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FINAL MASTER'S THESIS

Master's Degree in Chemical Engineering – Smart Chemical Factories

DESIGN AND IMPLEMENTATION OF A DATABASE FOR QRA MANAGEMENT

Memory and Annexes

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Abstract

In this project, bibliographic research is carried out on the European, Spanish, and Catalan legislation applied to establishments affected by the SEVESO directive. Research on the evolution of these regulations and the modifications between them is conducted, documenting the required information that each establishment must present according to its category. The literature refers to quantitative risk analysis and safety reports.

A database is designed for the collection of information from safety reports, basing its structure on the coding table of possible accidents of the Generalitat de Catalunya. Information on the location, industrial activity, meteorological conditions, substance involved, initiator of the possible major accident and the final event, are the fields introduced in the database.

An exploratory analysis of the database is carried out according to its location, meteorological conditions, including temperature, relative humidity, atmospheric stability, wind direction and velocity. The substance present, the possible basic accident and final event, specified together with the safety distances (intervention zone, alert zone, and domino effect zone) are also considered. In addition, the impact of each of these factors on the safety distances is studied.

Finally, an exploration via pattern recognition using principal component analysis and regression adjustment is done to investigate the existing relation between these factors, as a function of the final event, and the different safety distances.

Resum

En aquest treball s’ha dut a terme una recerca bibliogràfica sobre la legislació a nivell europeu, espanyol i català aplicat als establiments afectats per la directiva SEVESO. S’ha realitzat una investigació sobre l’evolució d’aquestes normatives i els canvis que presenten entre elles, documentant quina és a informació requerida que cada establiment ha de presentar segons la seva categoria. La literatura fa referència a l’anàlisi quantitatiu de risc i l’informe de seguretat.

S’ha dissenyat una base de dades per la recollida d’informació a partir d’informes de seguretat, basant la seva estructura en la taula de codificació de possibles accidents de la Generalitat de Catalunya. En aquesta base de dades s’ha introduït informació sobre la localització, l’activitat industrial, les condiciones meteorològiques, la substància involucrada, l’iniciador del possible accident greu i l’efecte final associat a aquest.

S’ha realitzat un anàlisi exploratori de la base de dades en funció de la seva localització, condiciones meteorològiques, destacant la temperatura, humitat relativa, estabilitat atmosfèrica, direcció i velocitat del vent. També s’ha tingut en compte la substància present, el possible accident bàsic juntament amb les distàncies de seguretat (zona d’intervenció, zona d’alerta i zona d’efecte dominó). Addicionalment, s’ha estudiat l’impacte de cada un d’aquests factors en les distancies de seguretat.

Finalment, s’ha realitzat una exploració pel reconeixement de patrons utilitzant la anàlisis de components principals i l’ajustament de la regressió per veure la relació que hi ha entre aquests factors, en funció de l’accident final, i les diferents distàncies de seguretat.

Resumen

En este trabajo se ha realizado una investigación bibliográfica sobre la legislación a nivel europeo, español y catalán aplicado a los establecimientos afectados por la directiva SEVESO. Se ha realizado una investigación sobre cuál es la evolución de esta normativa y los cambios que presentan entre ellas, documentando cuál es la información requerida que debe presentar cada establecimiento según su categoría. La literatura hace referencia al análisis cuantitativo de riesgo y al informe de seguridad.

Se ha diseñado una base de datos para la recogida de información a partir de informes de seguridad, basando su estructura en la tabla de codificación de posibles accidentes de la Generalitat de Catalunya. En esta base de datos se ha introducido información sobre la localización, la actividad industrial, las condiciones meteorológicas, la sustancia involucrada, el iniciador del posible accidente grave y el efecto final asociado al mismo.

Se ha realizado un análisis exploratorio de la base de datos en función de su localización, condiciones meteorológicas, destacando la temperatura, humedad relativa, estabilidad atmosférica, dirección y velocidad del viento. También se ha tenido en cuenta la sustancia presente, el posible accidente básico especificado junto con las distancias de seguridad (zona de intervención, zona de alerta y zona de efecto dominó). Adicionalmente, se ha estudiado el impacto de cada uno de estos factores en las distancias de seguridad.

Por último, se ha realizado una exploración para el reconocimiento de patrones utilizando el análisis de componentes principales y el ajuste de regresión para ver la relación existente entre estos factores, en función del accidente final, y las diferentes distancias de seguridad.

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To my friends Josep and Esteban for making these two years more enjoyable.

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1. Introduction

Technological risks are exhibited at the chemical industry when an activity has the capacity to produce a certain amount of damage due to the hazardous substance involved. Those chemicals are listed in Part 1 or in Part 2 of Annex I of RD 840/2015 and they are classified according to the European Regulation (EC) No. 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures known as CLP.

These risks can turn into major accidents when safety measures are not adequate. Releases can occur in the form of a major leak or spillage, followed by fires, or explosions, resulting from an undesired event or process during the operation of any establishment to which RD 840/2015 applies.

The effects of major accidents can cover large distances, which means that they can also affect the external population and are often more difficult to predict and evaluate. As a result, a set of methodologies has been developed to analyse and quantify such risks. These methodologies are referred to collectively as “risk analysis” [1].

A risk analysis is carried out to prevent the effects of potential major accidents and to contribute to their mitigation. Therefore, these situations need to be managed with detailed planning. So, the establishments affected are obliged to adopt measures and to limit the consequences that these situations can cause. One of the ways is presenting risk analysis and safety reports, as established in RD 840/2015.

1.1. Objectives of the project

The main objective of this project is the creation and analysis of a database of hazardous scenarios and their emergency planning distances (intervention zone, alert zone, and domino-effect zone) fed from quantitative risk analysis included in safety reports from chemical companies. The specific objectives of this project are:

- Make bibliographic research on the regulations applied to the establishments affected.
- Create a database for the collection of data from safety reports.
- Perform an exploratory analysis of the database.
- Carry out a pattern recognition of the different parameters.

1.2. Scope of the project

This project includes: i) the theoretical study of the legislation applied in the establishments affected, at European, Spanish, and Catalan level; ii) the creation of the database for the compilation of information from the safety reports; iii) the performance of an exploratory analysis of the database; and iv) the recognition of patterns of different parameters described in the database.

2. Framework regulation

This chapter provides an analysis of the different directives and regulations for prevention and control of major accidents involving hazardous substances in industrial facilities. It is divided into three sections: legislation at European, Spanish, and Catalan level (see Figure 1).

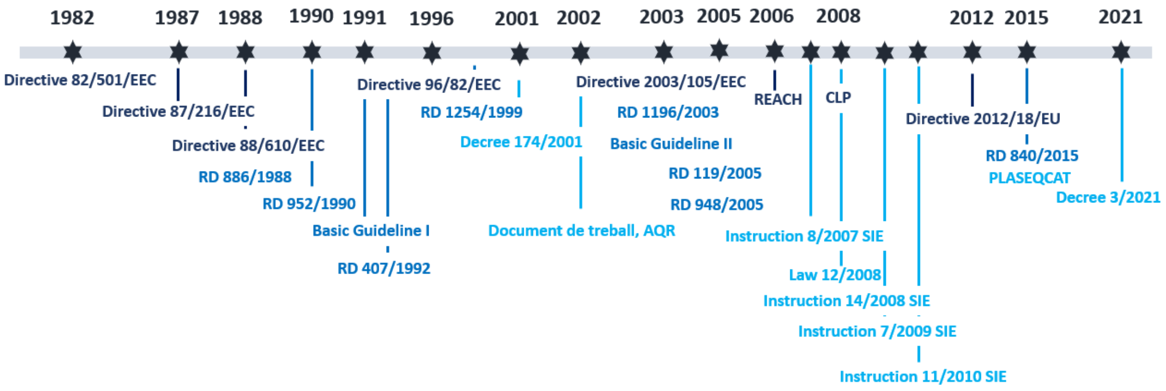

Figure 1. Framework regulation scheme, European level in dark blue, Spanish level in blue and Catalan level in light blue.

2.1. Legislation at European level

The European regulation for prevention and control of major accidents including hazardous chemical substances is known as the SEVESO Directive, created on the 24th of June 1982. It was developed after the catastrophic accidents that occurred in Flixborough, UK in 1973 and in the Italian town of Seveso in 1976. Its purpose was to minimize the occurrence of industrial accidents caused by hazardous chemicals that could affect the surrounding environment. Moreover, it provided a framework to standardize the legislation in the different countries of the European Economic Community (EEC).

SEVESO I (Directive 82/501/EEC) was a compilation of existing regulations in the EEC. Its main objective was to identify industries that integrated hazardous substances into their processes and the quantities they managed, to prevent major accidents [2]. In other words, the Directive established the obligation for those in charge of industrial activities to take the necessary steps to prevent major accidents and to limit their consequences for people and for the environment, as well as to identify any existing major-accident hazards at the establishment and to take the proper safety measures [3].

To do so, lower and upper threshold values of quantity for each hazardous substance were determined. Below the lower values, installations were not affected and above them, actions should be taken [2]. So, a distinction was made between the requirements to be satisfied by establishments depending on their inventory level of hazardous substances: Level I or high inventory level and Level II or low inventory level [4]. This classification was achieved using a list of toxic and dangerous products that delimited the effects on health produced by an exposure to toxic chemicals accidentally released. Therefore, the companies which were using hazardous chemicals in their process were required to officially report a safety assessment of hazards.

SEVESO I was modified by Directives 87/216/EEC on the 19th of March in 1987 [5] and 88/610/EEC on the 24th of November in 1988 [6]. The first amendment was done to clarify and to avoid different interpretations of the levels of limitations in Annexes I, II and III of the derogate SEVESO I. The second modification was made to extend the scope of applications to establishments storing hazardous substances, so a new Annex was added, containing the public information to be given in case of an accident [3].

On the 9th of December 1996 the Council of the European Union adopted Directive 96/82/EC (SEVESO II) and became mandatory for the industry on the 3rd of February 1999, on the control of major-accident hazards involving dangerous substances. Directive 96/82/EC derogated the previous Directive 82/501/EEC on the control of major-accident hazards of certain industrial activities [7].

SEVESO II was implemented as a response to the lessons learned from new accidents, such as the one in Bhopal, India in 1984. Its main objective was to achieve a higher level of protection for people, property, and environment. Therefore, the scope of the Directive was simplified and extended to include not only the so-called industrial activities, but also the storage of dangerous chemicals. Concerning the part of the simplification, the list of the industrial installations was deleted, which was replaced by a concept of industrial establishment characterized by the presence of hazardous substances. Regarding the storage applications, it was referred to the presence of a quantity of hazardous substances for the purpose of warehousing, depositing in safe custody or keeping in stock. Moreover, it was considered that the transport of dangerous substances through pipelines also could involve major-accident hazards [3].

To determine which chemicals were dangerous or not, there was a list of named substances (Annex I, Part 1) and a list of generic categories (Annex I, Part 2) such as toxic, flammable, and explosive substances. Depending on the quantities of hazardous substances presented on the establishment, it was classified as upper-tier or lower-tier. Also, it was assumed that the risk of the hazard increased with the quantities of substances presented at the installation [7].

Additionally, it was determined the technical aspects to be placed on the operator to provide a Major Accident Prevention Policy (MAPP), and for an upper-tier establishment, a Safety Report (SR) implemented by means of Safety Management System (SMS) [8].

A MAPP is a document whose objective is to give an overall insight into how the operator ensures a high level of protection for man and environment. This documentation should include the organization and personnel, the identification and evaluation of major hazards, the operation control. It should also include the management of change, the planning for emergencies and the monitoring performance [9].

A SR is a set of information relating to the establishment, the environment, the facilities, and the hazardous substances, which the company affected is under the obligation to submit to the competent authorities. So that, they can adopt the necessary measures to prevent and mitigate the consequences of major accidents that may occur in the establishment concerned. Also, it must certify that a prevention policy has been adopted, that accident risks have been identified and assessed, that the establishment is safe and reliable about major-accident hazards and that it has an Interior Emergency Plan (IEP) in place) [8].

Therefore, those companies, with potential major accident hazards due to the storage and use of hazardous substances, were required to submit a SR [8]. In general, the requirement for a detailed and demonstrative risk assessment in safety documentation (program, report, emergency plan) is a requirement for a complex and detailed analytical safety study, detailed hazard identification and risk assessment [10].

Directive 2003/105/EC of the European Parliament and of the Council of 16th of December 2003 which modified Council Directive 96/82/EC on the control of major-accident hazards involving dangerous substances entered into force. This amendment was made due to an extension of the scope to cover risks arising from warehousing and mining activities. Moreover, the lessons learned from new accidents as the one in a chemical plant in AZF, Toulouse in 2001 were incorporated [11].

This directive was introduced with the intention to reflect the latest results of studies on carcinogens and new substances dangerous for the environment, extending the scope of the directive. Also, to introduce new minimum deadlines for companies and industries to comply with the obligations imposed by the new amendment. To propose an improvement in the exchange of information, member states must provide the EC with basic information on accident industries. In general terms, to insist on the importance of operators’ participation in the creation of emergency plans, as well as in their training [11].

In 2006, the Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) was introduced. This new regulation, which entered into force on the 1st of June 2007, established a new legal framework regulating the development and testing, production, marketing, and use of chemicals. Its objective was to achieve a higher level of protection of human health and the environment from the potential risks posed by chemicals and to promote sustainable development. Therefore, REACH introduced a single system for all chemicals and ended the distinction between "new" (placed on the market after 1981) and "existing" (registered before 1981) chemicals [12].

To enhance the level of protection of human health and the environment, the same criteria should be used throughout the Union and the rest of the world for the identification of chemical hazards and the same labels should be used for their description [12].

Regulation (EC) No 1272/2008 on classification, labelling and packaging (CLP) of substances and mixtures, adopted in 2008, was intended to achieve harmonisation of the Union system with the United Nations Globally Harmonised System (GHS) [13]. Its main objective was to develop a new chemical hazard identification system, unifying it on a global scale. Hence, it was required a new system of hazard classification of substances and their mixtures involving a new hazard class and category system. Also, the introduction of signal words specifying the level of danger of the substance or mixture and the addition of new pictograms. Furthermore, some changes were implemented regarding the hazard statements (H) and precautionary statements (P). Therefore, it was needed that operators, importers and users of substances and mixtures to classify, label, and package their hazardous chemicals before placing them on the market. As a result, CLP regulation created the necessity for the revision of ANNEX I of the Seveso II Directive [13].

In July 2012, the new Seveso III (Directive 2012/18/EU) was published following its approval by the Parliament and the Council, considering the new international classifications of substances (CLP Classification) agreed by the United Nations, which allowed for better risk assessment and improved treatment of substances. In addition, conclusions from new accidents such as the case of Buncefield in 2005, were taken into consideration [14].

SEVESO III, on the control of major-accident hazards involving hazardous substances, amended and subsequently, repealed the previous Directive 2003/105/EC. It established measures for the prevention of major accidents which could result from certain industrial activities, hazardous substances, and the limitation of their consequences for human health and the environment. Its aim was to adopt appropriate precautionary measures to ensure a high level of protection of the whole European Union for citizens, population, and the environment in the event of a major accident. Therefore, its purpose was the preparation of emergency plans, involving the public in consultation and decision making [15].

The Directive covers establishments where hazardous substances may be present (e.g., during processing or storage) in quantities above the specified threshold. It excludes from the Directive certain industrial activities that are subject to other legislation providing a similar level of protection (e.g., nuclear establishments or the transport of dangerous substances) [14].

Those limits are specified in ANNEX I, which is divided into two different parts, listing the hazardous substances, including concentration thresholds. So, depending on the quantity of hazardous substances present, establishments are classified into lower and higher tiers, which are subject to stricter requirements [16].

Therefore, plants that contain or produce dangerous substances, are divided in “lower threshold plant” or an “upper threshold plant”, according to the quantity of the substances themselves (dangerous substances belong to Annex I part 1-2 of the aforementioned directives, i.e., material, products, by-products, remainder or intermediate products) [17]. Furthermore, the preparation of Safety Reports continues being required for establishments affected at a higher level [14].

Seveso III applies to more than 12,000 industrial establishments in the European Union where hazardous substances are used or stored in large quantities, mainly in the chemical and petrochemical industry, as well as in the fuel wholesale and storage sectors (including LPG and LNG) [16].

This Directive has contributed to the decrease in the frequency of major accidents, considering the high rates of industrialisation in the European Union. The Directive is widely considered as a reference framework for industrial accident policy and has been a model for legislation in many countries around the world [16].

2.2. Legislation at state level

The European Directive has been successfully implemented into national laws and regulations. This section will be focussed on the Spanish legal framework, distinguishing three different periods, due to the modifications of the EU Directive.

RD 886/1988 was published on the 15th of July 1988; and it was the introduction of SEVESO I into the Spanish regulation. Its purpose was the prevention of major accidents, specifying industrial activities. There were some limitations for the protection of population, environment, and property, as well as safety and health protection of people in their workplace. It was applied to both new industrial activities and to those already existing before its implementation [18].

This legislation was subsequently complemented by the provisions of RD 952/1990 of 29th of June 1990, in accordance with the European Directives 87/216/EEC and 86/610/EEC. According to this legislation, some new measures were approved to control the risk associated with major accidents involving hazardous substances. The criteria to meet by companies were more restrictive, thus the number of substances involved was increased as it was introduced a new category of hazard, the oxidizing class. In addition, it was decreased the quantities above which industrialists had to develop self-protection measures [19].

At the same time the Resolution of 30th of January 1991 was published. This set of provisions is not a set of technical regulations, although it is an interpretation and development of the regulation. This resolution published the Agreement of the Council of Ministers approving the Basic Directive I for the elaboration and homologation of the Emergency Plans for the Chemical Sector (EPCS). There are two types of EPCS, the internal emergency (PEI) which is prepared by the company itself and is activated in the event of an emergency whose consequences do not affect the outside of the installation and the external emergency (PEE) which is elaborated by the Autonomous Community based on the information provided by the industries affected by the R.D. on the prevention of major accidents [20].

Meanwhile, in accordance with Law 2/1985 of 21st of January 1985, and RD 407/1992 of 24th of April 1992, the basic regulation on Civil Protection was approved. Law 2/1985 established in Articles 5, 6 and 12 the classification of potential emergency activities and the identification of the centres, facilities, and installations in which those activities were carried out. It also regulated the obligations of industrialists to have a self-protection organization and an internal emergency plan for the prevention of risk [21]. Furthermore, RD 407/1992 included the essential requirements for the preparation of plans dealing with specific hazardous substances. Consequently, an Agreement was adopted on the 23rd of November 1999, approving the Basic Directive for the preparation and approval of the special plans for the chemical sector [22].

The implementation of SEVESO II required the approval of new regulation for its incorporation into Spanish law. RD 1254/1999 entered into force on the 16th of July 1999, and its purpose was the prevention of major accidents involving hazardous substances and the limitations of their consequences to protect people, property, and the environment. RD 1254/1999 was applied to establishments in which hazardous substances were present in quantities equal to or greater than those specified in Annex I of the Royal Decree, independently of the processes in the establishments and without differentiating between storage processes. Annex I of RD 1254/1999 also specifies other considerations to be taken into account, such as the sum of hazardous substances present in an establishment or the 2% rule [23].

RD 1196/2003 was approved, on the 19th of September 2003. The most significant modifications on its purpose were that accidents would be classified according to three categories, depending on the expected consequences. Category 1: accidents where the only expected consequence is damage to property on the establishment involved and no damage of any kind is expected outside the establishment. Category 2: those where consequences are expected to include possible casualties and damage to property on the establishment, while the external repercussions are limited to minor damage or adverse effects on the environment in limited areas. Category 3: those where potential casualties, severe damage to property or severe environmental disruption over large areas and outside the establishment are expected as consequences [24].

Moreover, it was introduced the Acute Exposure Guideline Levels (AEGL), Emergency response planning guidelines (ERPG), Temporary emergency exposure (TEEL) indices, according to different concentration limits, used to define planning areas [11].

Also, Basic Guideline II was approved, which clarified the concept of major accident hazard identification, underlining the importance of risk analysis related to start-up and shut-down operations, as well as loading and unloading, these operations being, together with maintenance, the main causes of accidents in process plants [24].

In addition, it was published RD 119/2005 of the 4th of February 2005 and RD 948/2005 of the 29th of July 2005. RD 119/2005 was introduced because of the initiation of an infraction procedure by the European Commission against the Spanish authorities, due to disagreements with administrative aspects [25]. The RD 948/2005 added important technical aspects, highlighting the modifications to Annex I, related to the incorporation of new criteria on hazardous substances [26].

EU Directive SEVESO III was adopted in Spain through RD 840/2015 on the 21st of September, on control measures for major-accident hazards involving hazardous substances. Its purpose was the prevention of major accidents and the limitations of their consequences for human health, property, and environment. Its range of application covers all establishments in which one or more hazardous substances are present in quantities equal to or greater than those specified on Annex I. This Royal Decree introduced important changes, such as the harmonisation of the categories of substances in Annex I with those corresponding to the new European system for the classification of substances and mixtures [27]

Also, a deadline was established for industrialists to adapt to the new regulations, which varies between 1 and 2 years from its publication, depending on the type of establishment. Minimum criteria were established considering the modification of an establishment as a modification with significant consequences for major accident hazards. For establishments affected at a lower level, routine inspections are mandatory every 3 years [27].

At the same time, RD 840/2015 contemplates the general structure of civil protection planning in the face of special risks, comprising the national plan, the plans of the autonomous communities and the municipal action plans [27].

2.3. Legislation at Autonomous Community level

In 1999, the Spanish Government implemented the SEVESO II Directive through RD 1254/1999, and it established the requirements for Autonomous Communities. Therefore, the Government of Catalonia approved its own law defining the procedures and measures to be taken to ensure risk management.

