³
Ground type	Concrete
Ground temperature	19.2˚C
Pool temperature	Ground temperature
Realease duration	60 minutes (by default)
Maximun average sustained release rate	1.43 kg/min, see Figure 6
Total smount hazardous component released	84.9 kg

The evaporation rate of the chemical has the following behavior during the leak:

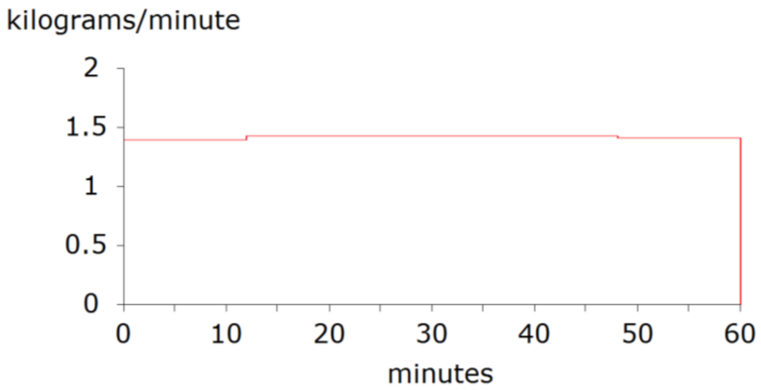

Figure 6. Evaporation rate of nitric acid at Site B. (ALOHA, 2016).

From the above, during the 60 minutes of analysis, the compound escapes from the pool, practically at the same rate, so there is enough chemical to continue evaporating after this lapse of time. Therefore, following consequences could occur:

3.4.1. Toxic area of vapor cloud, scenario 2

When carrying out the model run (Gaussian), the following dispersion chart of pollutants is generated:

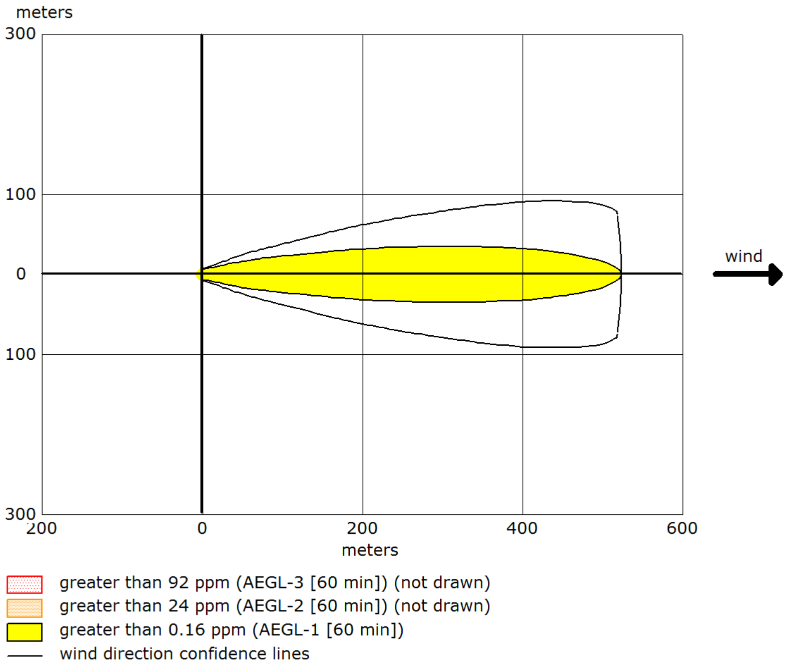

Figure 7. Toxic cloud of nitric acid due to the accident at Site B. (ALOHA, 2016).

It is interpreted from the above that the toxic cloud whose concentration exceeds AEGL-1 reaches almost 525 linear meters in wind direction (west-east) from the point of emission and extends from its central axis to both sides up to 35 linear meters; being able to produce in this zone discomfort, irritation, or certain asymptomatic, non-sensory effects over the general population (alert zone). AEGL-2 and AEGL-3 are nor reached at any point. If Figure 7 is superimposed on the location of the hospital's property, it results as follows (Figure 8):

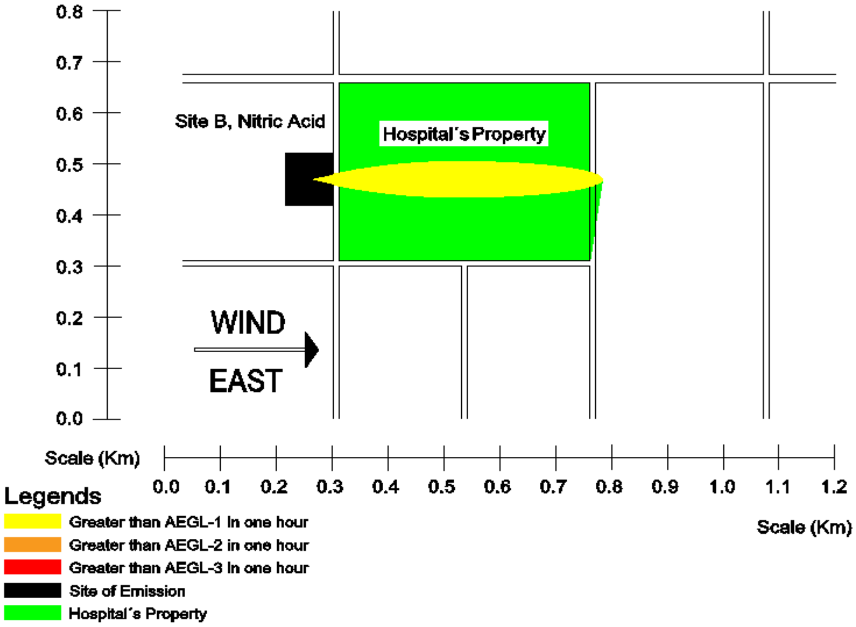

Figure 8. Area of the toxic cloud of nitric acid due to the accident at Site B and its spatial relation with the hospital's property.

Based on the above, if a nitric acid spill accident occurs at Site B, the toxic cloud produced would do affect the hospital's property in the middle sector (main buildings), which corresponds to approximately 15.98% the coverage of the land (11,500 m^2 of 143,932 m^2). In this case, concentration only surpasses AEGL-1 (alert zone).