The Catalan regulations are complemented by means of decrees, orders and instructions that develop procedures to implement regulations. It is done in accordance with the Catalan organisational model, which has the power to increase the safety requirements with respect to the State legislation, when it is considered necessary. Thus, the current model of industrial safety in Catalonia involves three public policies: it is based on a legal framework that establishes different types of safety standards; it defines, organises, and coordinates the different agents with specific functions; it defines their responsibilities and establishes sanctions, in the event of noncompliance, to guarantee the accomplishment of the objectives required [28].

In Catalonia, the general framework for major accidents is set out in Decree 174/2001 of 26th of June 2001, which incorporates the requirements of RD 1254/1999. Also, the announcement of Law 12/2008 of 31st of July 2008 on Industrial Safety, which regulates the aspects related to territorial planning around establishments and the regulations that develop it. Moreover, Decree 3/2021 of the 20th of December 2021, establishes the requirements that industrial risk assessment organisations must comply with to be authorised in Catalonia to carry out the assessment of Safety Reports [28].

Decree 174/2001 of the 26th of June 2001 came into force to make effective the application of Directive 96/82/EC (SEVESO II) and RD 1254/1999. The aim was to adopt measures to control the inherent risks in major accidents involving hazardous substances. Also, it determined the competent authorities that must carry out each of the functions, specified the administrative procedure for modification and updating of establishments or installations and included the required information data on the transport of hazardous substances by road, rail, or ship. Furthermore, this decree stipulated which establishments were affected by Article 9 of RD 1254/1999 and the mandatory documentation to be submitted by the owners of establishments affected by the Directive, in Safety Reports [29].

In September 2002 it was published in the guide *Document de treball, Anàlisi Quantitativa de Risc. Revisió de la metodologia i guia de criteris bàsics,* and it became clear that there were different approaches to the methodology and that they could lead to different results, which, if not harmonised, would make decision-making more difficult. This guide proposed a general structure to divide it into phases and listed the uncertainty factors associated with each of these phases. However, it is general and does not discard alternative methods. This guide was based on the Dutch Purple Book (Guidelines for Quantitative Risk Assessment, CPR 18E published by the Committee for the prevention of disasters, first revision of 1999) [30].

Instruction 8/2007 SIE, approved on the 30th of July 2007, was based on urban growth according to the effects established by existing major accident legislation. It set up tolerable criteria for the individual and social risk. Regarding the first one, it is considered intolerable when a vulnerable element is subjected to individual risk values of 10^{-6} $year^{-1}$ or higher. In relation to social risk, its tolerability is determined by a f-N limit plot, showing the cumulative frequency of events that can cause N + number of fatalities versus number of fatalities [31].

Later, the legal framework was constituted by Law 12/2008, on the 31st of July, on industrial safety. The purpose of this law was to regulate the general legal framework for industrial safety in Catalonia. To do so, it included market monitoring in this area, and the creation and regulation of the Catalan Industrial Safety Agency[32].

Instruction 14/2008 SIE, published on the 5th of November 2008, was focussed on criteria for carrying out Quantitative Risk Analysis in Catalonia (Purple Book and complementary criteria). Moreover, to make clearer the need to apply identical criteria in all cases, it included complementary criteria to the Purple Book (PB) in aspects that were not sufficiently detailed. Therefore, the specific objectives were: to establish without ambiguity that the QRA must be carried out in accordance with the PB and additional criteria included in this instruction; to reduce as far as possible the "degrees of freedom" that remain in the PB in order to guarantee fair treatment for all major accidents establishments and to promote the QRA as a tool for assessing the safety improvements that could be introduced in an establishment to reduce risk. In addition, it included the consideration of the domino effect when the specific initiator event was established [33].

Instruction 7/2009 SIE of 1st of April, determined the requirement to present a Quantitative Risk Analysis (QRA) in the processing of environmental authorization for new establishments or substantial changes of low level, as well as for high level establishments. Additionally, it also regulated the requirement and execution of a QRA for the industrialists of affected existing establishments [34].

In addition, there is Resolution IRP/971/2010, of 31st of March. Its main objective was to establish the general criteria for the preparation of safety reports and the control of the implementation for new vulnerable elements. It was based on the chemical risk in installations that manipulate hazardous substances and on the transport of hazardous substances by road and rail, nuclear risk, and flood risk [35].

Furthermore, Law 9/2014 was published on the 31st of July 2014, its purpose was to regulate, within the scope of the powers of the Catalan Government, the legal system applicable to the industrial safety of establishments, installations, and products. Although this law did not introduce any new mandatory technical requirements, it had changes to simplify administration and reduce bureaucratic requirements [36].

Instruction 11/2010 of the 29th of October was based on the criteria for the preparation and evaluation of the safety report to be prepared by establishments affected at a high level by the current legislation on major accidents. To do so, this instruction described the criteria to be considered in the preparation of Safety Reports and their evaluation. Its main objectives were the improvement of the process of selecting accident scenarios, and it established the criteria for determining the planning distances. Then, it promoted the incorporation of existing technological safeguards in the facilities and established the intervention and lethality distances that justify the adoption of additional safeguards to minimise the risk as much as is reasonably practicable [37].

In the Plan for the external emergency of the chemical sector (PLASEQCAT) published on the 10th of March 2020, it is possible to consult those companies and establishments that are under the European SEVESO III regulation. They are forced to apply a major accident prevention system and promote the implementation of a safety management system that ensures all aspects related to internal organisation, personnel, risk assessment, operational control and planning of emergency situations. It also provides information on the categorisation of accident scenarios classified according to the degree of risk and the defined zones [38].

Finally, Decree 3/2021 was published on the 20th of December 2021. Its purpose was to establish the procedures in which the owners of the establishments must provide, the evaluation of the documentation carried out by a control organisation, as well as the procedure to be followed to carry it out [39].

2.4. Elaboration and evaluation of the information to be submitted by the establishments affected

The purpose of this section is to describe the required information to satisfy the legal requirements for establishments affected by Decree 3/2021 and RD 840/2015 in Catalonia.

To do so, the first step is to identify all hazardous substances present in the establishment and to verify whether they are included in Parts 1 or 2 of ANNEX 1 of the RD 840/2015. Those chemicals are determined by the specific list set out in Part I of Annex I, or by the categories of substances and mixtures set out in Part II of Annex I.

If the amount of any hazardous product exceeds its lower threshold, but not the upper threshold, the installation would be classified at its lower level. If the amount present of any of the hazardous products exceeds its upper threshold, the installation would be classified at its upper level. However, if the quantities present of the hazardous substances do not exceed their respective lower thresholds, the installation would not be affected. Moreover, if the quantity present of a given product does not exceed 2% of that indicated as a threshold and if it is not considered a possible cause a major accident, it shall not be considered for determining the impact of the installation.

Consequently, the threshold quantities of hazardous substances determine: i) establishments not affected, ii) establishments exceeding the lower threshold, as set out in column 2 of Parts I and II of Annex I and iii) establishments exceeding the upper threshold, set out in column 3 of Annex I, Parts I and II.

The establishments affected at a lower level have to present:

- Quantitative Risk Analysis (QRA)
    - QRA coding data sheet
    - Major Accident Prevention Policy (PPAG)
    - Safety Management System (SGS)
    - Notification

While the establishments affected at higher level have to present:

- Quantitative Risk Analysis (QRA)
    - QRA coding data sheet
    - Notification
- Safety Report (SR)
    - SR coding data sheet
    - Basic information for the elaboration of the external emergency plan (IBA)
    - Major Accident Prevention Policy (PPAG)
    - Safety Management System (SGS)
    - Notification

According to this information required, it can be concluded that a QRA is mandatory in both cases, and that the most significant difference is whether the SR is compulsory or not. The total number of installations in an establishment where a Safety Report has to be made can be very large. Since not all installations contribute significantly to the risk, it is not worthwhile to include all installations in the QRA [30].

An QRA is a methodology used during the Risk Analysis (RA), it consists of a set of methodologies for estimating the risk posed by a given system in terms of human loss or, in some cases, economic loss. It is based on the application of mathematical models to determine the consequences of the accident scenarios and on the use of the corresponding frequencies to estimate the resulting risk over a given area. QRA is performed through a series of steps or activities which are schematized in Figure 2 [40].

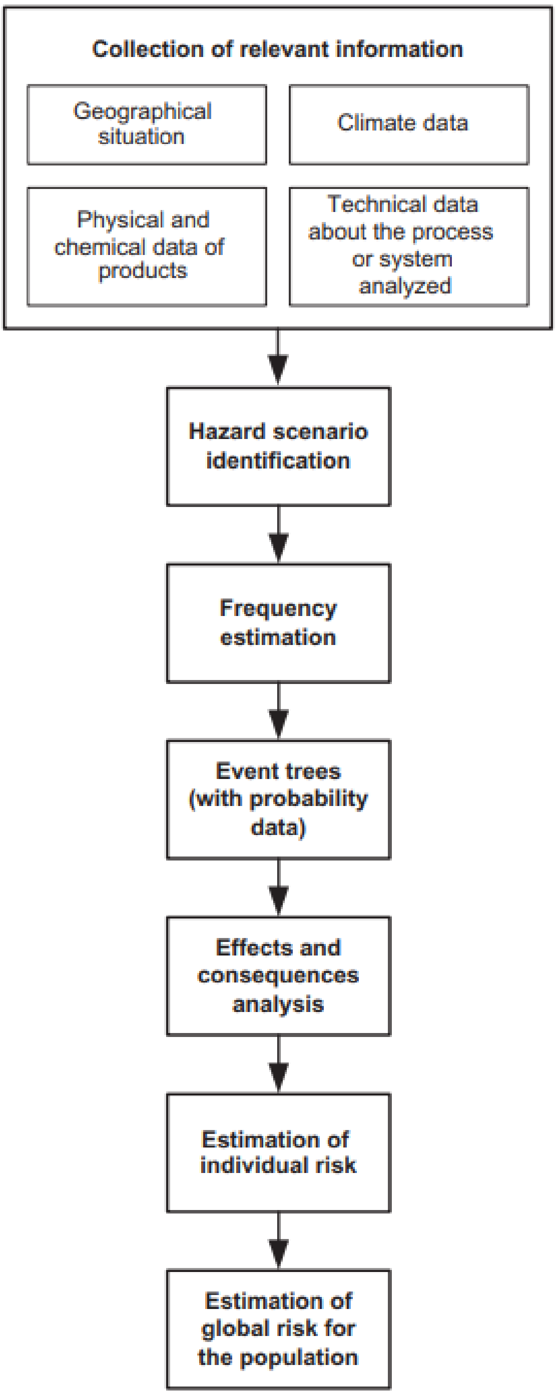

Figure 2. Main steps in a quantitative risk analysis. Source: [40]

In a QRA mathematical accident models and vulnerability models must be used to calculate the effects and consequences of each accident scenario. By combining the consequences with their corresponding frequencies, the individual risk (IR) can be obtained at any desired distance and iso-risk curves can be plotted [40].

The IR must be presented as contour lines on a normal topographic map. Frequencies of 10^{-4},10^{-5}, 10^{-6}, 10^{-7} and 10^{-8} per year must be displayed (Figure 3).

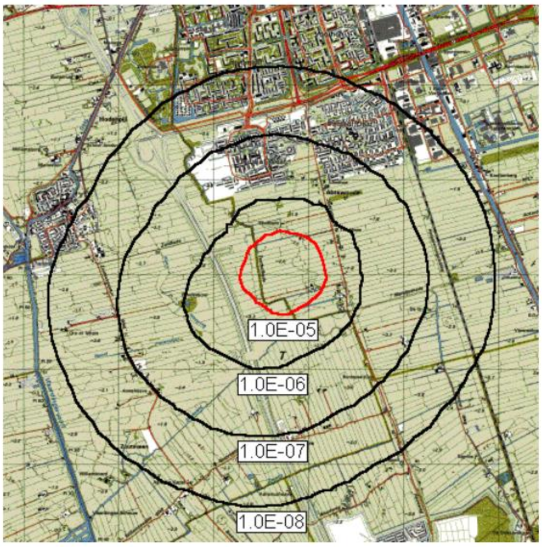

Figure 3. Example of Individual Risk contours. Source: [30]

While the societal risk must be plotted as an FN-curve (Figure 4), in which the x-axis represents the number of deaths, N. It is placed on a logarithmic scale and the minimum value should be displayed as 1. In addition, the y-axis represents the cumulative frequency of the accidents, with the number of deaths equal to N or more [30].

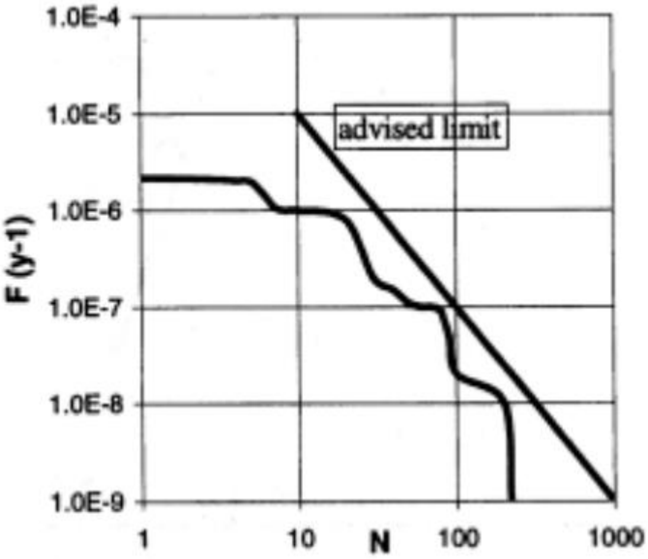

Figure 4. Presentation of the societal risk curve. Source: [30]

Focussing on the high-level establishments, a SR has the purpose of demonstrating which measures have been taken to prevent and limit the consequences of major accidents. Its main structure can be seen in Figure 5.

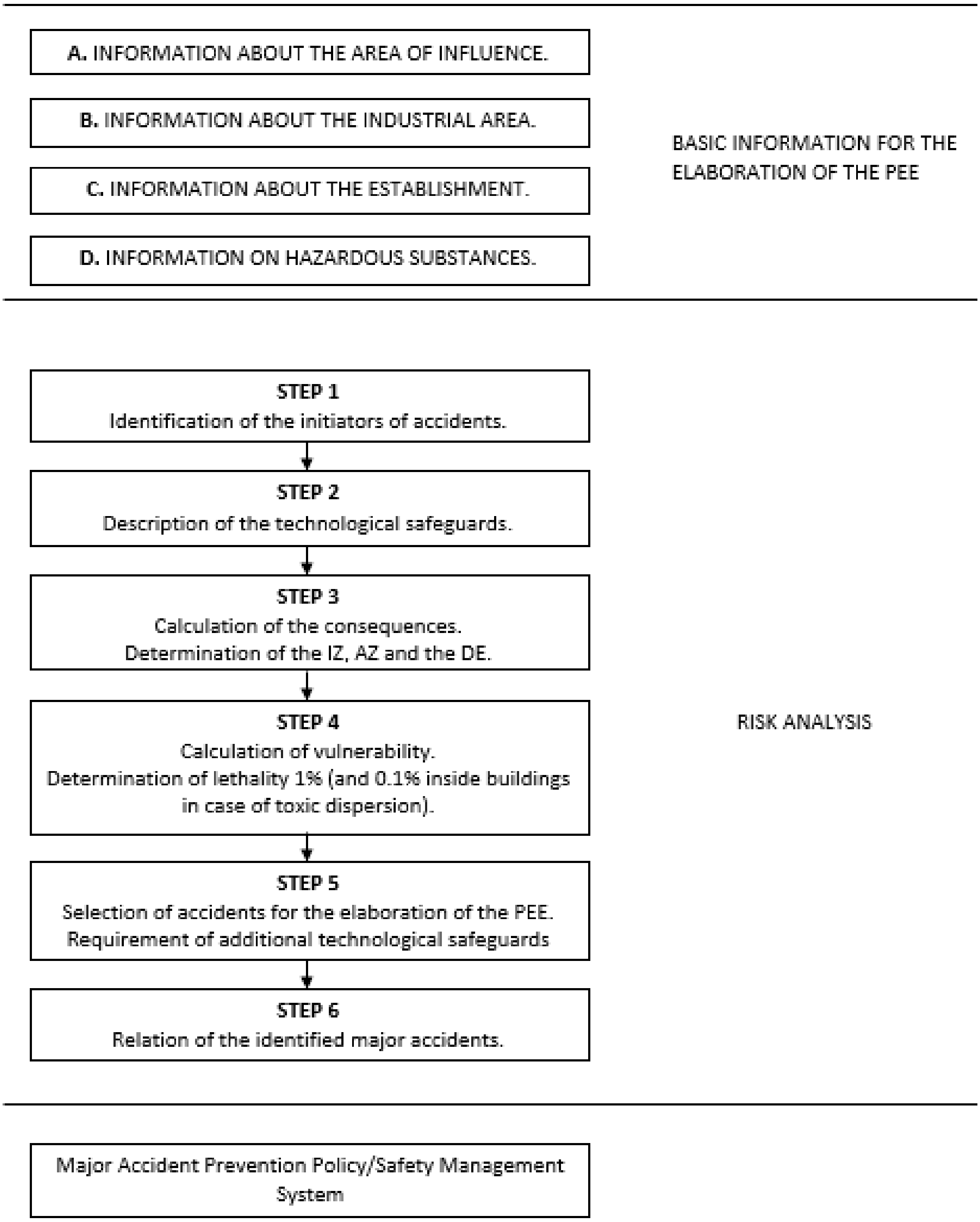

Figure 5. Structure of a Safety Report. IZ intervention zone, AZ: Alert zone; DE: Domino Effect zone; PEE: External Emergency Plan.

The first set of information that should include is related to the characteristics of the establishment's environment and surroundings, and the description of the installation. It also includes the identification of hazardous substances, including their Safety Data Sheets.

The second block is the RA, whose main objective is the prevention of the effects of a possible major accident in industrial installations and to mitigate the effects of the accident. i.e., to define vulnerable areas around the facilities where accidents may occur. It is done following the six different steps depicted in Figure 5, i.e., the identification of initiator events, the description of technological safeguards, the calculation of the Intervention Zone (IZ), Alert Zone (AZ) and the domino effect zone (DE). Further steps are the calculation of vulnerability, the selection for the elaboration of PEE and the relation of the identified major accidents.

IZ is the zone in which the consequences of accidents may produce a level of damage that justifies the immediate application of protection measures. AZ is the area in which the consequences of accidents cause effects which, although perceptible to the population, do not justify the immediate application of protective measures, except for critical population groups [41]. The DE Zone is the area in which potential accidents propagation must be considered (Figure 6) [42].

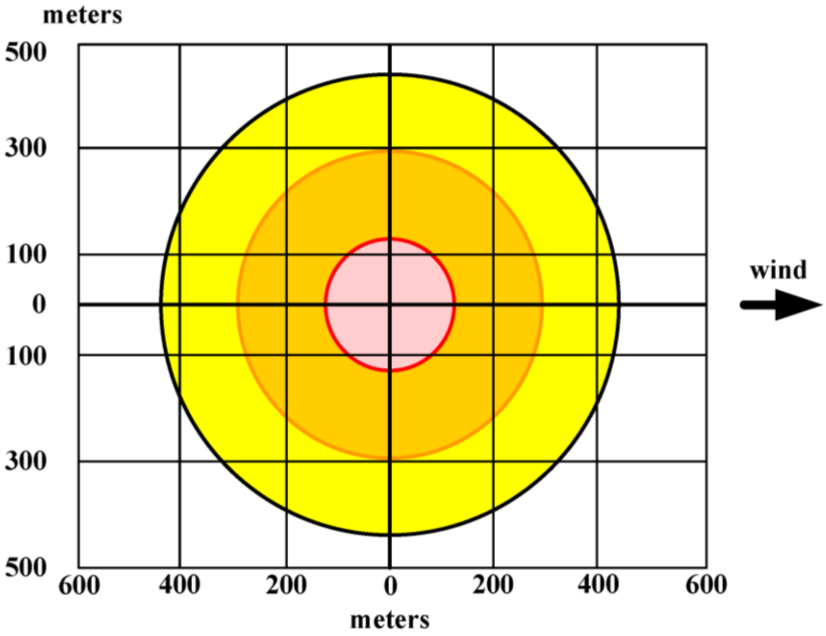

Figure 6. IZ in orange, AZ in yellow and DE in pink. Source: [43]

For the first step on hazard identification, it is required the identification of generic initiator events. For each of the initiators of accidents, the corresponding event trees will be prepared which will determine the final accidents.

The second step is the description of the safeguard's technologies, which details the prevention, control and mitigation safeguards existing in the establishments for the management of hazardous substances and the ones applied to the initiators event under study.

The third step is the calculation of the consequences (IZ, AZ, DE), aimed at determining the areas of emergency planning and domino effects associated with the final accidents resulting from the initiators event described in step 1. These computations are carried out in a justified way including the existing safeguard technologies in the establishment that have been identified in step 2. Those calculations are made using programs such as ALOHA and/or EFFECTS [44]. To this end, the source term must be calculated and associated with a given time, depending on the safeguarding technologies applied.

The fourth step is the calculation of vulnerability to determine the 1 % fatality areas and a 0.1 % inside the buildings in case of a toxic dispersion, associated with the final accidents caused by the initial accidents. So, it is needed to calculate the vulnerability by using tabulated data or graphs, or by applying analytical models (Probit equations).

The fifth step is the selection of the accidents to be included in the PEE and the recommendation of additional safeguards. Additionally, a criterion of distances from the intervention zone and lethal dose of 1 % is set. From these, the evaluator must recommend the study of additional technological safeguards to reduce the planning distances.

Finally, in step 6, these accidents are classified for use in the preparation of PEE. The purpose of the PEE is to have an emergency planning system that allows an effective response and management of incidents. It establishes the response structure, operations, and procedures necessary to manage any emergency in establishments affected by the regulations on major accidents involving chemical substances, with the aim of minimising the risk and guaranteeing the safety of people and the protection of property, infrastructure, and environment.

3. Data base description

In this chapter it will be explained in detail the database (DB) that is created for the collection of information from SR. Also, it will be justified the reason for each of the selected fields and the variables that are considered to analyse these data.