3.5. Analysis of accidents at Site C

To define the accidents in Site C, it is necessary to define the basic conditions of the dimethylamine. These aspects are shown in the following table:

Table 6. Storage conditions and release of dimethylamine by accident at Site C

Chemical	Dimethylamine
Type of accident	Various
Kind of tank	Vertical cylinder
Diameter	1.2 m
Length	3.05 m
Volume:	3.45 m^3
State of the chemical	Liquid
Temperature within the tank	Ambient temperature
Mass in the tank	2 ton
Liquid volumen	2.76 m^3
Percentage full by volume	80%
Shape that best represents the opening through which the pollutant is exiting	Circular opening
Opening diameter	0.05 m
Is leak thorugh a hole or short pipe/valve?	Valve
Bottom of the leak	0.4 m
Release duration	10 min
Maximun average sustained release rate	214 kg/min, see Figure 9
Total amount released	1,778 kg
Note	Note: The chemical escaped as a mixtured of gas and aerosol (two phase flow)

The conditions assumed for this accident (valve failure, valve opening size, tank filling volumes, etc.) are the typical ones that can occur in reality. However, this does not imply that different scenarios of hazardous pollutants releasing may occur. In those cases, the analysis procedure would be similar.

The evaporation rate of the chemical has the following behavior during the leak:

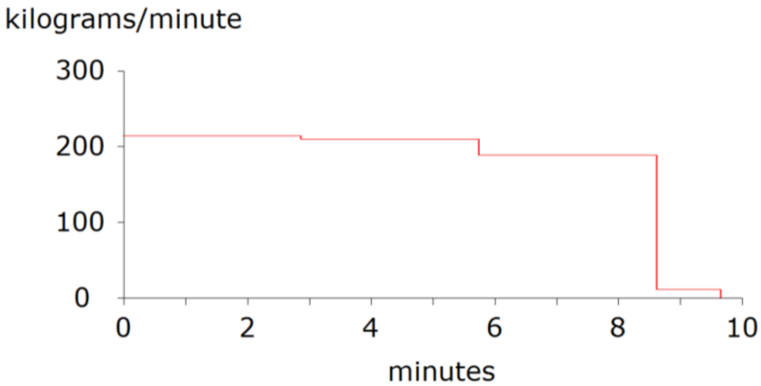

Figure 9. Evaporation rate of dimethylamine at Site C. (ALOHA, 2016).

From the above, during the first 10 minutes all the chemical evaporates to the atmosphere, without forming a pool first, due to its low boiling point (3.1°C). So, an analysis of 60 minutes by default in unnecessary. Therefore, following consequences could occur:

3.5.1. Toxic area of vapor cloud, scenario 3

When carrying out the model run (heavy gas), the following dispersion chart of pollutants is generated:

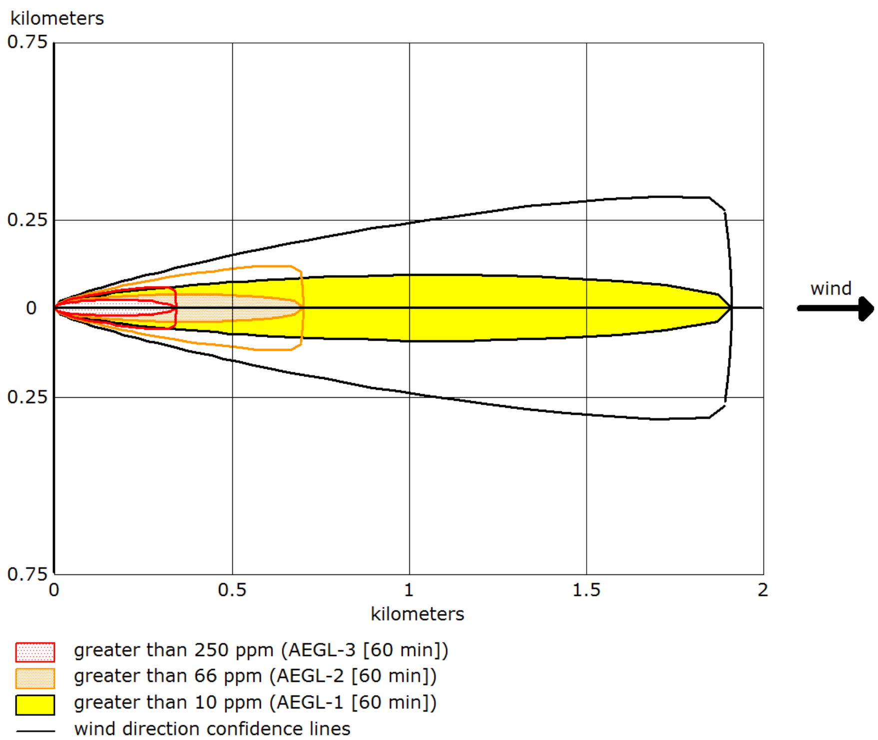

Figure 10. Toxic cloud of dimethylamine due to the accident at Site C. (ALOHA, 2016).

It is interpreted from the above that the toxic cloud whose concentration exceeds AEGL-1 reaches almost 1,890 linear meters in the direction of the wind (west-east) from the point of emission and extends from its central axis to both sides up to 98 linear meters; being able to produce in this zone discomfort, irritation, or certain asymptomatic, non-sensory effects over the general population (alert zone).

Also, the toxic cloud whose concentration exceeds AEGL-2 reaches almost 700 linear meters in the direction of the wind (west-east) from the point of emission and extends from its central axis to both sides up to 40 linear meters, being able to produce in this one Irreversible zone or other serious, long-lasting adverse health effects or an impaired ability to escape (intervention zone).

In addition, the toxic cloud whose concentration exceeds AEGL-3 reaches almost 335 linear meters in the west-east direction from the point of emission and extends from its central axis to both sides up to 23 linear meters, being able to produce life-threatening health effects or death zone.

If Figure 10 is superimposed on the location of the hospital's property, it results as follows (Figure 11):

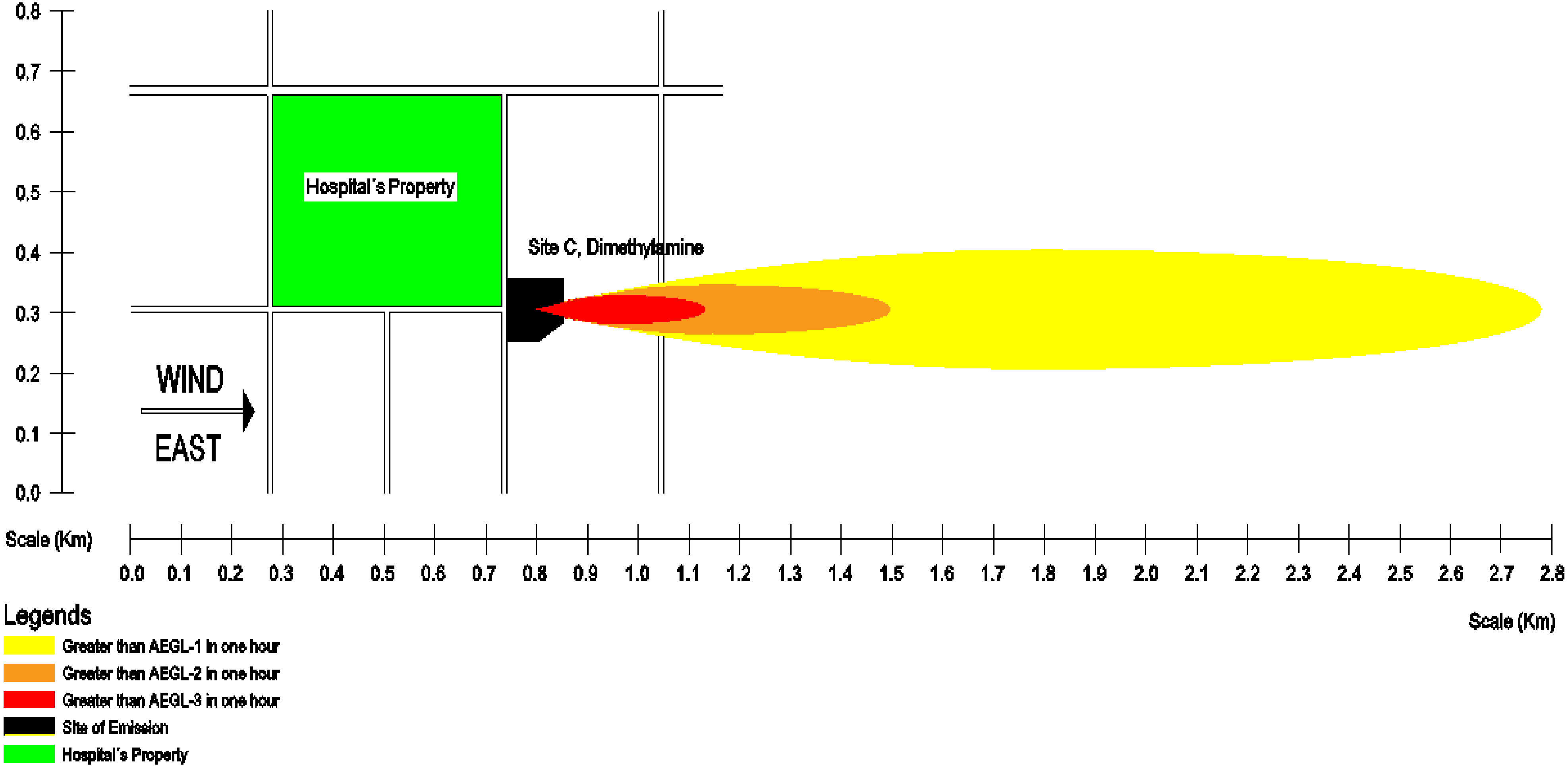

Figure 11. Area of the toxic cloud of dimethylamine due to the accident at Site C and its spatial relation with the hospital’s property.

Based on the above, if a leakage of dimethylamine occurs in Site C, the toxic cloud produced would not affect the hospital's property, although it would affect the urban sector to the east of the site of emission up to a distance of almost 2.8 km, in concentrations exceeding from AEGL-1 to AEGL-3.

Obviously if an accident of this nature happens, even though the toxic cloud would not almost impact the hospital's property, there will be health consequences in those who are reached by the air toxicity (in the rest of the industrial-residential zone). These peolple will attend the hospital and it will directly affect the demand of the healthcare services, so the capacity of response of this infrastructura and its effectiveness will be reduced.

3.5.2. Flammable area of vapor cloud, scenario 4

When carrying out the model run (heavy gas), the following dispersion chart of pollutants is generated:

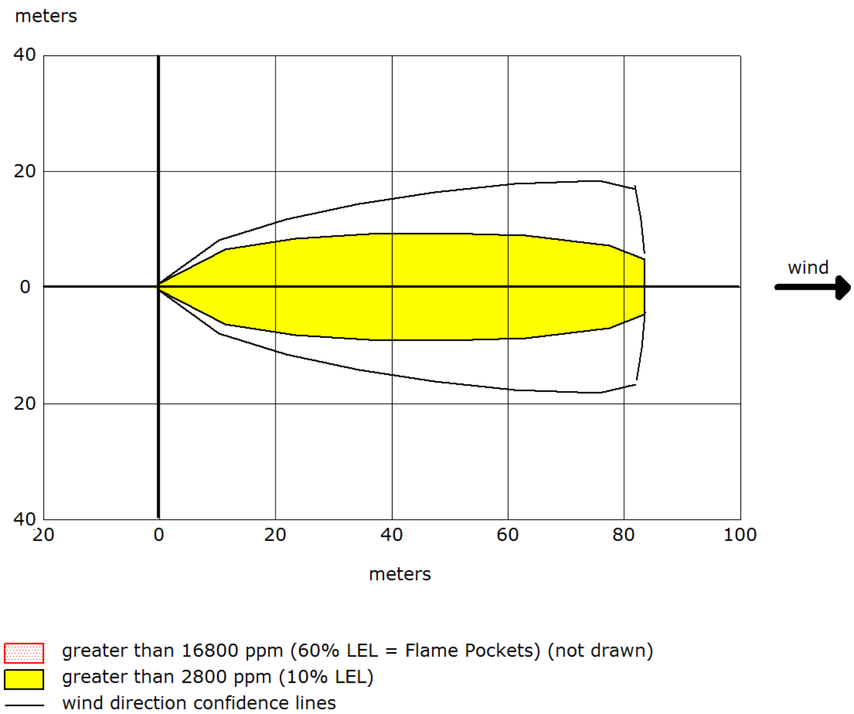

Figure 12. Flammable area of vapor cloud of dimethylamine due to the accident at Site C. (ALOHA, 2016).

Based on the above graph, it is observed that the flammable area of vapor cloud is present and reaches the yellow zone (10% LEL, enough to burn), which has a maximum distance of 84 linear meters in the direction of the wind (west-east) from the point of emission and extends from its central axis to both sides up to 10 linear meters. Due to its short extension and the wind direction, this accident would not affect the hospital's property, because it would almost exclusively be limited to the site of the emission.