The general design of the DB is based on the Generalitat de Catalunya's accident hypothesis coding table [45]. It shows the required parameters for a QRA, such as the substances involved, and the meteorology applied. Also, initiator events are divided into three categories: equipment, type, and the loss of containment (LOC), and then, there is the definition of the final accident. Finally, the calculated distances for the IZ, AZ, and DE zone are specified for each of the possible major accidents.

Additional information is considered. Firstly, general information about the company is collected, as well as its location (city and province), its general sector and the specific industrial activity, based on the International Standard Industrial Classification of All Economic Activities (ISIC) [46].

Furthermore, data concerning the meteorological conditions is included, which is an essential variable for the determination of the lethal consequences. It is contemplated the temperature and the relative humidity from the nearest weather station to the company (Figure 7). Accordingly, those values will be the annual average of the station [33].

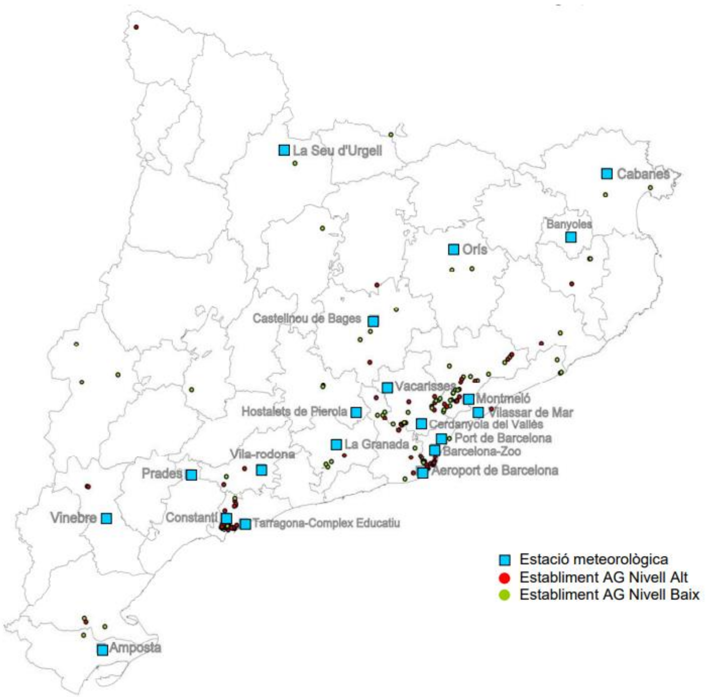

Figure 7. Weather stations. Source: [47].

Another important aspect to be considered is the atmospheric stability, which represents the level of turbulence that exists at a given moment and it is a function of wind velocity and solar radiation. At the same time, solar radiation depends on the angle of incidence of the sun's rays on the Earth's surface, the season of the year and the amount of clouds present in the atmosphere [48].

Stability can be classified in six different classes related to the Pasquil categories. Thus, stability A represents a very unstable atmosphere, B unstable, C slightly unstable, D neutral, E slightly stable and F stable. It has to be highlighted that an unstable atmospheric condition is characterised by the existence of a significant vertical movement of the air mass, a negative vertical temperature gradient, frequent fluctuations in the direction of the wind, strong insolation, etc. In contrast, a stable condition is characterised by a laminar flow of air layers (absence of turbulence), a positive vertical temperature gradient (thermal inversion), minimal fluctuations in the direction of the wind and a low level of sunshine [48].

According to Instruction 11/2010, two different meteorological conditions must be considered in each study of a potential major accident in an installation. The most probable Pasquill stability at the reference meteorological station, including the mean velocity for it, and the Pasquill stability F, including its mean velocity. In the case of overlapping the most probable with class F, the data of the second most probable is taken [37].

In addition, it is collected the wind velocity and its direction which will be associated with an atmospheric stability. The information about the wind is defined by the *wind rose*. The directions are usually given in 8 or 16 sections of 45º or 22,5º respectively, named according to the cardinal directions. The data of the wind are taken at a certain height, since they vary according to it, depending on the atmospheric stability and the roughness of the ground (Figure 8) [49]. Generally, the velocity recorded by the meteorological services refers to an altitude of 10 m.

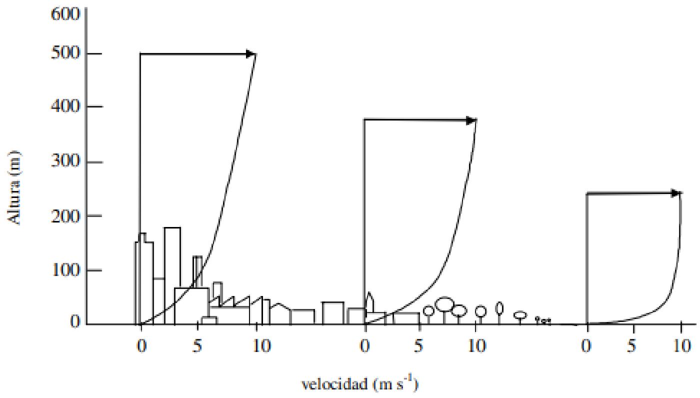

Figure 8. Velocity profile. Source: [49]

The next block of information is related to the hazardous substance involved in each possible major accident. For this purpose, the name of the substance, and the CAS number associated to each one is collected. Furthermore, the Global Harmonized System (GHS) classification has been considered to classify substances according to their hazards [50].

At the GHS hazards are grouped into three blocks, physical, health, and environmental. Within these three blocks, different subgroups can be distinguished. For the case of physical damage, this categorisation is divided into 17 possible classes (Table 1), for the case of health, into 10 (Table 2), and for the environmental one, it is subdivided into 2 groups (Table 3). This classification is established by the H-phrases of the substance. Concretely, all H200 phrases are for physical, H300 phrases are for health and H400 phrases are for environmental hazard [30].

Table 1. Type of physical hazards. Source: [50]

Explosive	Substance which in contact with water, emit flammable gases
Aerosols	Oxidising liquids
Oxidising gases	Oxidising solids
Gas under pressure	Organic peroxide
Flammable liquid	Corrosive metals
Flammable solid	Desensitized explosive
Self-heating substance	

Table 2. Types of health hazards. Source: [50]

Actuate toxicity (oral/dental/inhalation)	Cancerogenicity
Skin corrosive/irritation	Reproductive toxicology
Respiratory or skin sensitization	Specific target organ systemic toxicity – simple exposure

Serious eye damage/eye damage	Specific target organ systemic toxicity – repeated exposure
Germ cell mutagenicity	Aspiration toxicity

Table 3. Types of environmental hazards. Source:[50]

Hazardous to aquatic environmental (acute/chronic)	Hazardous to the ozone layer

The total amount of the substance considered to be released is included in the data base. Moreover, information about the source term and the release time of each possible accident is compiled [44]. Regarding the source term, it is useful to quantify the flow rate at which accidental releases of hazardous substances may occur and/or to estimate the release quantity and the duration.

In addition, a very important set of information that is considered is the information about the initiator event of any potential major accident. To do so, the classification described in the Instruction 11/2010 is taken into account. So, possible major accidents will depend on the initiating event, which is often a loss of containment (LOC), and on a set of circumstances that will determine the accident sequences that may follow afterwards [51].

LOCs of an installation should be included only if two conditions are fulfilled: i.e. (1) frequency of occurrence is equal to or greater than 10^{-8} per year and (2) lethal damage (1% probability) occurs outside the establishment's boundary or the transport route [30].

The initiating event field is divided into three different subcategories in the DB: equipment, type, and LOC. Referring to the first and second subgroup, these fields give information on where the major accident could happen. So, LOC scenarios can occur due to the accidental release of a hazardous chemical substance from a piece of equipment (such as stationary tanks, gas cylinders, pipes, pumps, heat exchangers, pressure relief devices, warehouses, etc.) or transport units (e.g., road tankers, rail tank wagons, ships, etc.) [52].

Those possible scenarios must be characterized. That is, their frequencies and consequences must be determined. To estimate the probable frequencies, values must be assigned to the frequency of the initiating event (e.g., rupture of a pipe) and to the probabilities in the accident sequence [51]. In this sense and according to BEVI these initiators are the ones seen in Table 4.

Table 4. Classification of equipment and Loss of containment (LOC) and its frequencies. Source: [51]

System	Instantaneous Release of the Complete Inventory	Release (at Constant Rate) of the Complete Inventory in 10 min	Continuous Release from a Hole With ds=10 mm
	Stationary Vessels		
Pressure vessel	$5 \cdot 10^{-7}$ year $^{-1}$	$5 \cdot 10^{-7}$ year $^{-1}$	$1 \cdot 10^{-5}$ year $^{-1}$
Reactor, process vessel	$5 \cdot 10^{-6}$ year $^{-1}$	$5 \cdot 10^{-6}$ year $^{-1}$	$1 \cdot 10^{-4}$ year $^{-1}$
Reactor vessel	$5 \cdot 10^{-6}$ year $^{-1}$	$5 \cdot 10^{-6}$ year $^{-1}$	$1 \cdot 10^{-4}$ year $^{-1}$
	Atmospheric Tanks		
Single containment tank	$5 \cdot 10^{-6}$ year $^{-1}$	$5 \cdot 10^{-6}$ year $^{-1}$	$1 \cdot 10^{-4}$ year $^{-1}$
Double containment tank	$1{,}25 \cdot 10^{-8}$ year $^{-1}$	$5 \cdot 10^{-8}$ year $^{-1}$	$1 \cdot 10^{-4}$ year $^{-1}$
Mounded tank	$1 \cdot 10^{-8}$ year $^{-1}$	-	-
	Heat Exchangers		
Hazardous material outside pipes	$5 \cdot 10^{-5}$ year $^{-1}$	$5 \cdot 10^{-5}$ year $^{-1}$	$1 \cdot 10^{-3}$ year $^{-1}$
Hazardous material inside pipes	$1 \cdot 10^{-5}$ year $^{-1}$	$1 \cdot 10^{-3}$ year $^{-1}$	$1 \cdot 10^{-2}$ year $^{-1}$
Distillation columns	$5 \cdot 10^{-6}$ year $^{-1}$	$5 \cdot 10^{-6}$ year $^{-1}$	$1 \cdot 10^{-4}$ year $^{-1}$

Road Tankers and Tank Wagons in an Establishment	Instantaneous Release of the Complete Inventory	Continuous Release from a Hole (Largest Connection Size)	Full Bore Rupture, Loading/ Unloading Hose	Leak of Loading/ Unloading Hose (ds = 0.1d, max. 50 mm)
Pressurized tank	$5\cdot10^{-7}$ year^{-1}	$5\cdot10^{-7}$ year^{-1}	$4\cdot10^{-6}$ h^{-1}	$4\cdot10^{-5}$ h^{-1}
Atmospheric tank	$1\cdot10^{-5}$ year^{-1}	$5\cdot10^{-7}$ year^{-1}	$4\cdot10^{-6}$ h^{-1}	$4\cdot10^{-5}$ h^{-1}

Centrifugal Pumps and Compressors	Catastrophic Failure	Leak (ds=10% d, max. 50 mm)
Without gasket	$1\cdot10^{-5}$ year^{-1}	$5\cdot10^{-5}$ year^{-1}
With gasket	$1\cdot10^{-4}$ year^{-1}	$4{,}4\cdot10^{-3}$ year^{-1}

Pipes	Full Bore Rupture	Leak (d=.1ds, max. 50 mm)
Φ <75 mm	$1\cdot10^{-6}$ year^{-1} / meters	$5\cdot10^{-6}$ year^{-1} / meters
for 75 < Φ <150 mm	$3\cdot10^{-7}$ year^{-1} / meters	$2\cdot10^{-6}$ year^{-1} / meters
Φ >150 mm	$1\cdot10^{-7}$ year^{-1} / meters	$5\cdot10^{-7}$ year^{-1} / meters

Depending on the meteorological conditions, the properties of the released material, and the plant's characteristics, various sequences could follow the accident initiating event and various final accident scenarios are possible [51]. So, the next step is obtaining information about the final accident.

It is important to mention that this category is divided into two different fields. Initially, there is the *Basic Scenario* which is classified into three different scenarios, such as dispersion, explosion, and fire. Then, there is the *Final Scenario* category, which gives more information about the previous one, considering the classes shown in Table 5.

Table 5. Final scenarios associated to a basic scenario. Source: [37]

Basic Scenario	Final Scenario
Dispersion	Flammable Dispersion
	Oxidizing Dispersion
	Toxic Cloud Dispersion
Explosion	Unconfined Vapour Cloud Explosion
	BLEVE
	Confined Vapour Explosion
Fire	Flash Fire
	Jet Fire
	Pool Fire
	Warehouse Fire

Going into detail on Table 5, dispersion refers to the evolution of a toxic or flammable gas cloud in the atmosphere. The dispersion of such a cloud takes place by diffusion and, essentially, transported by the wind: the cloud moves in the wind's direction but also perpendicular to the wind, both vertically and horizontally [53]. The basic scenario of dispersion is divided into 3 categories for the final scenario, giving place to flammable dispersion, oxidizing dispersion, and toxic cloud dispersion. This classification depends on the properties of the substance being dispersed.

Explosions are associated with a very fast release of energy that produces large quantities of expanding gas. Depending on the level of confinement in the atmosphere, there are two types of explosions: unconfined flammable vapour cloud explosion (UVCE), and confined vapour explosion (CVE) [49]. BLEVE is the acronym for Boiling Liquid Expanding Vapor Explosion. It is a type of vessel explosion, which can have a high energy content [54].

The Basic Scenario *fire* can be divided into 4 different subcategories, including flash fire, jet fire, pool fire, and warehouse fire. A flash fire occurs if a flammable gas or vapor is released in certain meteorological conditions and formed a cloud. The flammable cloud will disperse, increasing in size, and will move according to wind direction. If it meets a source of ignition, the mass between the flammability limits will burn very quickly, as the flames are propagated through the cloud. A pool fire is characterized by turbulent diffusion flames on a horizontal pool of fuel that is vaporized. The liquid receives heat from the flames by convection and radiation and may lose or gain heat by conduction toward/from the solid or liquid substrate under the liquid layer [55]. Additionally, a jet fire has a stationary and elongated flame (of large length and small amplitude) caused by the ignition of a turbulent jet of combustible gases or vapours [49]. Finally, warehouse fires are associated with higher average property losses per fire than most other occupancies. It must be considered that warehouses are properties that are used for the storage of commodities. Despite their common purpose, warehouses vary based on size, types of materials stored, design, storage configurations, construction and other factors [56].

Once the final scenarios are determined, it must be considered that their final frequencies will also depend on the properties of the released materials, the meteorological conditions (wind and atmospheric stability), the structure of the plant (layout, equipment congestion, and possible ignition sources), the existence of safety barriers (deluge systems and fireproofing), and the operators' training, among other factors.

To carry out the assessment of the consequences, RD 840/2015 determines the threshold values that must be considered on the application of models and risk zoning [41]. So, the area potentially affected by an accident is divided into different zones (IZ, AZ, DE) according to the type of hazard, the intensity of the effects, and the vulnerability of people and property. Table 6 shows the threshold values classified as a function of the type of accidents [42].

Table 6. Threshold values. Source:[37]

	Accident type	**Intervention Zone**	**Alert Zone**	**Domino Effect Zone**
Dispersion	Toxic Dispersion	AEGL-2, ERPG-2, and TEEL-2	AEGL-1, ERPG-1, and TEEL-1	-
Explosion	UVCE	$\Delta P = 125$ mbar	$\Delta P = 50$ mbar	$\Delta P = 160$ mbar
	CVCE	$\Delta P = 125$ mbar	$\Delta P = 50$ mbar	$\Delta P = 160$ mbar
Fire	Flash Fire	LFL	50% LFL	-
	Pool Fire	$250\ (kW\cdot m^{-2})^{4/3}\cdot s$ Equivalent to:	$115\ (kW\cdot m^{-2})^{4/3}\cdot s$. Equivalent to:	$8\ (kW\cdot m^{-2})$

		5 $(kW\cdot m^{-2})$ for 30 s	3 $(kW\cdot m^{-2})$ for 30 s	
	Jet Fire	250 $(kW\cdot m^{-2})^{4/3}\cdot s$ Equivalent to: 5 $(kW\cdot m^{-2})$ for 30 s	115 $(kW\cdot m^{-2})^{4/3}\cdot s$. Equivalent to: 3 $(kW\cdot m^{-2})$ for 30 s	8 $(kW\cdot m^{-2})$

Acute Exposure Guideline Levels (AEGL) are intended to describe the risk to humans resulting from once-in-a-lifetime, or rare, exposure to airborne chemicals. Each of the three levels of AEGL is developed for each of five exposure periods: 10 minutes, 30 minutes, 1 hour, 4 hours, and 8 hours [42].

- AEGL-1 is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience significant discomfort, irritation, or certain asymptomatic no sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.
- AEGL-2 is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.
- AEGL-3 is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Emergency Response Planning Guidelines (ERPGs) are defined as the concentration ranges at which adverse health effects could be observed. ERPG guidelines do not protect everyone, as hypersensitive individuals suffer adverse reactions to concentrations far below those suggested in the guidelines. It is divided into three levels [42] :

- ERPG-1 is the maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 h without experiencing other than mild transient adverse health effects or perceiving a clearly defined objectionable odour.
- ERPG-2 is the maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 h without experiencing or developing irreversible or other serious health effects or symptoms which could impair an individual's ability to take protective action.
- ERPG-3 is the maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 h without experiencing or developing life-threatening health effects.

Temporary Emergency Exposure Limits (TEELs) are temporary loss-of-containment events to use when ERPGs are not available. TEEL-0 is the threshold concentration below which most individuals will experience no appreciable risk to their health. TEEL-1 is the same as ERPG-1, TEEL-2 is the same as ERPG-2, and TEEL-3 is the same as ERPG-3 [42].

4. Data base exploratory analysis

This chapter shows the results of the analyses carried out on the variables of highest interest in the data base. To do so, an exploratory data analysis (EDA) has been done to investigate data sets and to summarise their main characteristics, using data visualisation methods. So, EDA is a set of techniques aimed at achieving a basic understanding of the data and the relationships between the variables being analysed.

In order to generate this EDA, it was decided to select general variables of the company, such as its location, according to the province and the city. Also, meteorological variables were considered (e.g., temperature, RH stability, wind velocity and direction). Lastly, the final accident described in the SR is investigated.

However, before starting with the EDA, it is interesting to highlight that this database is based on data collected from 15 different companies in Catalonia. From the different scenarios studied in each of the companies, a database was obtained with 626 records.

4.1. General aspects

To begin with, an analysis of the company is carried out, highlighting its location, defined by the province and the city. As mentioned above, since these data is obtained from companies located in Catalonia, the provinces are Barcelona and Tarragona.

From the information obtained, it is concluded that of the 626 entries in the database, 80% of the cases are located in Barcelona and the remaining 20% in Tarragona.

4.2. Meteorological conditions

Continuing with the analysis, this section focuses on the meteorological conditions, highlighting temperature, RH, atmospheric stability, wind velocity and its direction at each of the inputs, as seen in Figure 9 and Figure 10.

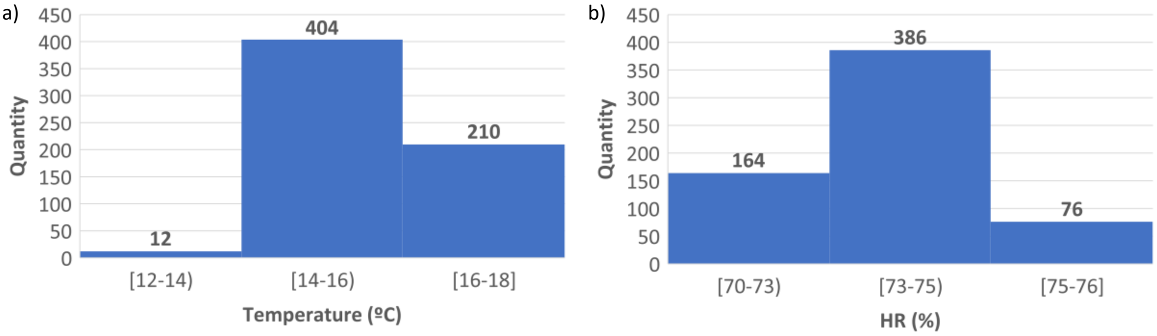

Figure 9. a) temperature and b) relative humidity

To begin with, in Figure 9 the extent of temperature and the HR is depicted. These data are obtained from the weather station from *Servei Meteorològic de Catalunya* closest to the company [47]. Analysing those values, it can be seen how temperature records range between 12 and 18 ºC. However, the most representative temperature is between 14-16 ºC, while the minimum one is in the range of 12-13 ºC.

In relation to the HR parameter, its values go from a 70 to 76 %, having its maximum quantity of records in a range of 73-75 % and it is minimum at 75-76 %.