3.5.3. Blast Area of Vapor Cloud, scenario 5

When carrying out the model run (heavy gas), the following dispersion chart of blast area of vapor cloud explosion ignited by spark or flame is generated:

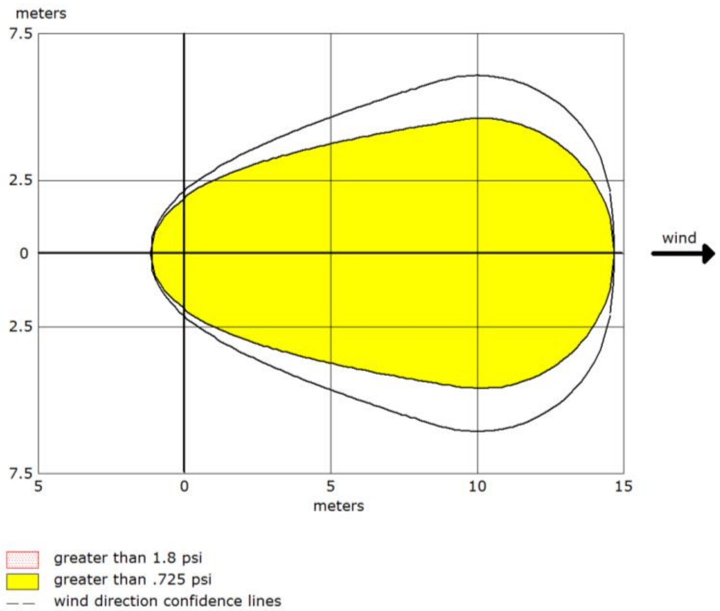

Figure 13. Blast area of steam cloud explosion ignited by spark or flame at Site C and its spatial relation with the hospital's property.

Based on the above graph, it is observed that the blast area of vapor cloud explosion ignited by spark or flame only reaches the yellow zone (greater than 0.725 psi), which corresponds with alert zone. The blast has a maximum length of 16 linear meters and extends from its central axis to both sides up to 4.5 linear meters.

Due to its relationship with the flammable area of vapor cloud (scenario 4) and according to its short extension and the wind direction, this accident would not affect the hospital's property, because it would exclusively be limited to the site of the emission.

3.5.4. Leaking tank (jet fire), scenario 6

For the jet fire's scenario, it was modeled using thermal radiation values given by "Real Decreto 1196/2003" (see Attachment 5). An exposure of 30 seconds was chosen because it is a magnitude that exists in legislation for both, alert and intervention zone.

The burning rate of the chemical has the following behavior during the jet fire (which is directly related with the time of leakage, 10 minutes).

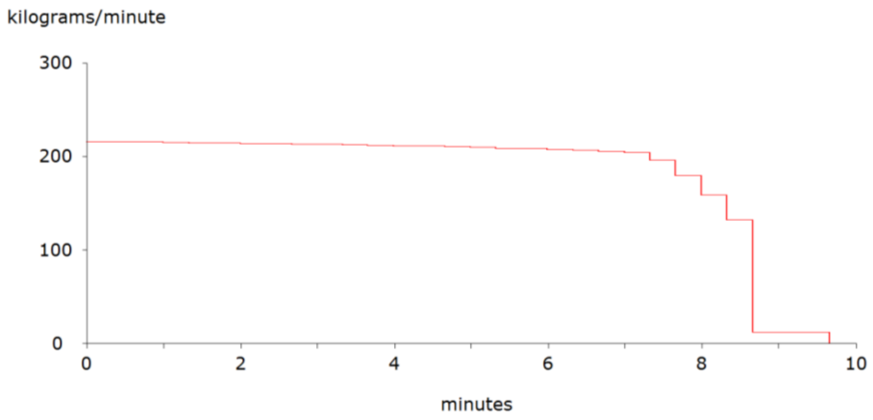

Figure 14. Burning rate of dimethylamine for a jet fire at Site C. (ALOHA, 2016).

When carrying out the model run, the following thermal radiation chart is generated:

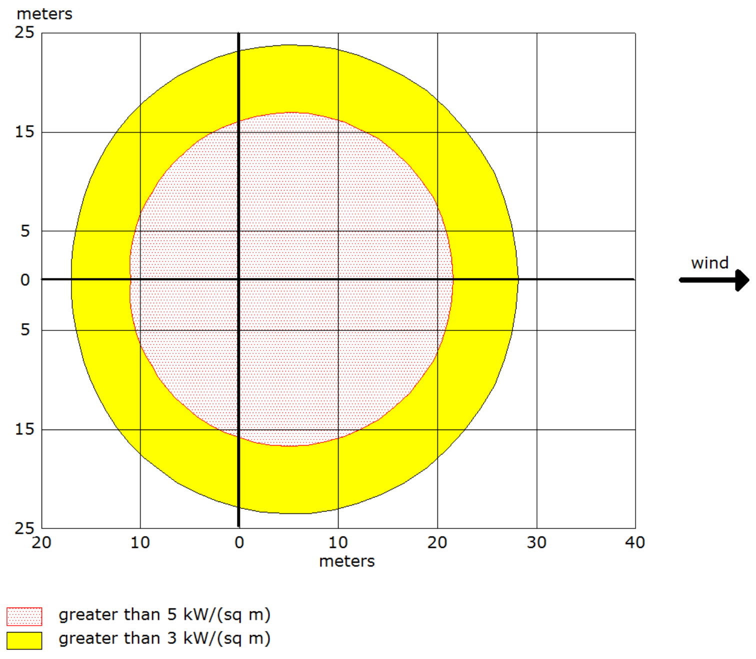

Figure 15. Thermal radiation caused by a jet fire accident involving dimethylamine at Site C. (ALOHA, 2016).

It is interpreted from the above that the thermal radiation -for a 30 second exposure- is round shaped and tends to follow the wind direction, being the most of it to the east of the source. The alert zone (yellow color), in which this radiation is greater than 3 kW/m^2, has a radius of approximately 23 linear meters. With regard to the intervention zone, in which the radiation is more than 5 kW/m^2, has a radius of approximately 17 linear meters.

Due to its short extension and the wind direction, this accident would not affect the hospital's property, because it would almost exclusively be limited to the site of the emission.