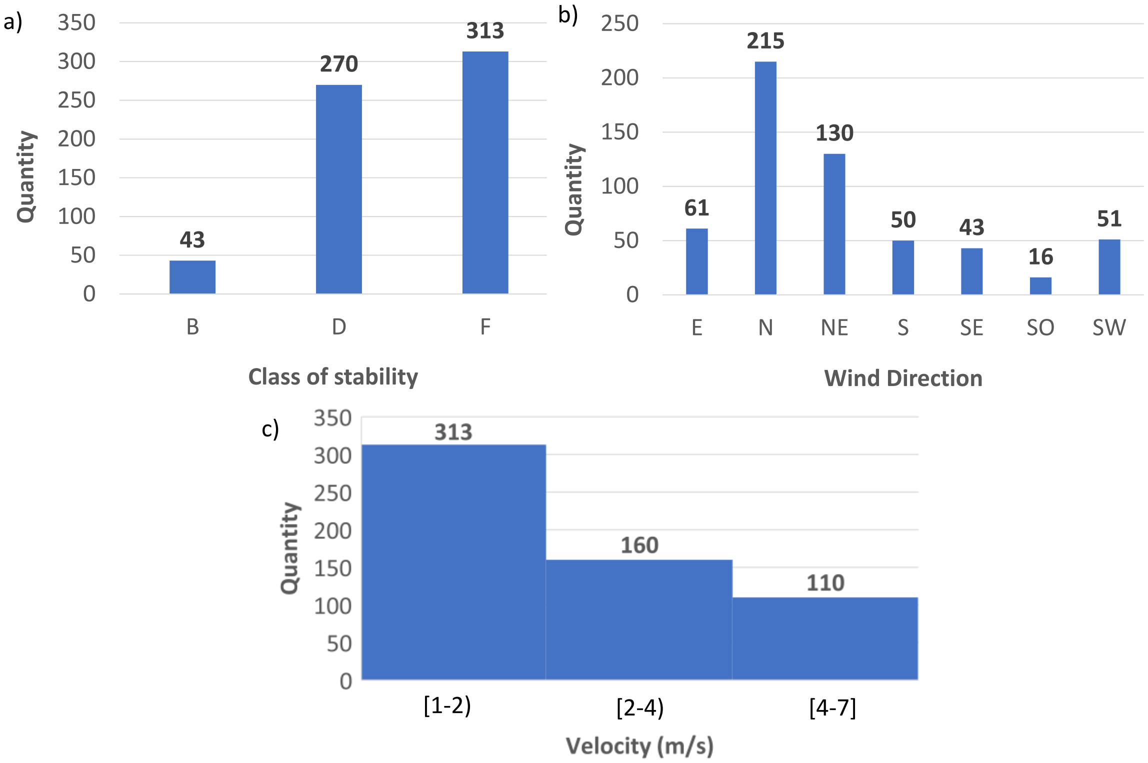

Figure 10. a) stability, b) wind direction and c) wind velocity.

Another variable plotted is the atmospheric stability (Figure 10a). To start with, it is important to highlight that during the preparation of a safety report, two atmospheric conditions must be considered. As discussed above (in chapter 3), these stability classes will refer to the most probable class and to stability class F.

Analysing the obtained graph (Figure 10a), this fact can be verified since half of the entries are F class. Consequently, there are 313 inputs for that class, while the other half varies between class D (270) and class B (43).

Finally, it is studied the effect of the wind, in terms of direction and velocity magnitude. Regarding the direction of the wind, it is important to keep in mind its classification, which depends on the cardinal points, such as North (N), South (S), East (E), West (W). From the values obtained in the histogram (Figure 10b), there are different possibilities for this wind direction, being the most representative N, and the least representative being SO.

In addition, there is the wind velocity (Figure 10c). This variable ranges from values of 1 to 7 m/s. However, the most significant is between 1-2 m/s and the least represented one is in a range of 4-7 m/s. Analysing these data (plots not shown), it is concluded that the results showing a stability class B are associated with a velocity of 2 m/s. Also, it is observed that all cases of stability F are associated with low velocities, i.e., those cases that have a velocity below 2 m/s. Therefore, high velocities in the range of 4-7 m/s belong to atmospheric stability D.

4.3. Substances

The next block of information to be analysed is the hazardous substance involved in potential major accidents. To do so, Figure 11 includes a visual representation of all substances mentioned in the safety reports reviewed.

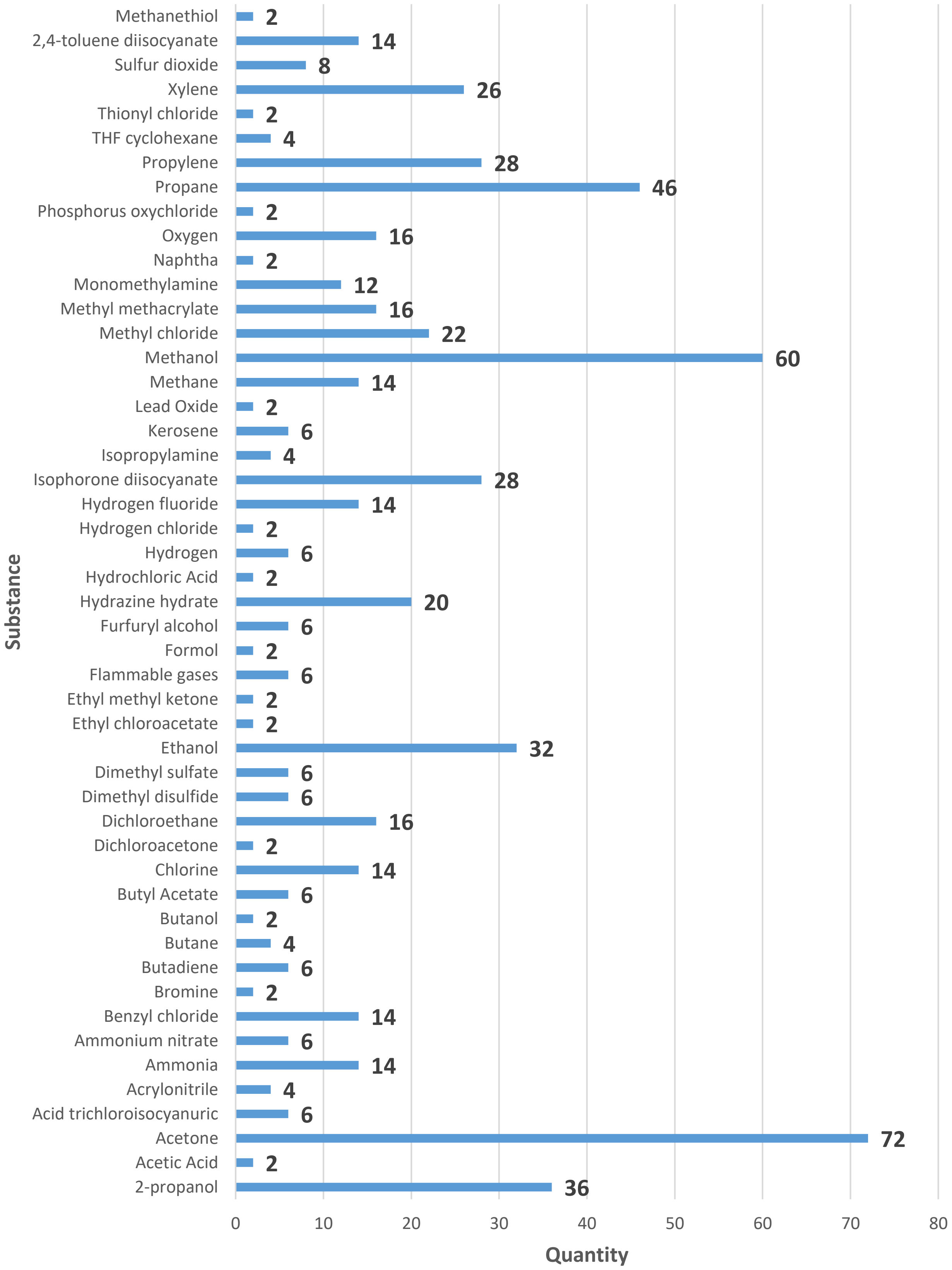

Figure 11. Hazardous substances included in the database.

According to the information provided in the figure above, a total of 49 different hazardous substances are observed. Among them, the most representative are acetone, methanol, and propane. In contrast, there is a set of 14 different substances being the less representative, since there are only two cases of each of these substances studied in the safety reports analysed.

Continuing with the analysis of the substances, Table 7 shows the GHS classification for each of them. This classification is related to the corresponding hazard statements (H-phrases) and it is divided into three different categories: physical, health and environmental, as it is classified in Table 1, Table 2, and Table 3.

Table 7. GHS classification for each substance.

Substance	**Physical Hazard**	**Health hazard**	**Environmental hazard**
2-propanol	🟨		
2,4-toluene diisocyanate		🟦	
Acetic Acid	🟨	🟦	
Acetone	🟨	🟦	
Acid trichloroisocyanuric	🟨	🟦	🟩
Acrylonitrile	🟨	🟦	🟩
Ammonia	🟨	🟦	🟩
Ammonium nitrate	🟨	🟦	
Benzyl chloride		🟦	
Bromine		🟦	🟩
Butadiene	🟨	🟦	
Butane	🟨		
Butanol	🟨	🟦	
Butyl Acetate	🟨	🟦	
Chlorine	🟨	🟦	🟩
Dichloroacetone		🟦	🟩
Dichloroethane	🟨	🟦	
Dimethyl disulphide	🟨	🟦	🟩
Dimethyl sulphate		🟦	
Ethanol	🟨		
Ethyl chloroacetate		🟦	🟩
Ethyl methyl ketone	🟨	🟦	
Flammable gases	🟨	🟦	🟩
Formol		🟦	
Furfuryl alcohol		🟦	
Hydrazine hydrate	🟨	🟦	🟩
Hydrochloric Acid		🟦	
Hydrogen	🟨		
Hydrogen chloride		🟦	
Hydrogen fluoride		🟦	

Isophorone diisocyanate		🟦	🟩
Isopropylamine	🟨	🟦	
Kerosene	🟨	🟦	🟩
Lead Oxide		🟦	🟩
Methane	🟨		
Methanethiol	🟨	🟦	🟩
Methanol	🟨	🟦	
Methyl chloride	🟨	🟦	
Methyl methacrylate	🟨	🟦	
Monomethylamine	🟨	🟦	
Naphtha	🟨	🟦	🟩
Oxygen	🟨		
Phosphorus oxychloride		🟦	
Propane	🟨		
Propylene	🟨		
Sulphur dioxide		🟦	
THF cyclohexane			
Thionyl chloride		🟦	
Xylene	🟨	🟦	🟩

Altogether, it is observed that of these 49 substances, 32 are physically hazardous, 40 are hazardous to health and 16 are hazardous to the environment. However, if it is analysed in detail, it is seen that there are 8 substances that are only categorised as being physically hazardous and 11 substances that are only classified as health hazards. Consequently, the remaining 33 substances are associated with a combination of 2 or 3 types of hazards.

Thus, there are 13 substances for the combination of physical and health hazard, 5 substances for health and environmental hazard, and the remaining 11 substances for the combination of the three hazard categories. These substances are acid trichloroisocyanuric, acrylonitrile, ammonia, chlorine, dimethyl disulphide, flammable gases, hydrazine hydrate, kerosene, methanethiol, naphtha and xylene.

4.4. Final accident

The following indicator to be analysed is the possible final accident, which is divided into: basic and specific scenario. Regarding the first classification, three different categories can be distinguished such as dispersion, explosion, and fire.

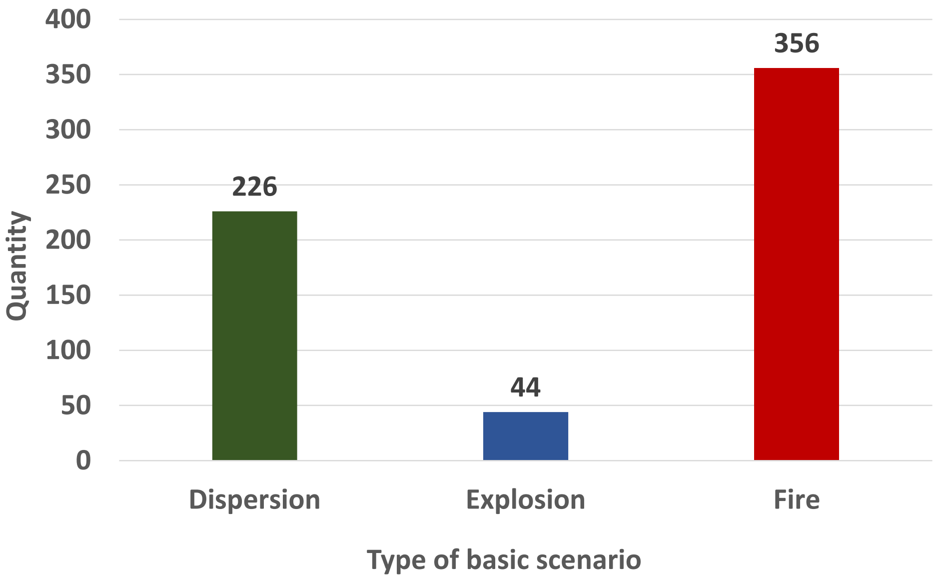

Figure 12. Basic scenario distribution

Figure 12 presents the results of the quantification of each of these cases, showing a 57% of the cases corresponding to the possible generation of a fire, 36% associated to dispersion and the remaining 7% belong to possible explosions that could be generated.

Once the basic scenario has been discussed, the following parameter to analyse is the specific scenario, considering the classification done in Table 5. Figure 13 shows the specific scenarios for each of the above-mentioned categories.

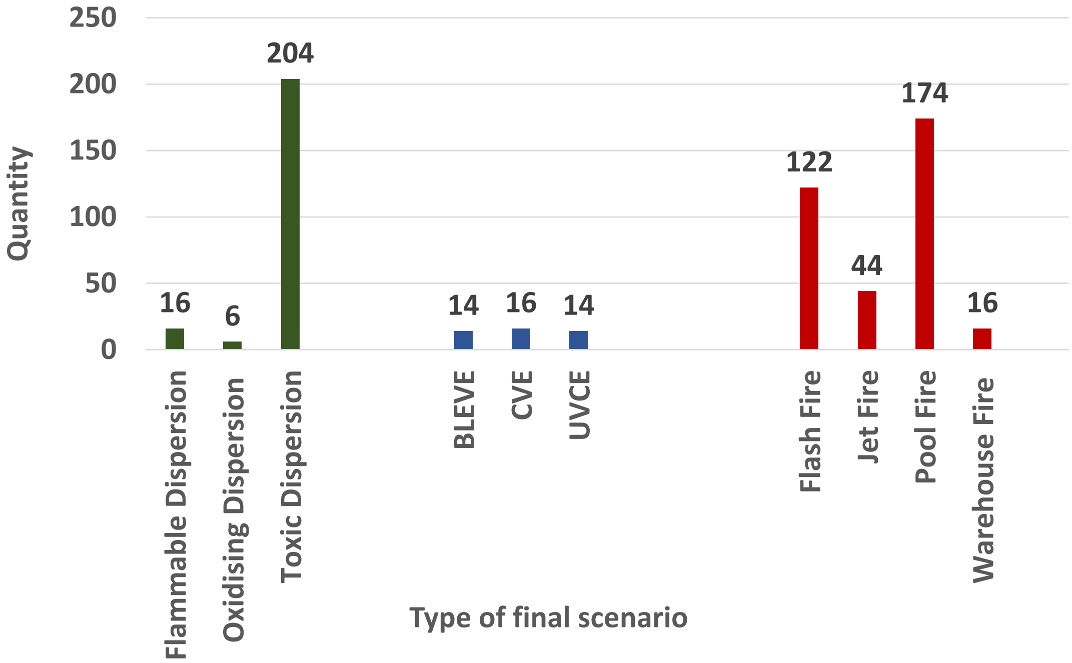

Figure 13. Final scenarios distribution.

Regarding the dispersion, it is divided into three different subcategories, flammable, oxidising and toxic. According to Figure 12, there are 226 possible cases registered for dispersion. Among them, toxic dispersion stands out with 204 associated entries, followed by flammable dispersion with 16 inputs and finally oxidising dispersion with the remaining 6.

Concerning explosions, this scenario is divided into three subcategories, BLEVE, CVE and UVCE. At a general view, 44 possible cases of explosions have been listed in the DB, including 16 for CVE and the remaining ones for BLEVE and UVCE, considering 14 inputs for each of those fields.

Finally, the last category to be analysed is the case of fire, which is divided into four different types, namely flash fire, jet fire, pool fire and warehouse fire. There are a total of 356 different entries in the database, in which pool fires stand out with 174 associated cases, followed by flash fires with a total of 122 different entries, and jet fires with 44 cases and finally, there are warehouse fires with the remaining 16 entries in the database, being the least representative.

4.5. IZ, AZ and DE zone

In this last section the safety distances, referring to IZ, AZ and DE zone, are analysed for each of the scenarios described above. Hence, it is possible to observe the impact caused by each of the possible final accidents in the risk zones.

4.5.1. Basic scenario

Firstly, the safety distances for the basic scenario, which includes dispersion, explosion, and fires, is studied. For this purpose, Figure 14 shows the minimum and maximum values of those distances.

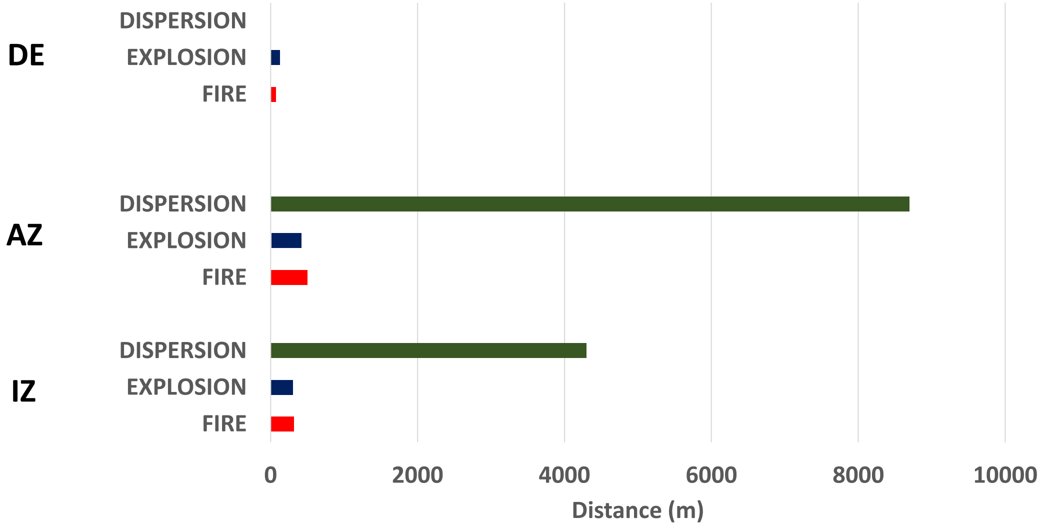

Figure 14. Intervention Zone, Alert Zone, and Domino Effect Zone for basic scenario.

On a general overview, it is seen that the distances of the AZ are the longest, i.e., they cover a larger range of distances than in the case of the intervention zones. This is because they depend on less restrictive threshold values. Furthermore, IZ will always have smaller distances since they are closer to the affected installation. Finally, in the case of the DE, these zones should be very short, because it is a marked zone where the domino effect can occur close to the installation, or even inside it. This fact can be demonstrated according to Figure 6.

In Figure 14 it is observed that the longest distances for IZ are for the cases of dispersion, worst cases reaching values of approximately 4300 m. This is followed by the case of fire and finally the explosion scenario.

Concerning the AZ distance, it is observed the same behaviour than in IZ. There is a higher range of values for the case of dispersion, followed by fires and finally the explosion case. Related to the dispersion case, it has a distance range of up to 8600 m. While the other two cases have much smaller distances, being 500 m in the case of fire and 400 m in the case of explosion.

Lastly, it is seen that the dispersion does not have a DE, as described in Table 6. In addition, it can also be observed that the explosion case has a longer range than the fire scenario, covering longer distances.

4.5.2. Specific scenario

According to the classification in Table 5, dispersion is divided into three subgroups, flammable, oxidative and toxic. In the case of explosion, it is categorised into BLEVE, CVE and UVCE, and finally in case of fire, it is divided into flash fire, jet fire, pool fire and warehouse fire.

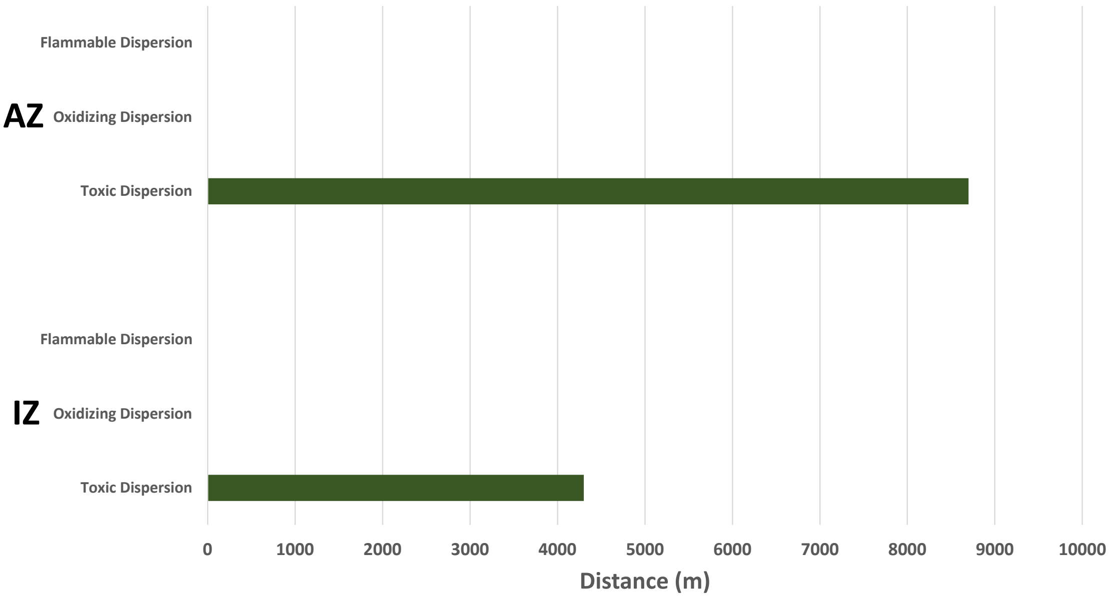

Figure 15. Intervention Zone and Alert Zone for dispersion.

Figure 15 shows the intervention and alert distances for the case of dispersion. It is seen that the oxidising and flammable dispersion does not contain inputs of risk zones registered. The fact that the distances are not displayed is because no threshold values for their calculation are indicated in Table 6, since its dispersion does not represent in itself a risk of toxicity. Furthermore, those distances are only observed for the case of the toxic dispersion, reaching up to 4300 meters for the intervention zones and 8700 meters for the alert zones.

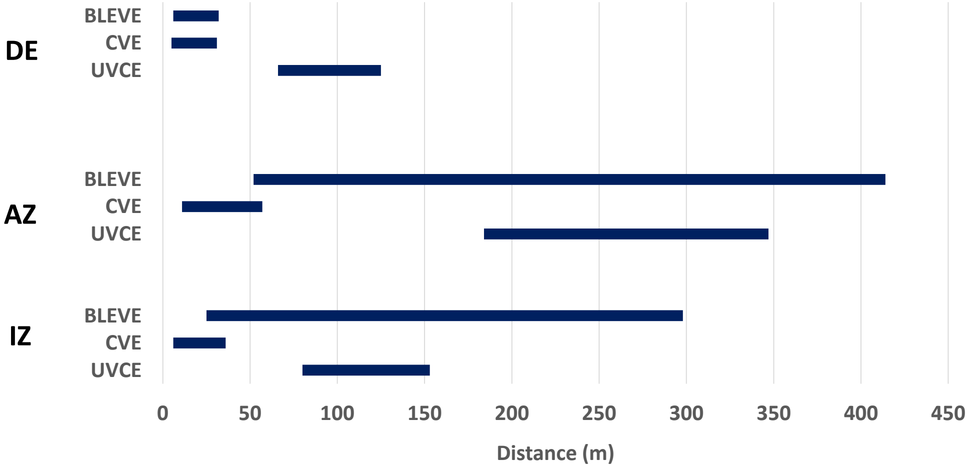

Figure 16. Intervention Zone, Alert Zone, and Domino Effect Zone for explosion

Figure 16 illustrates minimum and maximum risk zones for each of the explosion categories. From the intervention zone, it is seen that BLEVE has the longest range of distances, reaching a maximum of approximately 300 metres. This is followed by UVCE whose range is between 80-150 metres and finally the case of CVE with a maximum value of 40 metres.

In the case of the alert zones, the same pattern is observed as before, i.e., BLEVE has the highest distance range, reaching distances up to 420 metres, followed by UVCE with 350 metres and finally the case of CVE with a maximum distance of approximately 60 metres.

Finally, in the case of the distances of the domino effect, there is a change in behaviour: UVCE achieves the maximum distances with a range of 60-130 metres. However, the other two cases, BLEVE and CVE show the same range of values, reaching a maximum of 26 metres for each of them.

Therefore, by analysing the data obtained in the database, it is concluded that BLEVE is the one with the longest distance range. Whereas between UVCE and VCE, considering the threshold values in Table 6, it is seen that in the case of UVCE these distances are longer. This fact is due to its own definition since it is an unconfined explosion, it can expand more, and therefore reach longer distances, than in the case of CVE.

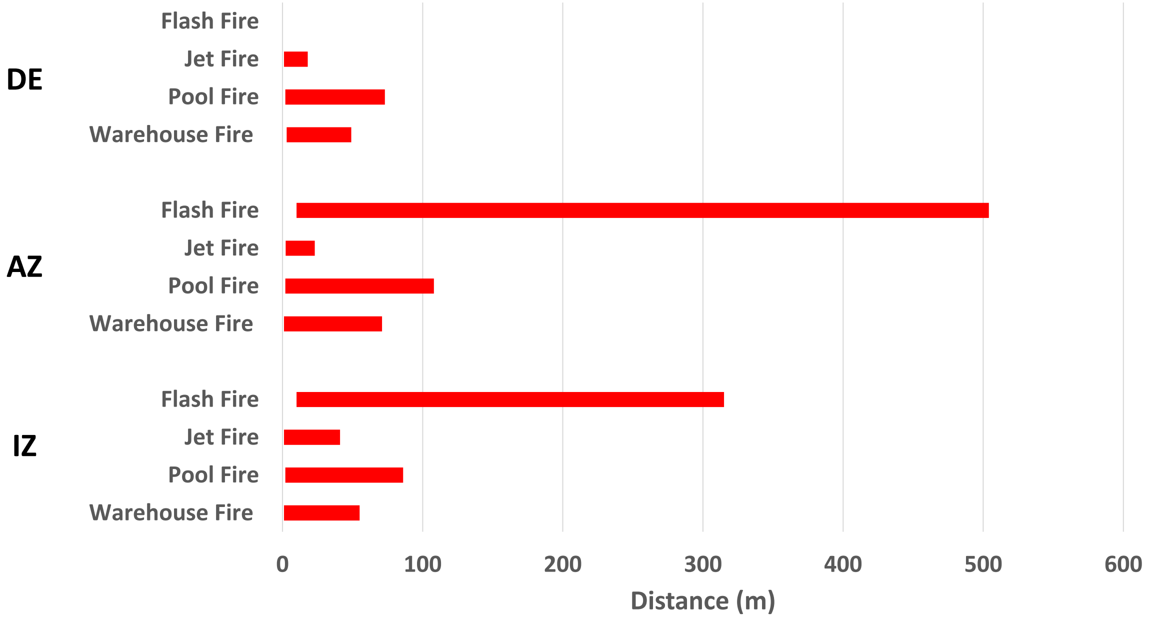

Figure 17. Intervention Zone, Alert Zone, and Domino Effect Zone for fire.

Figure 17 shows the different risk zones for each of the fire scenarios. Based on the intervention zones, a higher range of distances is seen in the flash fire case than in the other ones reaching maximum distances of up to 320 metres, while the other cases range between 40 and 80 metres.

In the case of alert distances, the same behaviour can be observed as in the previous case. The flash fire subcategory is the one with the largest range of distances, up to 500 metres. It is followed by pool fire, which has a maximum distance of 100 metres, and warehouse fire, which reaches a maximum of 70 metres, and the last one is jet fire, showing a maximum distance of 23 metres.

Finally, the case of the domino effect zones is analysed, in which it is seen that there is no impact for flash fire, as described in Table 6. The pool fire has the highest range of distances, getting values of up to 70 metres, followed by the warehouse fire, reaching 50 metres, and finally the jet fire, obtaining maximum values of up to 18 metres.

4.6. Impact on safety distances

In this section it is analysed the effect of different parameters described in the database on the safety distances (IZ, AZ and DE zone). To do so, the risk zones are plotted, depending on different factors, to visualise how they are affected. Only the most representative figures will be shown, to illustrate the result.

To begin with, the global behaviour for all entries in the database is plotted. Figure 18 presents the frequency of each of the zones, using a distribution of data. As a result, it can be seen how the 3 different zones are organised.

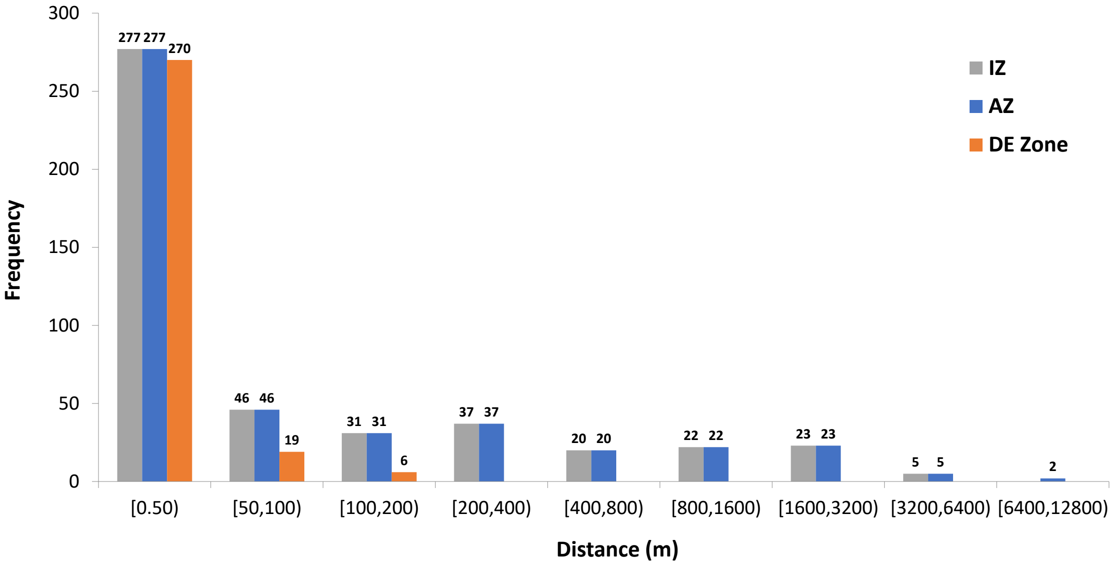

Figure 18. Intervention Zone, Alert Zone, and Domino Effect Zone for the total number of inputs.

Regarding the IZ, it is observed that the most representative distance with 277 cases is around 0-50 metres. From this point on, there is a range of distance values, between about 100 metres and 3200 metres, which have approximately the same frequency. Ending with 5 inputs, which have an intervention distance of less than 6400 metres.

Concerning AZ, it shows the similar performance as IZ, although it reaches longer distances. In other words, its behaviour begins with a maximum frequency at small distances, below 50 metres. Then a range of distances is established, where its frequency remains apparently constant, and finally there are two cases with distances greater than 6400 but less than 12800 metres.

Finally, the trend in the values for the DE zone is shown. In this case, its greatest representation is also found at distances between 0 and 50 metres. This is followed by the range between 50 and 100 metres and finally, there are six database entries with distances between 100 and 200 metres.

4.6.1. Meteorological conditions

Once it is shown a general idea of the frequencies of the different safety distances, the effect of the meteorological conditions is studied. For this, the focus is set on temperature, relative humidity, wind stability and wind velocity. Wind direction is outside the scope.

Based on the temperature (Figure 19), it is seen that the most reported temperature range is [14-16), since it is the one with the highest density of entries recorded in the database. Thus, the information obtained in Figure 9a is confirmed. From a general point of view, the three distances show the same behaviour for the different temperature ranges determined.

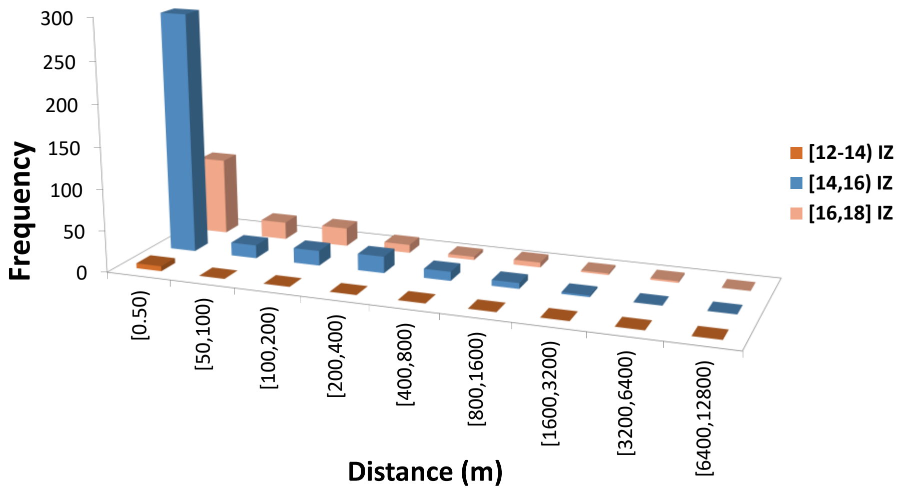

Figure 19. Intervention Zone for temperature.

The most significant range of distances in IZ is found at 0-50 m, decreasing when the distance increases. In the case of the range [16,18), these distances reach longer, below 6400 m. While in the case of

[14,16), a maximum distance of 3200 m is achieved. Finally, in the range [12,14), it is seen that the density of those cases is very low, and refers to the range of [0,50) only.

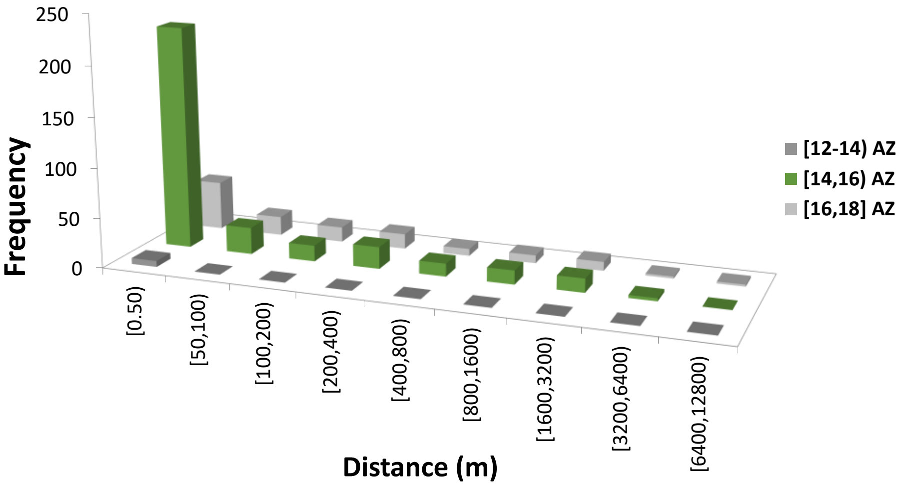

Figure 20. Alert Zone for temperature.

In the case of the AZ (Figure 20), the same pattern can be observed as in the previous case. For the range of [12,14), its maximum distance will be less than 50 m. In relation to the [16,18) case, it can also be observed that the maximum distances reached are longer than the range of [14,16).

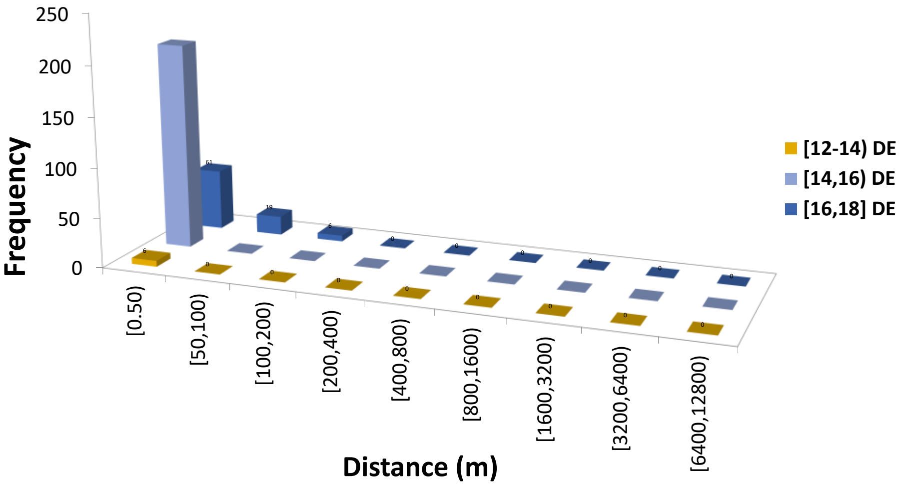

Figure 21. Domino Effect Zone for temperature.

Finally, the effect in the DE zones (Figure 21) is observed. Again, the same pattern is found as in the other cases. Therefore, [16,18) has more influence within longer distances, and the [12,14) at shorter distances.

The next parameter to take into account is the relative humidity (Figure 22, Figure 23 and Figure 24). It is divided into three main ranges, whose maximum density is [73,75), in accordance with Figure 9.

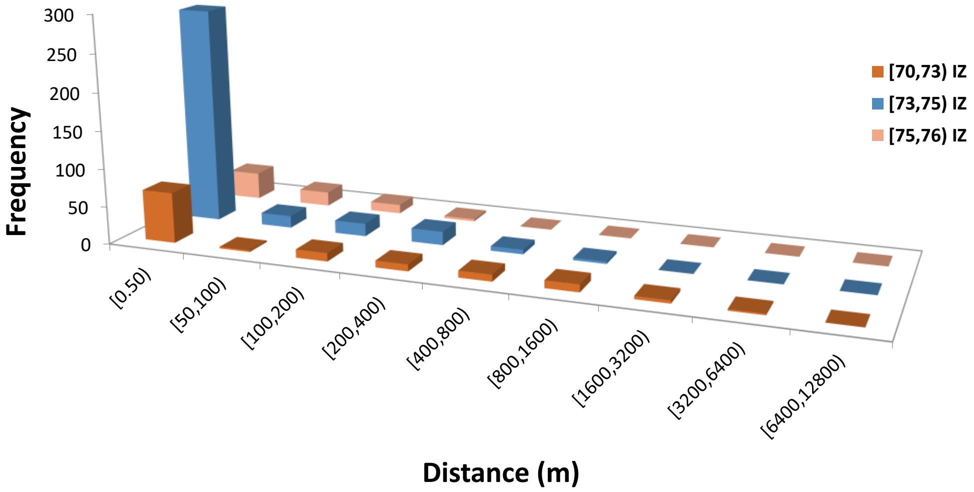

Figure 22. Intervention Zone for relative humidity.

Analysing the values obtained for the IZ (Figure 22), it is seen that the most representative distance is between [0-50) m. However, it should be noted that for a relative humidity between [70-73), the distances are longer, even reaching values of up to 6400 metres, while the other two cases offer shorter maximum distances having a lower frequency of inputs.

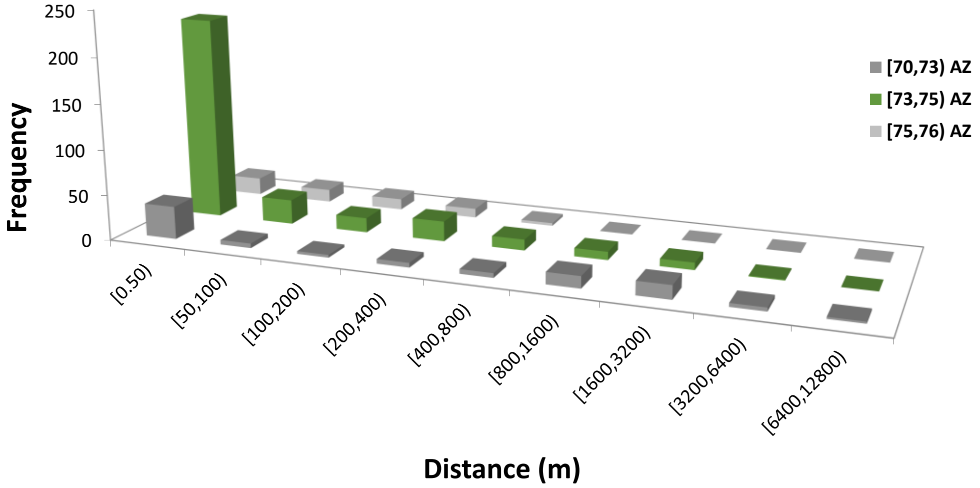

Figure 23. Alert Zone for relative humidity.

For the case of the AZ (Figure 23), the same pattern is seen as for the IZ. The maximum density of inputs in the DB will have a maximum distance between [0-50). Highlighting that for a low relative humidity, the values of these distances are longer.

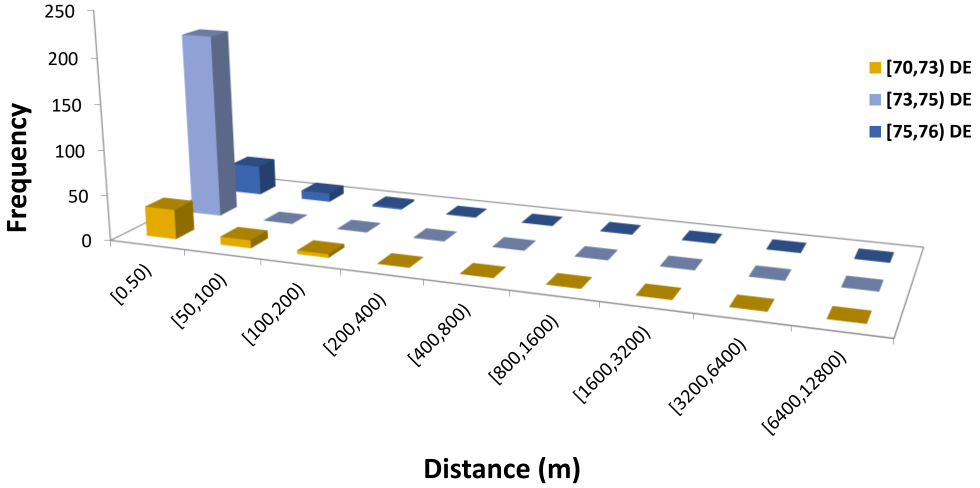

Figure 24. Domino Effect Zone for relative humidity.

In the ED (Figure 24), it is again seen that the most representative distance is [0-50) m for all three cases. It is noted that the range of [73-75) only has an effect in that range of distances. While [70-73) and [75-76], reach distances of less than 200 m.

The next parameter to visualise is the effect of stability, (Figure 25, Figure 26, and Figure 27). For this purpose, it should be reminded that the stability category according to the entries in this database is divided into three classes, B, D and F.

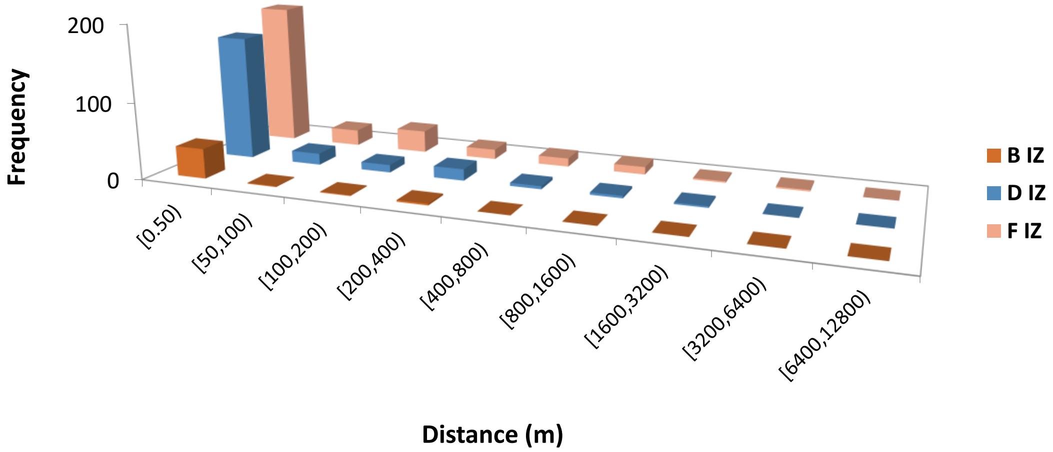

Figure 25. Intervention Zone for stability.