It is important to clarify that the simulated jet fire is flame shaped, has a maximun length of 18 meters and lasts 10 minutes burning. Nevertheless, Figure 15 is about the thermal radiation produced as a result from this jet fire, not a drawing of it. It assumes a hole in any point of the tank circunference.

3.5.5. Leaking tank (BLEVE and fireball/pool fire), scenario 7

For the BLEVE's scenario, it was assumed an external fire event that provokes the explosion of the dimethylamine's tank. It is typical that 80% of the gas leaking in the explosion forms the fireball and the remaining 20% constitutes a subsequent pool fire. At BLEVE, ALOHA automatically calculates that the internal pressure of the tank is 62.6 psi, and that its temperature reaches 48.0°C at that time prior to the fireball. Regarding the latter, thermal radiation limits given by "Real Decreto 1196/2003" (see Attachment 5) were used. An exposure of 30 seconds was chosen because it is a magnitude that exists in legislation for both, alert and intervention zones. When carrying out the model run, the following thermal radiation chart is generated:

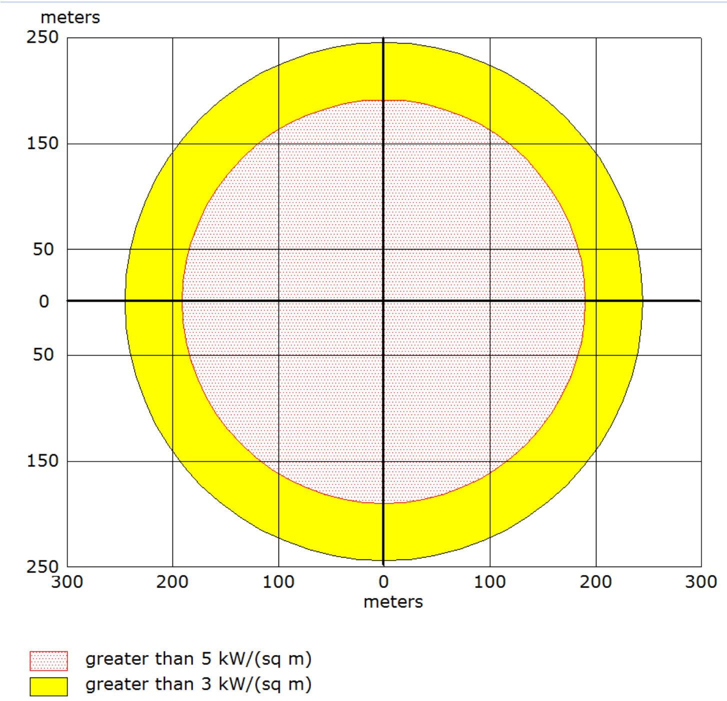

Figure 16. Thermal radiation caused by an accident with fireball involving dimethylamine at Site C. (ALOHA, 2016).

It is interpreted from the above that the alert zone (yellow color), in which the thermal radiation is greater than 3 kW/m^2, has a radius of approximately 250 linear meters. With regard to the intervention zone, in which the thermal radiation is more than 5 kW/m^2, has a radius of approximately 190 linear meters. It must be highlighted, that the fireball has a diameter of 66 linear meters and its burning time lasts 6 seconds. If Figure 16 is superimposed on the location of the hospital's property, it results as follows (Figure 17):

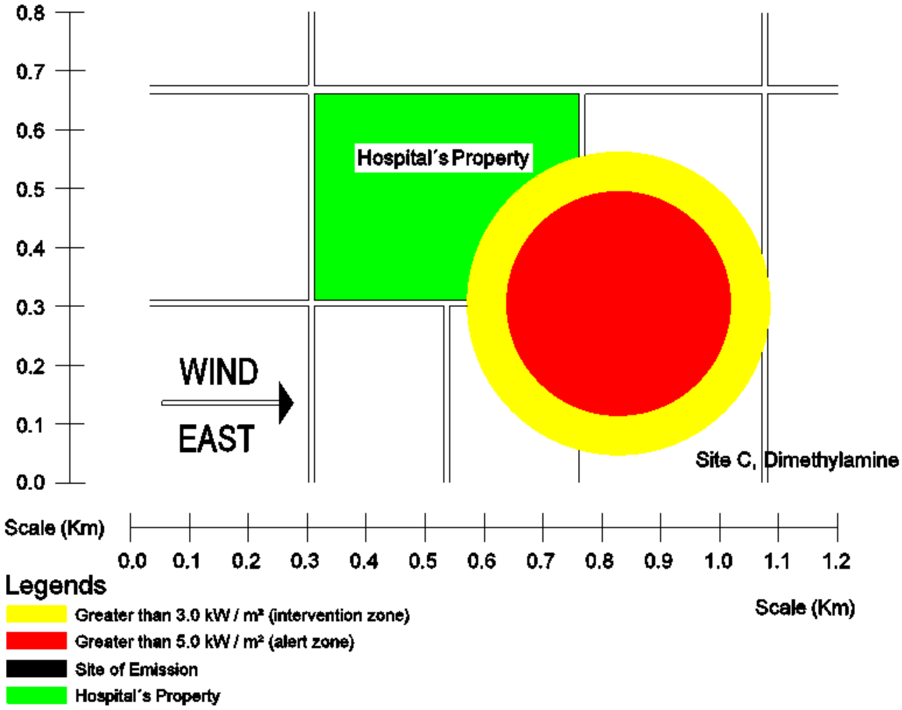

Figure 17. Fireball's thermal radiation caused by an accident involving dimethylamine at Site C and its spatial relation with the hospital's property. (ALOHA, 2016).

Based on the above, a thermal radiation from fireball of a half kilometer diameter can be generated for 30 seconds exposition time. That is, not only affects a 23.56 % of the hospital's property (33,914 m^2 land area of 143,932 m^2), but also the out-of-hospital coverage that surround it in 110,033.37 m^2. For all this area, the thermal radiation values for both, alert and intervention zone, are reached.

One again, it is observed that this accident not only affects the hospital directly. Also, there will be health consequences in those who are reached by the thermal radiation in the specified dosage (for the people in the rest of the industrial-residential places).

Finally, the resultant pool fire has a diameter of 12 linear meters and its burning time lasts 56 seconds. There are no more details about the thermal radiation produced by the pool fire.

3.6. Summary of the analysis

Taking into account the simulated accidents in the different scenarios and considering only direct impact on the coverage of the hospital, the following table summarizes the results:

Table 7. Results of accident scenarios at Sites A, B and C.