In the case of IZ distances (Figure 25), the behaviour in class B, D and F is practically the same. They achieve maximum representation at distances ranging between [0,50) m. As the distance increases, the frequency decreases. For stability B, it has a maximum value around 400 m, for D class, its largest distance could be found in a range of [1600,3200) while in F category, the maximum value is in [3200,6400).

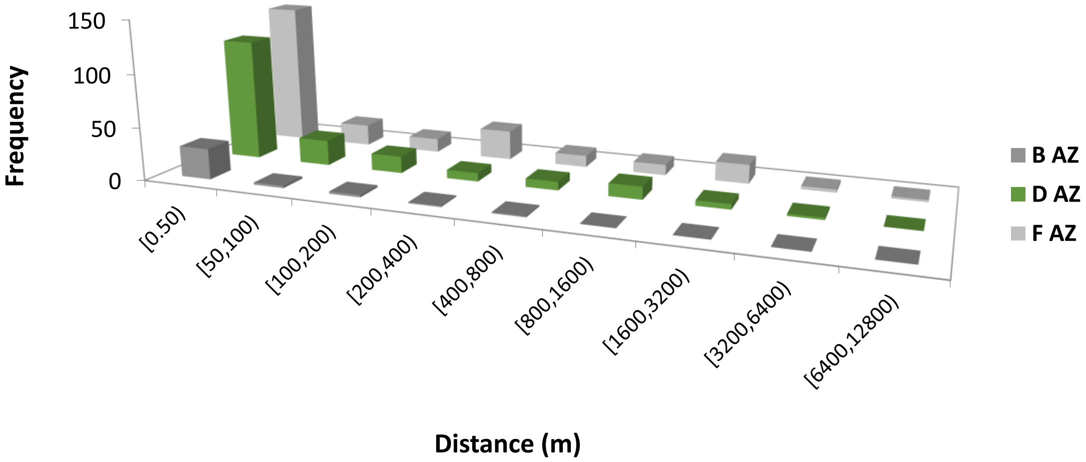

Figure 26. Alert Zone for stability.

In Figure 26, the same response is observed as in the intervention zones. For stability D and F, there is a representative distance between [0,50) m. However, for class F, distances are even higher than 6400 m, but lower than 12800 m. Meanwhile, for stability D and B, their maximum distance reached is between 1600 and 3200 m.

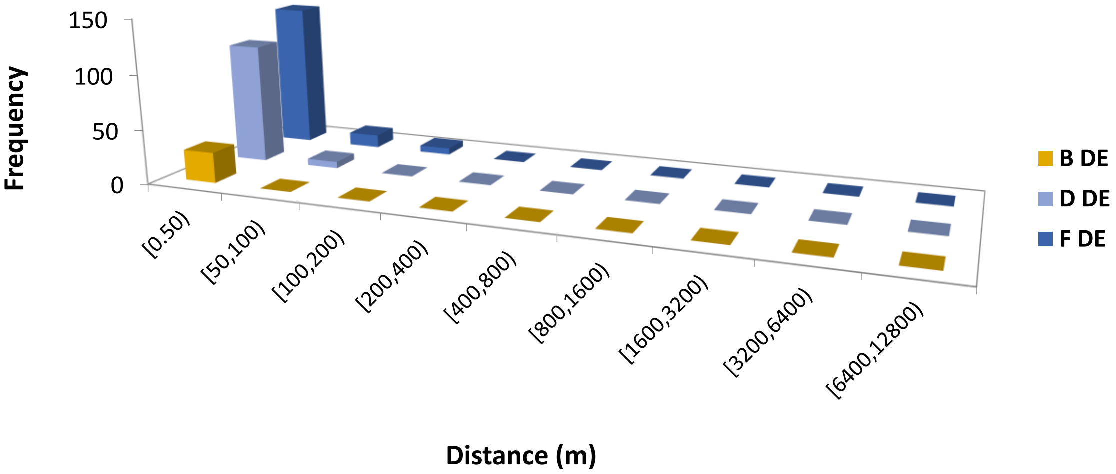

Figure 27. Domino Effect Zone for stability.

Finally, there are the domino effect zones (Figure 27). It is shown that both class D and F have their maximum frequency in the range between [0,50), while for stability B, its maximum representation is less than 50 metres.

In general terms, stability is a very important factor to be considered. It is concluded that the distances originating from the F class are larger. This is because class F is the worst category in terms of atmospheric stability since it is very stable. Moreover, it is seen that the distances coming from class B are the shortest, since this stability is the most unstable, consequently the most suitable for atmospheric conditions. Therefore, the distances that correspond to class D are those between the two previously mentioned classes.

The final factor to consider about meteorological conditions is wind velocity (Figure 28, Figure 29, and Figure 30).

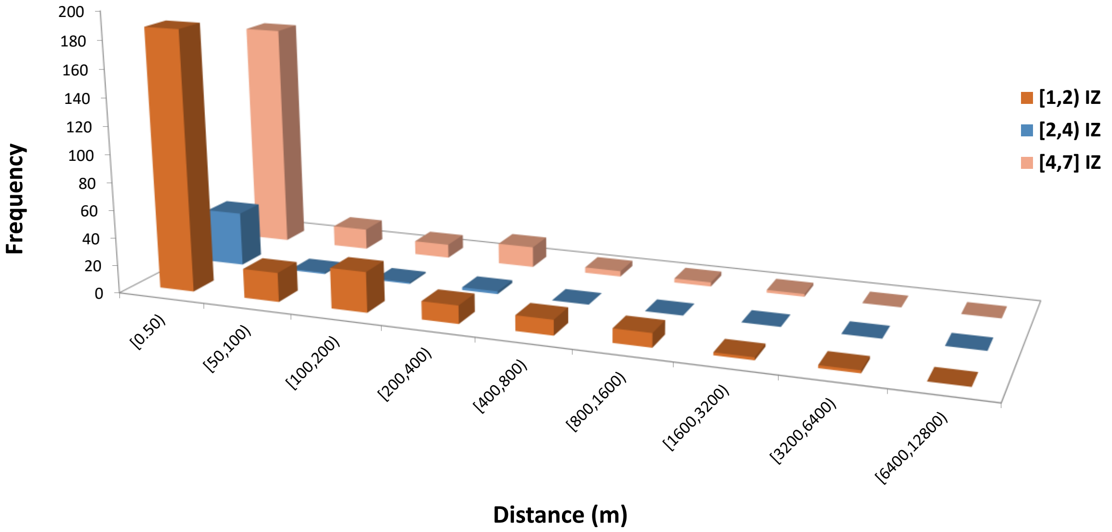

Figure 28. Intervention Zone for wind velocity.

In relation to IZ (Figure 28), it is found that its maximum density of values is in the range of [0,50) for all three cases. However, in the for [1,2), it is observed that it can reach longer distances, even lower than 6400, while for the other cases, they do not exceed 3200 m.

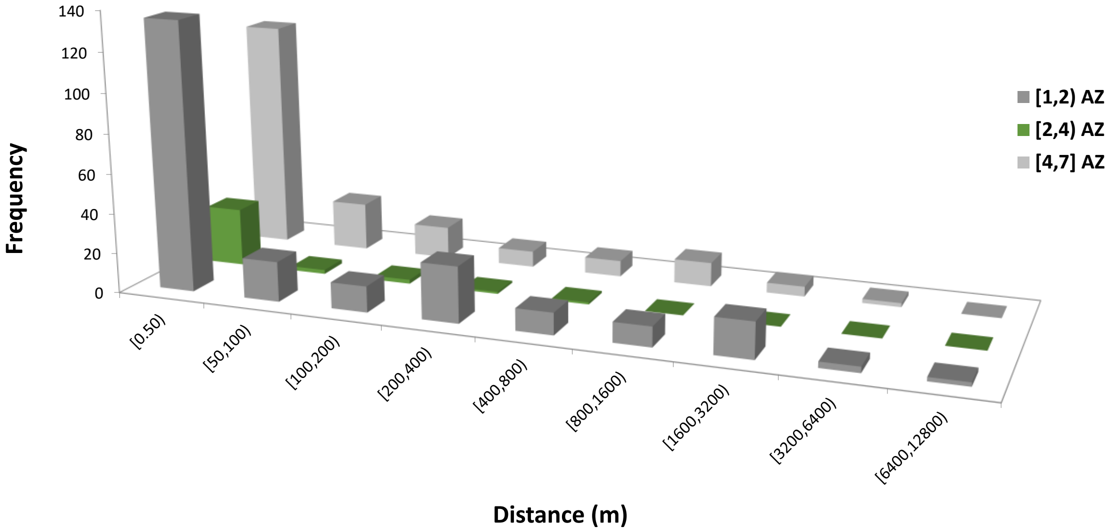

Figure 29. Alert Zone for wind velocity.

For AZ (Figure 29), the same behaviour is observed as in the previous case. However, the distance range with the highest density of cases is [0-50). It should be noted that for low velocities, the distance can be longer than for higher velocities. Thus, the distance range is 12800 m for low speeds, followed by 6400 m for high speeds and finally very short distances for intermediate velocities.

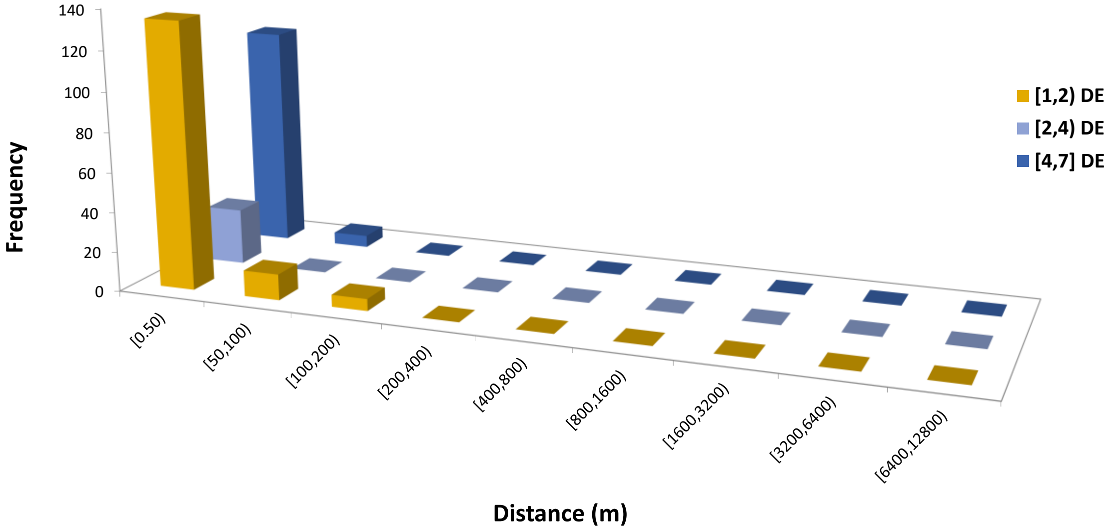

Figure 30. Domino Effect Zone for wind velocity.

In the DE (Figure 30), their maximum frequency is also found at distances of [0-50), for the three different cases. It emphasises that the low velocity range reaches longer distances than the other two cases, around 200m. Whereas at medium velocities the distances collected are shorter.

It should be remarked that in the previous analysis, a relationship between the velocities and the stability of the system was found. Therefore, it is concluded that in the case of low velocities, [1,2) is related to a stability class F. While medium velocities, around 2 m/s, are related to B stability, and finally, high velocities are those corresponding to D stability.

This is because the lower the wind velocity, the more constant the atmospheric stability will be and therefore the more difficult it will be to disperse the consequences of a possible major accident. The same behaviour occurs at higher velocities, corresponding to a stability D, which is a neutral class producing an unstable stability and consequently a higher dispersion in the atmosphere. And therefore, the safety distances in this case are smaller.

4.6.2. Basic Scenario

Once some of the most representative parameters of the meteorological conditions are discussed, it is time to analyse the different potential scenarios and their effect on the safety distances. To do so,

Figure 31, Figure 32, and Figure 33 show the different distances according to their classification, i.e. dispersion, explosion, or fire.

At a first look, it is seen that in the case of fires, there is a higher frequency at short distances, between [0,50) m. The same behaviour is observed for explosions, although this frequency is lower than for fires. Meanwhile, in the case of dispersion, its distribution oscillates between distances [0,12800)

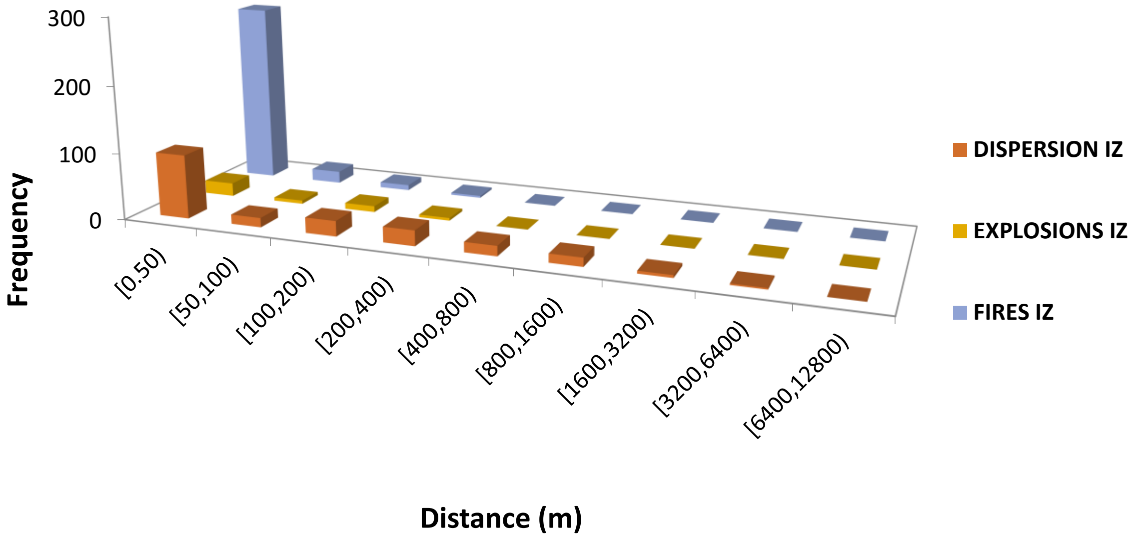

Figure 31. Intervention Zone for basic scenario

Moving on to the IZ (Figure 31), it shows that for these three cases, the highest frequency is found at short distances. Although for the case of dispersion, this has a distribution up to longer maximum distances than the other two cases, reaching distances between 3200 and 6400 metres. This fact is because fire and explosion are scenarios that are not extended over time, while dispersion is, reaching greater distances.

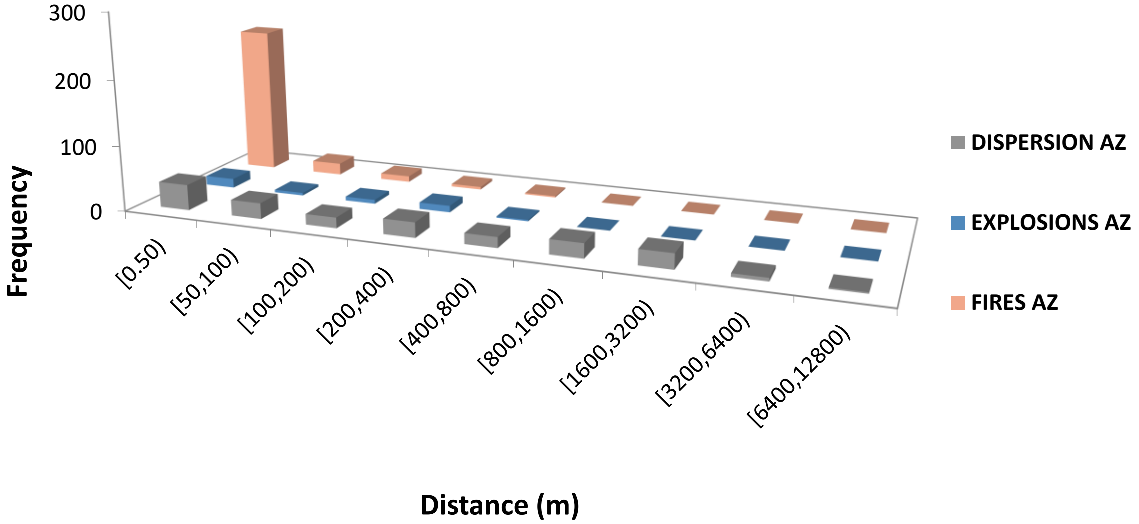

Figure 32. Alert Zone for basic scenario

For the AZ (Figure 32), the frequency of fires is much higher than in the other cases. Despite the high frequency, the maximum distances reached are short. The same behaviour is seen in the case of explosions, although with less frequency, since in the database there are fewer inputs related to explosions, and the distances reached are longer than in the case of fires. Finally, in the case of dispersion, the distribution of data points is equal over a greater range of distances, between 50 and 6400 metres.

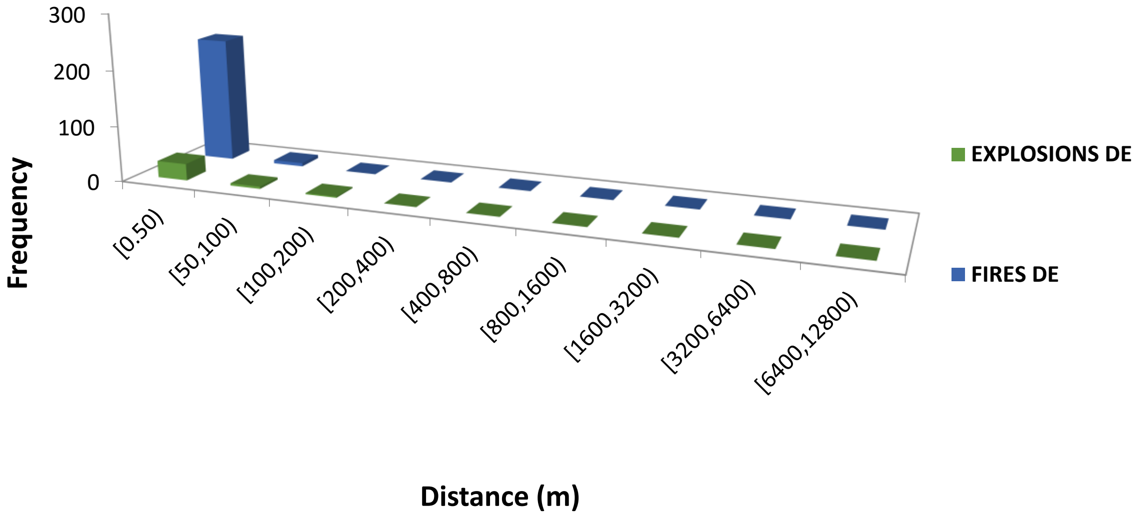

Figure 33. Domino Effect Zone for basic scenario

The DE (Figure 33) is only defined for the case of fires and explosions, because it is not considered in the dispersion, as it has been determined in Table 6. In the two cases plotted, the range of distances between 0 and 50 stands out due to the higher frequency associated with it.

4.6.3. Specific Scenario

Since the basic scenarios are analysed, the effect of each of the specific scenarios will be studied, based on Table 5. Therefore, the frequency distribution for the different risk zones is analysed, considering the possible final events.

Considering dispersion, it is only considered the toxic category. Figure 34 shows the distribution of risk zones according to that class. As discussed above, the dispersion does not take into account the domino effect.

Looking in detail at the case of toxic dispersion, it is observed that there are differences between the behaviour of IZ and AZ. Consequently, it is concluded that in the case of the IZ, there is a representative range between [0-50) m, although the distance continues to increase, but with less density. Meanwhile, in the case of the AZ, this distribution remains constant as the distance increases, but with a higher density. Thus, AZ reaches longer distances than IZ, because of its threshold values as seen in Table 6.

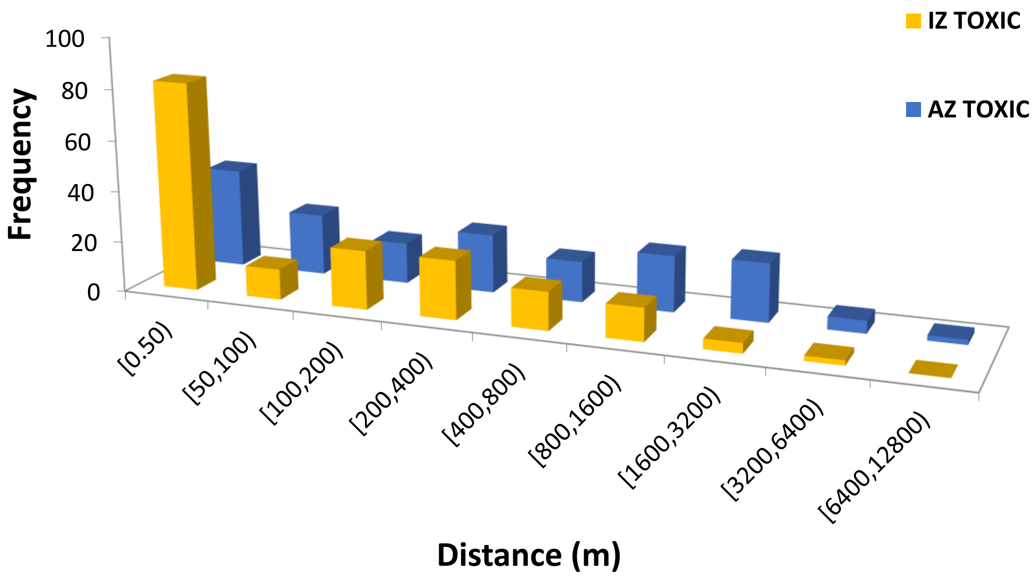

Figure 34. Intervention Zone, Alert Zone for dispersion

To further analyse the effect of distances on possible final accidents, the case of explosions will be analysed (Figure 35, Figure 36, and Figure 37). It must be considered that explosions are divided into BLEVE, VCE and UVCE.

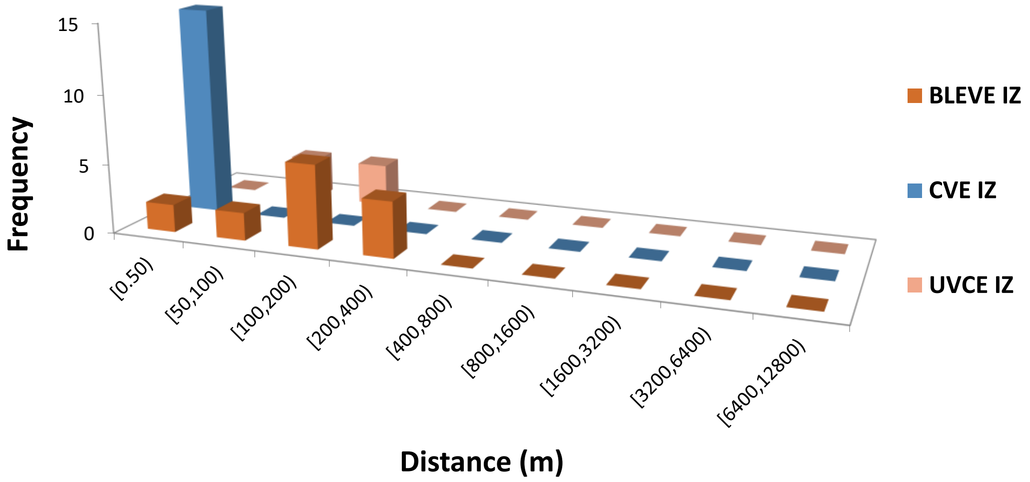

Figure 35. Intervention Zone for explosions.

Going into detail in the IZ (Figure 35), a different behaviour is observed in each of the categories. Starting with the case of BLEVE, it is seen that the IZ only affects a range of distances between [0-400) m. In the case of cloud explosions, for VCE the only range that appears is the [0-50) m range and in the case of UVCE there is a distribution over the [50-200) m range. This difference between them is due to the fact that UVCE is produced in an unconfined atmosphere, thus causing the cloud to move over longer distances. The opposite is the case for the VCE, which could be produced in a confined atmosphere, reaching shorter distances.

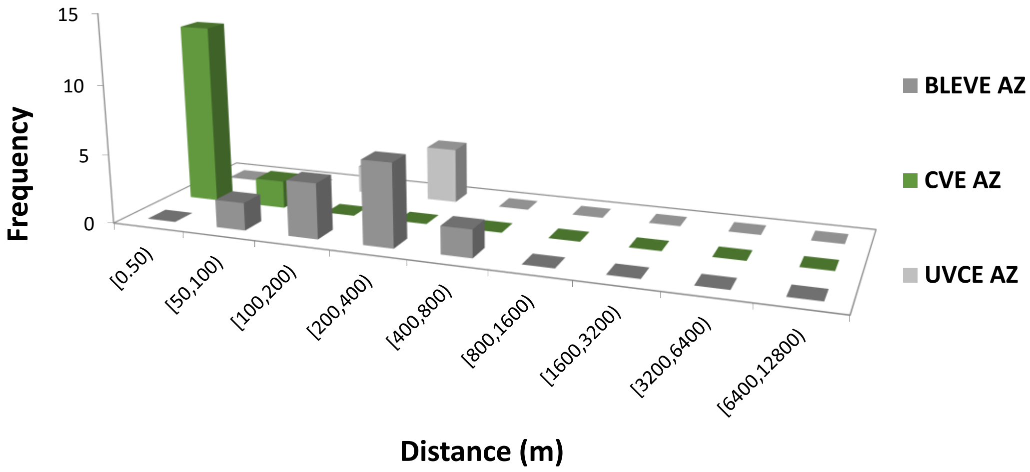

Figure 36. Alert Zone for explosions.

In the case of AZ (Figure 36), the maximum distances are offered by BLEVE, reaching distances of up to 800 metres. On the other hand, the same behaviour can be seen between UVCE and VCE as for IZ. This means that in the case of unconfined explosions, the distances reached are in the range of [200-400) m, while for confined explosions, the distribution of distances do not exceed 100 metres.

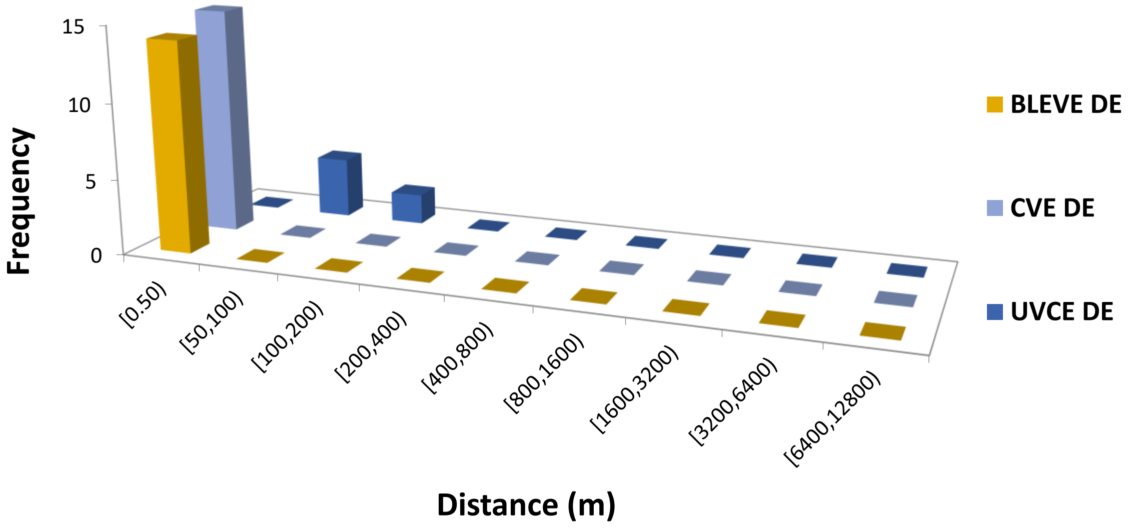

Figure 37. Domino Effect Zone for explosions.

Finally, for the DE (Figure 37), it is concluded that in the case of VCE and BLEVE their behaviour is quite similar, showing distances in the range of [0-50) m. Although in the case of UVCE, the range of distances reached is greater, between [100-200) m.

The final scenario to be analysed is the fire category, which is divided into flash, jet, pool, and warehouse (Figure 38, Figure 39, and Figure 40). In general terms, it is observed that the most outstanding case among all of them is pool fire, due to its higher density.

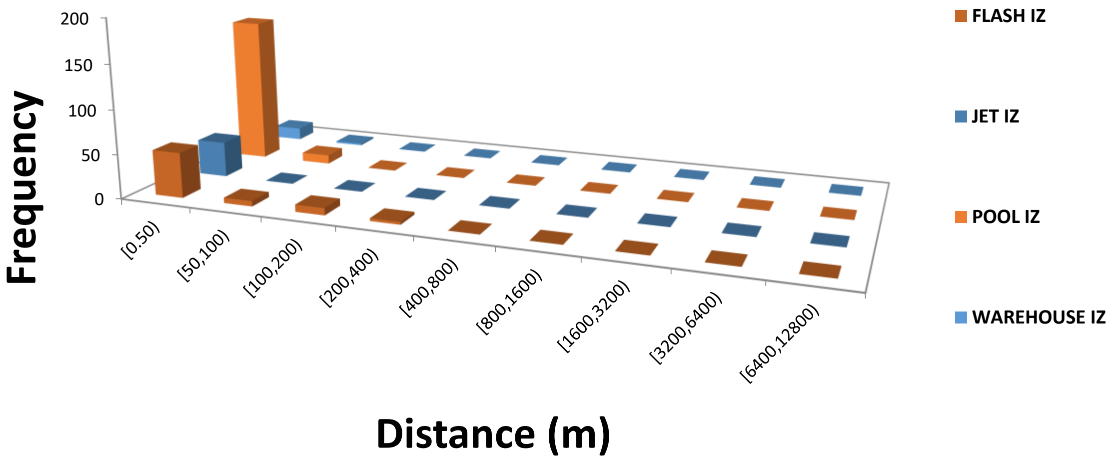

Figure 38. Intervention Zone for fires.

In relation to the IZ (Figure 38), as discussed above, the most significant case is the pool fire, due to its high density, because there are more entries in the database related to this category than the others. However, the distances are reported in the range of [0-200) m. For the jet and warehouse categories, their behaviour is the same, they are defined by short distances, between [0-50) m. In the case of flash, it has the most pronounced distribution in this range, reaching maximum distances of around 400 metres.

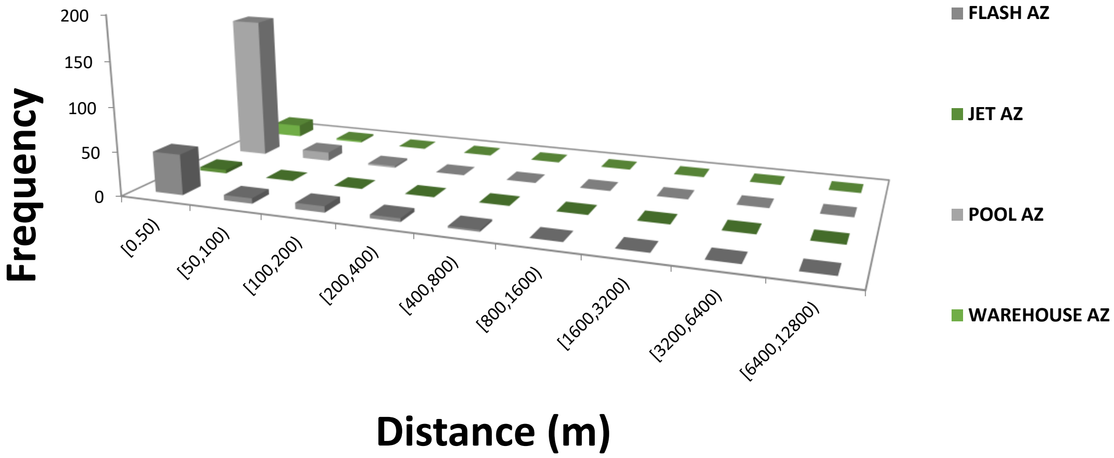

Figure 39. Alert Zone for fires.

In the case of AZ (Figure 39), the same pattern is observed as in the case of IZs. Consequently, a higher density of cases can be found for the pool fire, at distances of less than 200 metres. It also shows that in the cases of jet fire and warehouse fire, the distances are in the range of [0-50) metres, while in the case of flash fire, the distribution is spread out over distances up to a maximum of 400 metres.

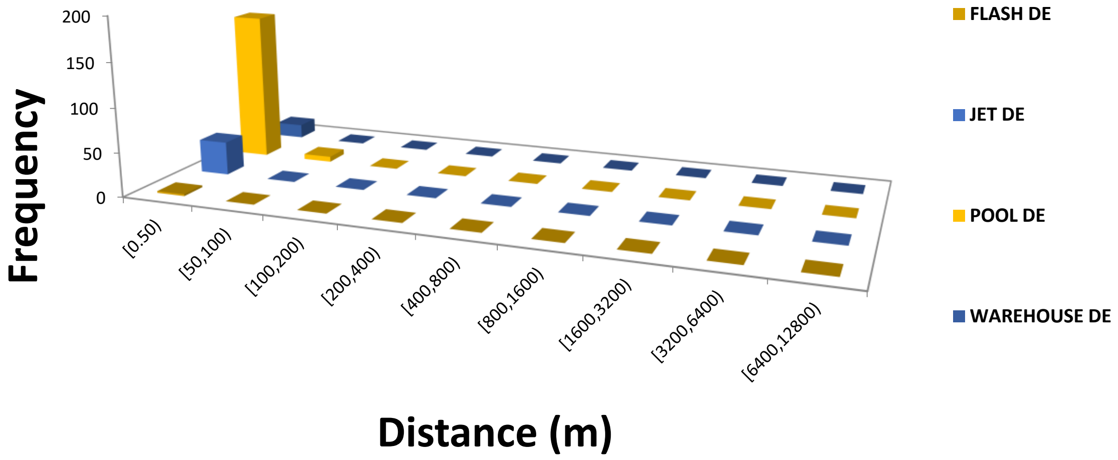

Figure 40. Domino Effect Zone for fires.

Finally, in the analysis of the DE (Figure 40), it is seen that in the case of the flash fire, this category does not apply to it. This is due to the fact that the fire produced is so fast, there is no time for the domino effect of the accident to occur. In the case of warehouse and jet fire, it does occur, although at distances of less than 50 metres. On the other hand, in the case of pool fire, it could reach distances of less than 200 metres, although its maximum frequency is between 50 and 100 metres in length.

5. Data base pattern recognition

Pattern recognition is a scientific discipline whose aim is to recognize scenarios in a variety of categories or classes. To do so, a method called multivariate analysis is used. It is a statistical technique that can be used to simultaneously explore whether multiple risk factors (referred to as independent variables) are related to a certain outcome (referred to as dependent variable).

This process is carried out using the Minitab software and using the Principal Component Analysis (PCA). It is a technique that is widely used for applications such as dimensionality reduction, lossy data compression, feature extraction, and data visualization. PCA is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables.

PCA is mathematically defined as an orthogonal linear transformation that transforms the data to a new coordinate system. So, that the greatest variance by a projection of the data comes to lie on the first coordinate (called the first principal component), the second greatest variance on the second coordinate, and so on. The goal of PCA is to explain the maximum amount of variance with the fewest number of principal components, which are linear combinations of the original variables that explain the variance in the data.

Since Minitab is used, it is important to underline that it only analyses quantitative variables and not qualitative variables (categorical variables). Regarding the first set, the values are numbers that usually represent a control or measurement. While the values of a categorical variable are mutually exclusive categories or groups.

To start the analysis, the first step is to introduce the data into Minitab's multivariate analysis section. In *Variables*, it specifies the columns of data to be analysed. However, if there is a missing value in any of the columns, Minitab ignores the entire row, so it excludes missing values from the calculation of the correlation or covariance matrix.

The next step is to enter the number of principal components to be calculated by Minitab. However, if the number of components to enter is unknown, it is possible to leave this field blank. If no number is specified, Minitab calculates the maximum number of components, which is equal to the number of variables. Then by using the output, it is determined how many components explain most of the variation in the original variables.

Finally, it is necessary to select the type of matrix to be used in order to calculate the principal components. Correlation matrix is used when variables have different scales, and it is desired to weight all variables equally. Covariance matrix is employed when variables use the same scale or when variables have different scales, but there is a desire to give more emphasis to variables with higher variances. Therefore, a correlation matrix is selected for this analysis.

As a result of the multivariate analysis of PCA, new variables to be studied will be obtained. These will be linearly proportional to the initial variables of the database. Once it is determined which are the most significant principal components for the analysis (only for quantitative variables), the regression study will be carried out. Its objective is to discover the relationship between a set of predictors and a continuous response using the ordinary least squares method. For this purpose, the main principal components determined before will be introduced, together with the categorical variables to study the response in the IZ, AZ and DE zones.

Therefore, the steps to be performed for this pattern recognition study are shown below in Figure 41. Hence, the PCA study on the quantitative variables is firstly performed to determine the number of principal components required. Then, the regression study is carried out, considering together the previously determined PCs and the categorical variables, to see if there is a relationship in the set of variables.

Figure 41. Steps to be considered.

Therefore, the first step to carry out the PCA is to define the quantitative independent variables. For this purpose, temperature, relative humidity, wind velocity, quantity of substance, source term, duration time and the different frequencies (basic, initiator, and final) are considered. In this analysis stability, wind direction, substance and LOC equipment are out of scope, because they are categorical variables.

The first result of the PCA will be the determination of the minimum number of principal components needed to explain the maximum variance of the data. To choose the number of principal components, two different parameters will be taken into account. Firstly, the cumulative variance in each of the principal components, and secondly the eigenvalue in each of them. Regarding the cumulative variance, the principal components that explain an acceptable level of variance must be conserved. Concerning the eigenvalues, those with a higher value should be retained, in this case, it is based on the Kaiser criterion that uses only the principal components with an eigenvalue greater than one.

Once the number of principal components has been chosen, the next step is to interpret each principal component in terms of the original variables. To do this, the magnitude and direction of the coefficients of the original variables must be examined. The larger the absolute value of the coefficient, the more important the corresponding variable is in the calculation of the component. Thus, as a final result of the PCA, new variables will be obtained, which are proportional to the initial variables.

The next step is to perform a regression adjustment to describe the correlation from a set of predictors to a continuous response. Hence, in this case, the predictors will be the new variables found during the PCA together with the categorical variables of the database. Those variables will be the stability, the substance, and the LOC equipment. Meanwhile, the response will refer to the safety distances, i.e., the IZ, AZ and DE zone.

Consequently, the following step is the numerical calculation of the PCs, considering the coefficients determined before and the original variables. Then, they are introduced into Minitab, and together with the categorical variables, the regression adjustment is made.

As a first step, it is necessary to determine whether the association between the variables and the response is statistically significant by comparing the p-value of the term with the significance level to evaluate the null hypothesis. In this study an alpha of 0.05 is selected, indicating a 5% risk of concluding that there is an association when there is no real association. Therefore, if the p-value $\leq \alpha$, the association is statistically significant while if the p-value $> \alpha$, the association is not statistically significant. As a result, variables with a p-value greater than or equal to 0.05 are discarded from the study. The regression adjustment is then re-run, considering only the significant variables (those with a p-value of less than 0.05).

As a result of the regression, an equation to calculate the response (IZ, AZ, DE zone) as a function of the parameters determined to be significant is obtained. From there, the responses are calculated using the equation provided, and the results are compared with those reported in the DB. Finally, both values are compared, and the residuals obtained are analysed to see if the model fits correctly.

It must be assumed that during the modelling of real case parameters, there is some error associated with it. Since the effect on safety distances is being studied in this analysis, the results obtained, and the possible associated error, will have units of metres.

The parameter to be studied is the effect of basic scenario on the different safety zones. For this purpose, it is divided into the different 3 cases, dispersion, explosion, and fires, in order to be able to determine their behavior define basic scenario.

5.1. Dispersion

The results obtained by applying the PCA are seen in Table 8, for the determination of the number of principal components. It should be noted that the analysis is performed considering only 141 cases, and 85 are discarded because they must have blank parameters.

Table 8. Analysis of the eigenvalues and eigenvectors of the correlation matrix for dispersion

Eigenvalue	2.0587	1.8007	1.6385	1.0947	0.8772	0.6585	0.4901	0.3309	0.0507
Proportion	0.229	0.200	0.182	0.122	0.097	0.073	0.054	0.037	0.006
Cumulative	0.229	0.429	0.611	0.733	0.830	0.903	0.958	0.994	1.000

The selection of the most appropriate number of principal components can be done in two different ways. The first is to use the cumulative proportion to determine the total amount of variance explained by the principal components and the second one refers to the eigenvalue criterion, in which those with larger variances are selected.

In this case, it is concluded that 4 principal components would be sufficient. Therefore, doing the PCA analysis allows to go from having 9 quantitative variables to only having 4 new variables, which are linearly proportional to the initial ones.

To understand each principal component in terms of the original variables, it is necessary examine the coefficients. Table 9 shows the combinations of each of these new parameters to be studied.

Table 9. Eigenvalues for dispersion.

Variable	PC1	PC2	PC3	PC4
TEMPERATURE_ºC	-0.140	-0.376	0.387	0.304
HR_%	-0.081	0.579	-0.132	0.002
Uw_m/s	0.117	0.173	-0.021	-0.662
QUANTITY_kg	-0.299	0.494	0.330	0.005
SOURCE _TERME_kg/s	-0.303	0.318	0.489	0.192
DURATION_TIME_s	0.037	0.129	-0.346	0.614
BASE_FREQUENCY_y-1	0.132	0.302	-0.436	0.180
INICIATOR_FREQUENCY_y-1	0.617	0.136	0.291	0.121
FINAL_FREQUENCY_y-1	0.616	0.145	0.298	0.096

Finally, it is concluded that by performing the principal components analysis, from the 9 initial variables, we can be left with 4 new variables, which are linearly proportional. Being:

- PC1: initiator and final frequencies.
- PC2: relative humidity and quantity.
- PC3: temperature, source term, and base frequency.
- PC4: wind velocity and duration time.

Once the qualitative variables have been reduced from 9 to 4, linear regression is performed to see the effect on safety distances. In this case, the PCs and the categorical variables are considered.

In linear regression, the first step is to determine whether the association between the response and the term is statistically significant. For this, the responses to be studied will be the safety distances (IZ, AZ and DE) and the predictors will refer to PC1, PC2, PC3, and PC4 together with the categorical variables, stability, substance, and equipment of LOC. Therefore, wind direction is outside the scope of the study because it is a parameter whose effect on the safety zones is related to the distribution of the surroundings.

5.1.1. Intervention Zone

Initially, a linear regression analysis is performed for continuous and categorical variables in the database, to calculate the IZ, obtaining the results in Table 10.

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Table 10. Analysis of Variance for dispersion for IZ

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	32	50931907	1591622	10.29	0.000
PC1	1	3091017	3091017	19.99	0.000
PC2	1	3016300	3016300	19.51	0.000
PC3	1	3085400	3085400	19.96	0.000
PC4	1	3037630	3037630	19.65	0.000
SUBSTANCE	2	1861314	930657	6.02	0.003
STABILITY	24	42171652	1757152	11.36	0.000
FINAL_SCENARIO	2	3880	1940	0.01	0.988
Error	151	23346791	154615		
Absence of adjustment	143	23083628	161424	4.91	0.010
Error due to replications	8	263163	32895		
Total	183	74278698			

First of all, as a general analysis, it is seen that Minitab does not take into consideration Equipment, type and LOC. This fact is due to the assumption that little information exists in this field. Therefore, only the regression considering the principal components, together with substance, stability, and final scenario, is studied.