Scenario	Type of accident	Consequences	Impact on hospital's property	Affected area (m^2) of the hospital
1	Evaporating pool of aqueous ammonia	Toxic area of vapor cloud	AEGL-1 (alert zone)[6]	4,100
2	Evaporating pool of nitric acid			11,500
3	Leaking tank (not burning) – dimethylamine	Toxic area of vapor cloud	None	
4		Flammable area of vapor cloud (flash fire)		
5		Blast area of vapor cloud explosion		
6	Leaking tank (jet fire) – dimethylamine	Thermal radiation area		
7	Leaking tank (BLEVE and fireball/pool fire) – dimethylamine		Alert and intervention zones[7]	33,914

Based on the above, the hospital as such, is affected directly in the simulations of accidents 1, 2 and 7. However, the surroundings are hit by gaseous pollutants, overpressures, and thermal radiation in the different scenarios, so this affects the hospital's capacity of response in case of emergency. Therefore, intervention (preventive and corrective) actions are needed to mitigate or eliminate the risk of happening of any scenario.

[6] AEGL-1 (alert zone): 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. This area is related with perceptible effects by the population, but their magnitudes do not justify the intervention, except for critical population groups.

[7] In addition to the alert zone, the intervention zone is related to an area with consequences of accidents that produce a level of damages which justify the immediate application of measures of protection.

Regarding to the wind direction confidence lines drawn because of the analysis of scenarios 1-6, it is shown how the toxic cloud and the distribution of the overpressure produced, have a considerable range of displacement due to typical variations in the direction of the wind, Therefore, the mentioned results of the simulations are not static or definitive, but are only guidance.

However, if the variations in wind direction are drastic (which might be feasible), the distribution of the affectation could be very different and scenarios in which there was no impact to the hospital's property, they could have. In fact, it does not seem advisable to unify industrial production areas where hazardous chemicals are managed, with residences and hospitals in the same population area.

4. Conclusions

a) In general, the predominant direction of the wind makes that the affections caused on the hospital by the accidents at Sites A and C (involving aqueous ammonia and dimethylamine), are minimal or null in the dispersion of toxic clouds. On the contrary, with the predominant wind direction, a release in Site B (nitric acid) produces a cloud of vapors from nitric acid that goes through the hospital's property right in the middle and distributes within it, almost completely. In this case, the concentration of toxic clouds would only reach AEGL-1 (alert zone), so these effects are not disabling and are reversible upon cessation of exposure. Nevertheless, due to the characteristics of the patients in a place like this, they can be considered as a critical population group.

b) The flammable vapor cloud, the blast area of vapor cloud and jet fire's thermal radiation threat zone caused by accidents at Site C (related with dimethylamine) do not reach the hospital's property and are practically distributed within the boundaries of the industrial company (very close to the source).

c) The most dangerous case for hospital impact is BLEVE and fireball/pool fire at Site C. According to the consequences to human health, the fireball produces thermal radiation that exceeds the reaches intervention zone (pain, burns of second degree and death). It could also destroy the facilities, so in such a situation, the hospital would be physically disabled.

d) As mentioned before, a hospital can never stop working and must also be solvent in dealing with emergency situations. Therefore, any impact to human health of people outside the hospital's property (in any of the scenarios) will indirectly affect this facility, as these people will attend to it for medical care and will saturate its services. This means that as part of the operations and organization of the hospital, it is necessary to plan and anticipate what to do in such case. If the hospital does not have sufficient response capacity to care for those affected, it will have to refer them to other health centers, consuming resources and valuable time that would put the people at greater risk.

e) Variations in wind direction could change the distribution of the consequences on the hospital's property (for all the simulated scenarios). Because of this, it is for sure that the obtained results are not static or definitive. So, considering hospital patients as a critical population group and according to the "Real Decreto 1196/2003", it is not advisable to unify industrial production areas where hazardous chemicals are managed, with residences and hospitals in the same alert zone. Therefore, they should not coexist.

5. Recommendations

For Caja Costarricense de Seguro Social:

a) Considering the results of this project but without taking into account the "Real Decreto 1196/2003" (because it does not apply for Costa Rica), to promote a teamwork with agrochemical industry companies that surround the hospital, to assess the risk of toxic, radiative or overpressure pollution, if case of accidents related with spills, leaks, fires, and explosions, originated in the facilities of these companies. To do this, it would be necessary to work with real data of substances and quantities, as well as to have access to the factories and warehouses, to obtain reliable results. The study can be extended to other facilities at risk such as close gasoline service stations. If the "Real Decreto 1196/2003" were applied in Costa Rica, locating a hospital within alert zones provoked by industrial accidents would not be allowed.

b) In view of the above and given that the hospital has not been designed yet, to incorporate in the construction plans, solutions in infrastructure and resistance of materials to the fire, suitable electromechanical connections and many other aspects that mitigate the impact of the accidents considered in this Mater`s Final Project.

c) To promote an emergency care commission, in coordination with the industry surrounding the hospital, to develop an articulated response plan for addressing possible accidents of spills, leaks, fires, and explosions, which affect not only the hospital but also to the residential and industrial zone.

For the agrochemical companies at Sites A, B, and C, to promote the security of the infrastructure, their occupants and neighbors, and to benefit the business economy (given that it is cheaper to prevent than to correct), it is recommended:

d) On a periodic and planned basis, conduct a detailed review of the facilities to determine the likelihood of accidents occurring from containers containing liquid chemicals, continuous leaks in pressurized tanks, fires, and explosions.

e) Based on the above, to generate a plan to apply preventive and corrective actions in order to reinforce primary control systems through operational tasks or projects. Consider at least the aspects that can be consulted in Attachment 6.

f) To update their facilities, considering the "Manual de Disposiciones Técnicas Generales Sobre Seguridad Humana y Protección Contra Incendios" developed by the Unidad de Ingeniería de Bomberos del Benemérito Cuerpo de Bomberos de Costa Rica. This mandatory document is used in the design and construction of all civil works projects destined to occupy people temporarily or permanently, whether new buildings or remodeling excepting residential single-family units, and for the design and installation of fire systems (both, active and passive protection), in the organization of events in which a concentration of more than 50 people is projected, and in the safety inspections carried out by the authorities. The above, according to Decreto No. 37615-MP, Gaceta No. 66 of April 5th, 2013, which informs that the Benemérito Cuerpo de Bomberos de Costa Rica adopts and incorporates the NFPA (National Fire Protection Association) standards that correspond.

6. Nomenclature

AEGL, Acute Exposure Guideline Levels for Airborne Chemicals.

BLEVE, Boiling Liquid Expanding Vapor Explosion.

CCSS, Caja Costarricense de Seguro Social.

CPR, Committee for the Prevention of Disasters.

ERPG, Emergency Response Planning Guidelines.

IMCR, Meteorological Institute of Costa Rica.

LEL, Lower Explosive Limit.

LOCs, Levels of Concern.

MAGRAMA, Ministerio de Agricultura, Alimentación y Medio Ambiente de España. Nowadays, it is known as MAPAMA, Ministerio de Agricultura y Pesca, Alimentación y Medio Ambiente de España.

MFP, Master's Final Project.

NOOA, National Oceanic and Atmospheric Administration.

TEEL, Temporary Emergency Exposure Limits.

UEL, Upper Explosive Limit.

USEPA, United States Environmental Protection Agency of the United States of America.

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8. Attachments

Attachment 1

Accidents with toxic substances:

a) ***Evaporating pool***. It happens when a liquid substance at ambient temperature spills on a surface (depending on where it is), forming a pool and tends to evaporate according to its physical properties. If the liquid is flammable and comes into contact with an ignition source, a fire pool may occur. It is interesting to determine the concentrations and dimensions of the toxic cloud that is formed in the accident site by applying an appropriate gas model (Gaussian or heavy gas) for dispersion of pollutants in the air, as well as an analysis of thermal radiation if the fire pool happens. (Nolan, 2011 and ALOHA, 2016).

b) ***Leaking tank (not burning).*** If the compound is a gas at ambient temperature but it is storaged as a pressurized liquid or if it is cooled due to that its boiling point is under the ambient temperature, an accidental opening in the container or a fail in the valve that retains it, will make it to evaporate until the pressures and temperatures internal and external to the tank were balanced, generating a continuous leak and forming a toxic cloud. It is necessary to determine their concentrations and the dimensions of it, from the site of the accident. The analysis can be performed using an appropriate gas model (Gaussian or heavy gas) for dispersion of pollutants in the air. (Nolan, 2011 and ALOHA, 2016).

Accidents with flammable and toxic substances:

a) ***Flash fire.*** When a flammable vapor cloud encounters an ignition source, the cloud can catch fire and burn rapidly in what is called a flash fire. Potential hazards associated with a flash fire include thermal radiation, smoke, and toxic byproducts from the fire. In this accident, it is important to estimate the flammable area of the vapor cloud (the area where a flash fire could occur at some time after the release begins). Its analysis can be performed using an appropriate gas model (Gaussian or heavy gas) for dispersion of pollutants in the air. (Nolan, 2011 and ALOHA, 2016).

b) ***Blast.*** It occurs when a flammable chemical is released into the atmosphere, it forms a vapor cloud that will disperse as it travels downwind. If the cloud encounters an ignition source, the parts of the cloud where the concentration is within the flammable range (between the Lower and Upper Explosive Limits) will burn. The speed at which the flame front moves through the cloud determines whether it is a deflagration or a detonation. In some situations, the cloud will burn so fast that it creates an explosive force (blast wave). The severity of a vapor cloud explosion depends on the chemical, the cloud size at the time of ignition, the type of ignition, and the congestion level inside the cloud. Its analysis can be performed using an appropriate gas model (Gaussian or heavy gas) for dispersion of pollutants in the air and explosions. (Nolan, 2011 and ALOHA, 2016).

c) ***Jet fire.*** A jet fire, also referred to as a flame jet, occurs when a flammable chemical is rapidly released from an opening in a container and immediately catches on fire (much like the flame from a blowtorch). It produces a stationary flame of great length and small width, like that of a blower, which is kept constant until the fuel is exhausted. It is the same phenomenon that applies to security torches to eliminate unwanted byproducts or excess gases. It has a limited range, but it is especially dangerous as far as the domino effect is concerned, since the flame is directional and constant. In this case, it is important to estimate the magnitude and size of the thermal radiation produced from the accident site, so its analysis is done using an exclusive model for jet fires. (Nolan, 2011 and ALOHA, 2016).

d) ***BLEVE and fireball.*** It occurs when a tank containing a liquefied gas fails completely, as a result of the contents of the tank heating up (by the action of an external source). Some of the released flammable chemical will burn in a fireball, while the remainder will form a pool fire. The amount of the chemical involved in the fireball and/or the pool fire will depend on the conditions at the time of release. In this case, it is important to estimate the reach of the fireball and the magnitude and size of the thermal radiation produced from the accident site, so its analysis is done using an exclusive model for fireballs. (Nolan, 2011 and ALOHA, 2016).

e) ***Pool fire*****.** It occurs when a flammable liquid forms a pool on the ground and catches on fire. It can also occur on water. In this case, it is important to estimate the time of burning, amount of burned chemical, the dimensions of the pool fire, the magnitude and coverage of the thermal radiation produced from the source, so its analysis is done using an exclusive model for pool fires. (Nolan, 2011 and ALOHA, 2016).

Attachment 2

- **AEGL-1:** It is the airborne concentration -expressed as parts per million or milligrams per cubic meter (ppm or mg/m^3)- 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. The coverage that reaches this parameter is called **alert zone**. This area is related with perceptible effects by the population, but their magnitudes do not justify the intervention, except for critical population groups.
- **AEGL-2:** It is the airborne concentration (expressed as ppm or mg/m^3) 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. The coverage that reaches this parameter is called **intervention zone**. This area is related with consequences of accidents that produce a level of damages which justify the immediate application of measures of protection.
- **AEGL-3:** It is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible people, could experience life-threatening health effects or death.
- **ERPG-1:** It is the maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing more than mild, transient adverse health effects or without perceiving a clearly defined objectionable odor. The coverage that reaches this parameter is called **alert zone**.

- **ERPG-2:** It is the maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms which could impair an individual's ability to take protective action. The coverage that reaches this parameter is called **intervention zone**.
- **ERPG-3:** It is the maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.
- **TEEL-1:** It is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience notable discomfort, irritation, or certain asymptomatic, nonsensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure. The coverage that reaches this parameter is called **alert zone**.
- **TEEL-2:** It is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape. The coverage that reaches this parameter is called **intervention zone**.
- **TEEL-3:** It is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience life-threatening adverse health effects or death.

Attachment 3

It must be said that the "Comisión Técnica de Prevención y Reparación de Daños Medioambientales de la Dirección General de Calidad y Evaluación Ambiental y Medio Natural del Ministerio de Agricultura, Alimentación y Medio Ambiente de España" developed a document entitled "Análisis de herramientas de evaluación de la difusión y comportamiento de agentes químicos en el marco de la normativa de responsabilidad medioambiental". In this document, a set of selection criteria was proposed that would help to choose from the available market offer of simulators, the most appropriate software to model the behavior of the agents causing the damage in the vectors soil, water (superficial and ground water) and atmosphere. The above, according to the requirements requested at Ley 26/2007 of October 23, on Environmental Responsibility. In the analysis, the simulation models available on the market were classified as follows:

- Analytical models, also known as screen models. Useful for a first approach to the problem focused on decision making. Generally, the equations considered in this type of models allow to obtain a simple result. They try one or two-dimensional simulations and are reasonably demanding as to the need for input data. These models are easy-to-use and do not require complex input data packages, because are based on very simplified starting assumptions (homogeneous and isotropic media). The absence or difficulty of obtaining the input data is, in most cases, a basic decision criterion for the use of this type of models.
- Numerical models. They require more complex input data, so obtaining or processing this information is significantly more difficult than in analytical models and tend to require more time for their correct application. Their use generally involves obtaining specific data from the facility by conducting field tests. They allow 3D simulations and are often used for complex conceptual models, in which spatial and temporal variations are considered. Although these models theoretically give a more realistic result than the analytical models, they require a more exhaustive analysis in the initial phase of development of the conceptual model, which generally requires an expert user.

Among the criteria studied to compare each model are: human factor (organizational scope, individual area), activities / facilities (storage, production processes and facilities, auxiliary processes and facilities), external elements (natural, infrastructure and supplies, socioeconomic aspects, atmosphere, soil, groundwater, surface water, habitat, wild species, soils), product or substance, amount involved, physical characteristics, conditions of service, prevention and control systems, means and time of intervention, meteorological conditions, hydrogeological conditions, reference levels and routes of exposure.

Finally, the adequacy to the conceptual model of the installation was assessed, the accident hypotheses raised, the availability of the input data and the need for experience or technical knowledge for the application of certain models.

After having identified the models available on the market with regard to the atmospheric dispersion of pollutants and having made a pre-selection (SCREEN 3, ALOHA, AERMOD, CALPUFF, PHAST, EFFECTS, CAMEO and DEGADIS), it was concluded that the more functional software was ALOHA for the case of analytical models and the PHAST for the numerical ones.

Since ALOHA is a free software, whose implementation offers technically appropriate results in the determination of contaminant immission levels from accident simulation, its use was recommended by the "Comisión Técnica de Prevención y Reparación de Daños Medioambientales". If someone wants to do further analysis (which will require more input and greater technical knowledge of the tool), PHAST is better and is not in the inventory of applications acquired by the University of Barcelona.

Based on the above, it was considered for purposes of the present work that the ALOHA could fulfill the expectations for a preliminary analytical simulation and in case of throwing important risk results, one could choose to deepen specific accidental situations with other software and with the accompaniment of the government and the private companies that had relation with the cases.

Attachment 4

The reference values from the point of view of losses in facilities that delimit the zones of overpressure are:

- Overpressure $\geq$ 1.813 psi (125 mbar), intervention zone.
- Overpressure $\geq$ 0.725 psi (50 mbar), alert zone.

Attachment 5

The reference values from the point of view of human health that delimit the zones of thermal radiation are:

- Intervention zone: delimits the area around the fire dart subjected to a radiation of 5 kW/m^2 with a maximum exposure time of 30 seconds. This applies for a thermal radiation dosage of 250 $(kW/m^2)^{4/3}\cdot s$.
- Intervention zone: delimits the area around the fire dart subjected to a radiation of 3 kW/m^2 with a maximum exposure time of 30 seconds. This applies for a thermal radiation dosage of 115 $(kW/m^2)^{4/3}\cdot s$.

Attachment 6

Actions to reinforce primary control systems (those that act on the amount involved in a possible accident and also on the probability of that accident occurring):

- Inventory of chemicals being handled.
- Evaluation of the location of the facilities with each other and identification of the activities carried out in them (processing, storage, services, human resources, loading, and unloading).
- Disposal of electromechanical equipment and containers with hazardous chemicals with respect to safety distances in order to avoid injury to people (personnel or neighbors), internal facilities and external properties.
- Adequacy of equipment and facilities. That is, the construction and characteristics of facilities and equipment should be in accordance with their function. Consideration should be given to: plant distribution according to purpose, adequate access, escape routes, compartmentalization, selection of building materials, electrical installation, fire doors, minimizing the possibility of spills and losses. The equipment must be equipped with the necessary detection and control instrumentation (automation).
- Prevention and protection against fire. To do this: avoid the concentration of large quantities of flammable products and separate incompatible products; disperse the storage; compartmentalize areas; include remote operated isolating valves; store liquefied gases at low pressure and temperature; separate the sources of ignition from the areas with flammable materials and orient them so that the wind does not direct the flames towards the flammable ones; consider safety and exit areas at reasonable distances from the possible fire outbreak; have sufficient sloped deposit for the spill to slide into the bucket; have suitable blocks: diameter, slope, distance from the tank; apply thermal insulation to chemical deposits; reduce retention of substances in process equipment; inert chemicals in case of leak; keep facilities ventilated; promote open facilities to prevent the accumulation of flammable vapors; controlling static electricity; place fire equipment separate from potentially dangerous equipment but at the same time with easy access to it; bury water pipes in the fire system and have adequate fixed and portable extinction equipment.
- Prevention and protection against explosions. About this: avoid overfilling containers; promote natural ventilation; avoid contamination of products and equipment; install gas detectors; apply measures to isolate, cut and disperse leaks; control chemical

reactions to prevent explosions; control the reaction temperature and consider depressurizing and insulation system.

- Prevention and protection against spills and leaks. If a liquid is spilled: have buckets in the storage tanks and have the possibility of transfer of product from one tank to another in case of breakage; collect the purges by pumping systems and put small deposits so that the chemical does not fall to the ground and infiltrate; use foams to prevent spilled liquid from escaping; incorporate instruments and materials that allow product adsorption and minimize the effects of the spill such as tubular, pillows, mats, rolls, special adsorbents, solidifying granules, skimmers, pumps and vacuum cleaners. If the size of the deposits is reduced, the evaporation surface area is minimized and the emission of the contaminant will be reduced and consequently the toxic cloud will also be decreased.