By analysing the values obtained, it is possible to determine whether the association between IZ and the variables is statistically significant. It is concluded that PC1, PC2, PC3 PC4, stability and substance are the only factors to be taken into account because their p-values are lower than 0.05, so the other factors are not significant for this study.

As a result of the regression adjustment, a model is obtained which gives an independent regression equation for each of the substances. Eq 1 is a mathematical simplification for each of the equations obtained, although it should be noted that "a" varies according to the substance (Table 11) and b to stability (Table 12). This model explains approximately 66.91 % of the variation in the response.

$$IZ = 1933 + 5071*PC1 + 1220*PC2 + 2753*PC3 + 989*PC4 + a + b \qquad \text{Eq 1}$$

Table 11. Value of a for each substance in meters and n is the number of inputs.

Substance (n)	a	Substance	a
Sulphur dioxide (8)	1567	**Furfuryl alcohol (6)**	55
Bromine (2)	593	**2,4-toluene diisocynate (14)**	0
Dichloroacetone (2)	555	**Hydrochloric Acid (2)**	-54
Chlorine (14)	540	**Methanol (30)**	-54
Acid trichloroisocyanuric (6)	450	**Oxygen (16)**	-233
Ethyl chloroacetate (2)	280	**Ammonia (14)**	-256
Hydrogen chloride (2)	217	**Benzyl chloride (6)**	-279
Hydrogen fluoride (14)	179	**Ammonia nitrate (6)**	-363
Dimethyl sulphate (6)	174	**Hydrogen (2)**	-472

Acrylonitrile (2)	128	**Acetone (14)**	-530
Thionyl chloride (2)	109	**Hydrazine hydrate (20)**	-676
Phosphorus oxychloride (2)	64	**Isophorone diisocyanate (28)**	-695
Formol (2)	45		

When analysing the coefficients of the individual substances, it is seen that not all of them have the same impact on the IZ calculation. This is because some values are larger than others, so they will give different distances in the end.

For this case, it is observed that the substances with the highest impact for the calculation of the IZ are Sulphur dioxide, Bromine, Dichloroacetone, Chlorine, Acid trichloroisocyanuric and Ethyl chloroacetate. While the substances that have the least impact are Benzyl chloride, Ammonia nitrate, Hydrogen, Acetone, and Hydrazine hydrate.

It is worth mentioning that some of the substances described for the IZ calculation appear only twice in the database, as shown in Figure 11. Those substance are Bromine, Ethyl chloroacetate, Hydrogen chloride, Thionyl chloride, Phosphorus oxychloride, Formol. Therefore, the coefficient obtained as a result for each of these substances will not be very accurate in the results.

Table 12. Value of b for each stability in meters.

	B	**D**	**F**
b	0	-393	109

In the case of stability, the coefficients obtained have positive, negative and zero values. In the case of type B stability, the coefficient obtained indicates that there is no effect on the safety distance. On the other hand, the values of D and F make sense because of their context, i.e., because stability F is the worst category, it is expected that the distances will be larger, hence a higher coefficient compared to the D case.

Finally, it should be determined whether the model meets the assumptions of the analysis. This is done by using the residual plots. According to the information in Figure 42, it is seen that the residuals between the theoretical (calculated) and experimental (database) intervention zones are around -1000, 1000 metres.

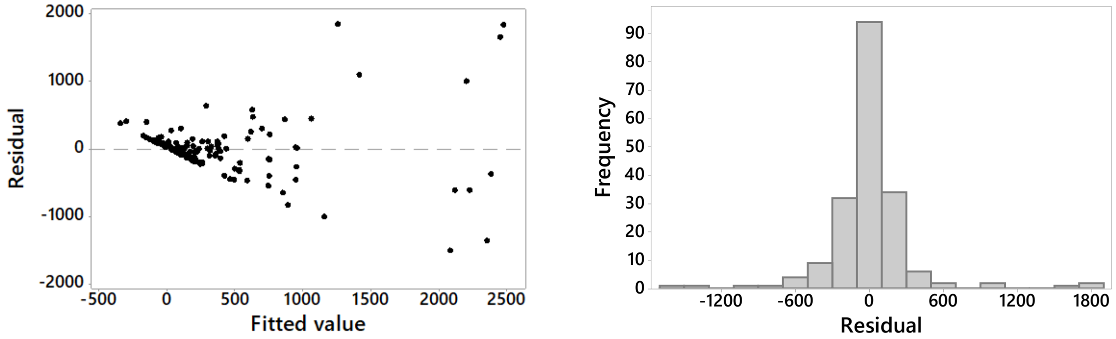

Figure 42. Residual plots for dispersion in IZ.

From the plot, it is also deduced that the model fits better when the distances are short, because the larger the distance, the larger the error between the two and the larger the residual.

Analysing the residual plot, it is seen that there are atypical cases in the fitted regression model, because it is observed that some points are far from the zero value. It can be seen that there are also influential values, because there are points that are far away from the others, but in the x-direction.

5.1.2. Alert zone

In the case of AZ, based on the results obtained from the p-values, it is concluded that the most significant parameters are PC1, PC2, PC3 and PC4 for the qualitative and substance and stability (Table 13).

Table 13. Analysis of Variance for dispersion for AZ.

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	28	197198917	7042818	9.50	0.000
PC1	1	8752997	8752997	11.81	0.001
PC2	1	8770976	8770976	11.83	0.001
PC3	1	8570165	8570165	11.56	0.001
PC4	1	8279730	8279730	11.17	0.001
SUBSTANCE	2	8245126	4122563	5.56	0.005
STABILITY	22	163730254	7442284	10.04	0.000
Error	141	104506131	741178		
Absence of adjustment	129	99455799	770975	1.83	0.119
Error due to replications	12	5050331	420861		
Total	169	301705047			

Finally, a regression model is obtained for AZ that explains 65.36 % of the variance, whose equation depends on PC1, PC2, PC3, PC4, substance and stability. As a result, the equation depends on a constant and six different coefficients, one for stability (Table 14) and for substance (Table 15).

$$AZ = 3565 + 10574 * PC1 + 2555*PC2 + 5724*PC3 + 2052*PC4 + c + d \quad \text{Eq 2}$$

Table 14. Value of c for each stability in meters.

	B	**D**	**F**
c	0	-963	320

From these values, it is possible to determine that in the case of stability B, there will be no associated effect, so, if this stability is the predominant one, the equation will only depend on the substance and the value for the principals' components. For the case of stability D, the obtained coefficient has a negative sign, which means that the initial value of the constant will be reduced, concluding that these distances will be shorter. Finally, in the case of stability F, the coefficient obtained is +146, making the distance calculation longer. These results are significantly relevant since, as previously mentioned, stability F is the worst possible category in terms of atmospheric conditions, so the distances should be longer, as it is expected by using this equation.

Table 15. Value of d for each substance in meters and n is the number of inputs.

Substance (n)	**d**	**Substance (n)**	**d**
Sulphur dioxide (8)	2721	**Acrylonitrile (2)**	280
Dichloroacetone (2)	2463	**Formol (2)**	191
Bromine (2)	2118	**2,4-toluene diisocynate (14)**	0
Hydrogen chloride (14)	1998	**Ammonia nitrate (6)**	-55
Thionyl chloride (2)	1544	**Furfuryl alcohol (6)**	-61
Hydrochloric acid (2)	1505	**Methanol (30)**	-90
Chlorine (14)	1222	**Ammonia (14)**	-434

Acid trichloroisocyanuric (6)	1188	**Acetone (14)**	-460
Ethyl chloroacetate (2)	1022	**Benzyl chloride (6)**	-584
Dimethyl sulfate (6)	589	**Hydrazine hydrate (20)**	-1334
Phosphorus oxychloride (2)	544	**Isophorone diisocyanate (28)**	-1453
Hydrogen fluoride (2)	443		

The coefficients obtained range from 2721 to -1453. Thus, the distances that will be reached will be different depending on the substance. By analysing them, it is concluded that Sulphur dioxide, Dichloroacetone, Bromine, Hydrogen chloride, and Thionyl chloride has more effect on the AZ, as their coefficient is higher. While in the case of Acetone, Benzyl chloride, Hydrazine hydrate, and Isophorone diisocyanate the coefficient is very low, even with a negative sign.

Again, it must be considered as some substance (Bromine, Ethyl chloroacetate, Hydrogen chloride, Thionyl chloride, Phosphorus oxychloride, Formol.) only appear two times in the DB, the coefficients obtained for their determination could not be accurate.

When comparing these coefficients with those of the IZ table, some similarities are found. The substances with the highest and lowest coefficients remain the same ones in both models. However, there are some exceptions, such as the case of furfuryl alcohol, which for the IZ has a higher contribution than in the case of AZ.

Finally, in the analysis of the residuals, it is observed that there are several atypical points, due to their alignment with the zero axis, although there are also deterministic points on the same zero axis (Figure 43). It concludes that the equation can reach errors of 400 metres, although the highest error density can be found in shortest distances, between the 0 and 500 m.

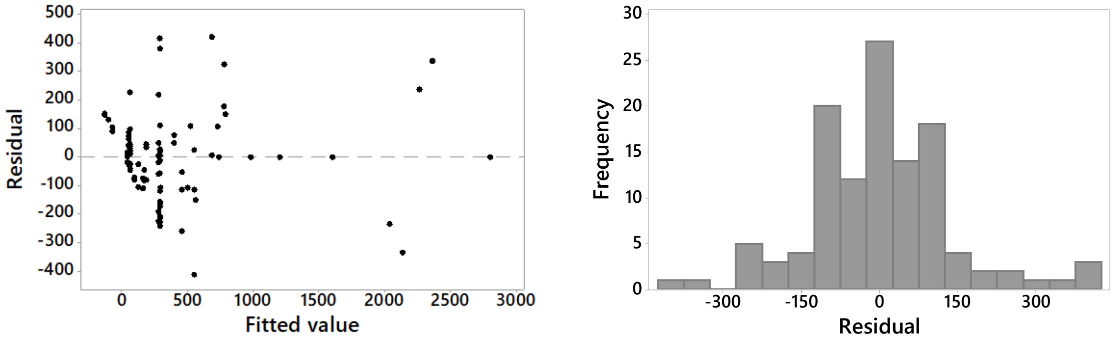

Figure 43. Residual plots for dispersion in AZ.

Analysing the plot, it is seen that in the cases where the distances are shorter, the model performs better. While in the case of longer distances, around 2500 metres, the calculated distances show a higher relative error.

5.2. Explosion

For the case of the explosion, as a result of the PCA it is obtained that with 3 principal components (Table 16), the method would be able to detail 97.9% of the variance. Thus, it would go from analysing 9 variables to analysing only 3 of them, which are linear and proportional to the initial ones. It should be noted that for the PCA, only 12 cases have been used, because 32 of them do not present all the possible variables to be analysed.

Table 16. Analysis of the eigenvalues and eigenvectors of the correlation matrix for explosions.

Eigenvalue	2,6666	1,2296	1,0000	0,1038	0,0000
Proportion	0,533	0,246	0,200	0,021	0,000
Cumulative	0,533	0,779	0,979	1,000	1,000

The new variables to be analysed will be combinations of the initial parameters. In PC1 there is a description of the quantity, the source term, and the final frequency. While in PC2 the initiator frequency can be considered and in PC3 the wind velocity (Table 17). For this study, the temperature, RH, and duration time has not been considered, as those values are very equal between them. In addition, the basic frequency is not taken into account because those values are very similar to each other, and when normalised, they are associated with a single value.

Table 17. Eigenvalues for explosions.

Variable	PC1	PC2	PC3
Uw_m/s	0,000	0,000	-1,000
QUANTITY_kg	0,546	-0,403	0,000
SOURCE _TERME_kg/s	0,546	-0,403	-0,000
INICIATOR_FREQUENCY_y-1	0,333	0,737	0,000
FINAL_FREQUENCY_y-1	0,541	0,361	0,000

5.2.1. Intervention Zone

In the case of the IZ, the variables PC1, PC2 and PC3 are analysed together with the categorical variables, and finally the result is that of all of them, the most significant is the substance. This is due to the fact that this variable is the only one with p-values lower than 0.05 (Table 18).

Table 18. Analysis of Variance for explosions in IZ.

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	9	151867	16874,1	3,55	0.005
PC1	1	14233	14232.8	4.37	0.046
PC3	1	45088	45088.2	13.84	0.001
STABILITY	2	47855	23927.7	7.34	0.003
SUBSTANCE	6	100302	16716.9	5.13	0.001
Error	27	87973	3258.3		
Absence of adjustment	15	87660	5844.0	224.05	0.000
Error due to replications	12	313	26.1		
Total	37	284928			

Adjusting the regression model of the data to the substance variable, a model with an R^2 of 69.12 % is obtained. The equation obtained (Eq 3) as a result to calculate the IZ depends on three different coefficients, two of them related to the principal components, and a coefficient (e) that varies according to the substance and stability involved (Table 19).

$$IZ = e + 0.00599 \cdot PC1 - 223.6 \cdot PC3 \quad \text{Eq 3}$$

In relation to the values of PC1 and PC3, it should be noted that the first refers to the amount of the substance involved, the source term and the final frequency. In the case of PC3, it only depends on the velocity. Therefore, this velocity will have an increasing effect on the distances because the principal coefficient is negative. So the higher the velocity, the greater the distances.

Table 19. Value of e for each substance and stability in meters.

SUBSTANCE (n)	STABILITY	e
Acetone (14)	B	624
	D	1106
	F	400.8
Benzyl chloride (8)	B	551
	D	1033
	F	328.5
Lead Oxide (2)	B	315
	D	797
	F	92
Methanethiol (2)	B	597
	D	1079
	F	374
Monomethylamine (2)	B	606
	D	1088
	F	383
Propane (8)	B	701
	D	1183
	F	477.9
Propylene (8)	B	619
	D	1101
	F	396.1

This equation only considers these 7 substances because they are the cases introduced to make the analysis. In case of an explosion of another type of substance, it would not be possible to study its behaviour with the equation obtained. However, it should be considered that in Lead Oxide, Methanethiol, and Monomethylamine, due to the fact that there are two entries in the database, the coefficients obtained may not be very accurate.

The distances for each of the substances are longer when the stability is class D than when the stability is class B or F. In the case of explosions, it is worth mentioning that stability could only affect the case of unconfined explosions, since it would not be a delimiting factor in the other cases.

Finally, the residuals of this study are studied, comparing the theoretical values, which refer to those calculated with the equation, along with the values provided in the database. In Figure 44, it is possible to see that there are some atypical values, due to the fact that they present a higher error in the calculation of the distance. Thus, those values are giving a fitted value of 150-200 m, but considering a posible error of 100 m.

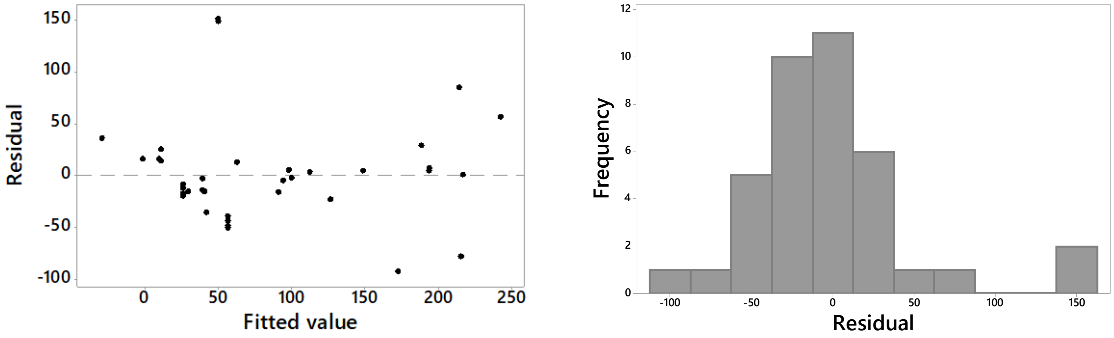

Figure 44. Residual plots for explosion in IZ.

5.2.2. Alert Zone

According to the regression model for the case of the alert zones, based on the results obtained, it is possible to conclude that substance and final scenario are significant factors (Table 20).

Table 20. Analysis of Variance for explosions in AZ.

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	11	565167	51378.8	22.68	0.000
PC1	1	731	731.0	0.32	0.575
PC3	1	7138	7138.0	3.15	0.089
STABILITY	2	7055	3527.5	1.56	0.231
SUBSTANCE	5	107823	21564.5	9.52	0.000
FINAL_SCENARIO	2	84214	42107.0	18.59	0.000
Error	24	54367	2265.3		
Absence of adjustment	12	53551	4462.6	65.66	0.000
Error due to replications	12	816	68.0		
Total	35	619534			

As a result of this regression model fitting, an equation is obtained that depends on substance and final scenario. This model manages to provide an adequate response to 90.07 % of the data. The equation (Eq 4) is determined with a constant coefficient for each of the substances, and two variable coefficients (f and g) that are dependent on the substance and the type of explosion (see Table 21 and Table 22).

$$AZ = 247.5 + f + g \qquad \text{Eq 4}$$

Table 21. Value of f for each substance in meters and n is the number of inputs.

Substance (n)	f	Substance	f
Propane (8)	112.5	**Methanethiol (2)**	-11.4
Propylene (8)	112.5	**Benzyl chloride (2)**	-26.9
Acetone (14)	0	**Monomethylamine (2)**	-195.5

For the case of the substance coefficient, positive and negative values and even zero have been obtained. For this, each of these substances will have a different impact on the distance. In the case of propane and propylene, the distance will increase, while for Benzyl chloride and Monomethylamine, the distance will be smaller. Although, it must be considered that for Lead Oxide, Methanethiol, and Monomethylamine, as there are two inputs in the database, the coefficients obtained may not be very accurate.

Table 22. Value of g for each specific scenario in meters.

	CVE	UVCE	BLEVE
g	-211.1	112.5	0

In the case of the coefficient for the type of explosion, positive, negative, and null values have also been obtained by BLEVE. Analysing them, it is possible to see that in the case of the unconfined explosion, the coefficient is higher, which makes sense because it is a non-confined explosion, and therefore, it can expand over a distance. This contrasts with the CVE, in which the explosion is confined.

Finally, in the analysis of the residuals (Figure 45), it is possible to see that their most representative range of error is between 0 and 100 metres. However, it is observed that there are some cases, which could present an error of higher than 50 meters when the distance to predict is higher than 250 metres.

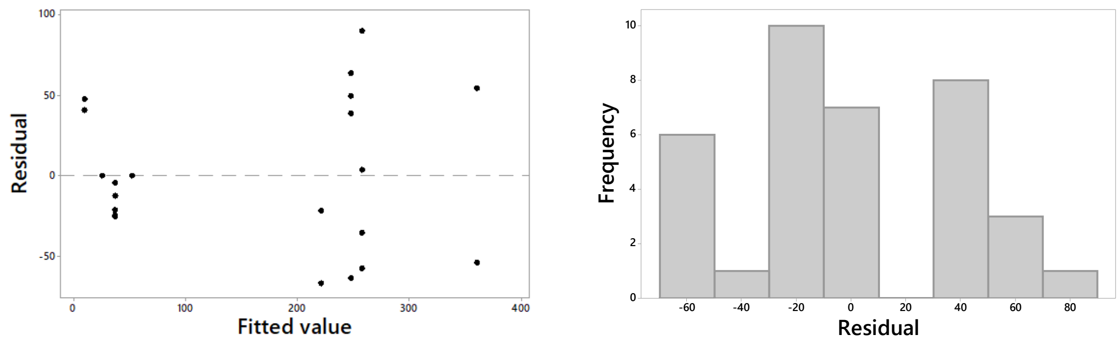

Figure 45. Residual plots for explosion in AZ.

5.2.3. Domino Effect

As a result of the analysis of the regression adjustment for the domino effect, it is found that the most significant parameter is final scenario (Table 23). Therefore, quantitative variables, stability and substance are not taken into account in this case.

Table 23. Analysis of Variance for explosions in DE.

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	11	29630.1	2693.64	24.17	0.000
PC1	1	419.0	418.98	3.76	0.064
PC3	1	236.4	236.39	2.12	0.158
STABILITY	2	233.6	116.82	1.05	0.366
SUBSTANCE	5	195.9	39.18	0.35	0.876
FINAL_SCENARIO	2	4184.7	2092.36	18.78	0.000
Error	24	2674.2	111.43		
Absence of adjustment	12	2466.6	205.55	11.88	0.000

Error due to replications	12	207.6	17.30
Total	35	32304.3	

As a result of the regression analysis, Eq 5 is obtained, which depends on a constant and a coefficient dependent on the final scenario determined (Table 24). This equation is able to explain 85.66 % of the variance.

$$DE = 22.43 + h \qquad \text{Eq 5}$$

Table 24. Value of h for each final scenario in meters.

	CVE	UVCE	BLEVE
h	-9.05	68.74	0

Based on the coefficients obtained for each of the models, the same conclusion can be reached as in the previous case. That is, the BLEVE will have no effect on the domino effect. However, in the case of unconfined vapour explosions, the distances will be greater because the vapour dispersant will have expanded over time, and therefore, the distances will be greater. The opposite is applicable to confined explosions, which occur in confined spaces reaching lower distances.

To finish with, a comparison is made between the DE values calculated with the equation and the values obtained in the BD. As a result, it is possible to see the different residuals of this comparison, without reaching maximum values of 40 metres of error, moreover its maximum density is between 0 and 5 metres (Figure 46). Although for 90 metres, errors of 30 or even 40 metres could be reached.

Moreover, three different zones of points can be distinguished in Figure 46. According to the values previously found, it could be concluded that the points on the right correspond to the UVCE case because the distances are longer. On the other hand, that the points described on the left correspond to the VCE because they have a negative coefficient. Finally, the distances of the BLEVE would refer to the intermediate points, around 20m.

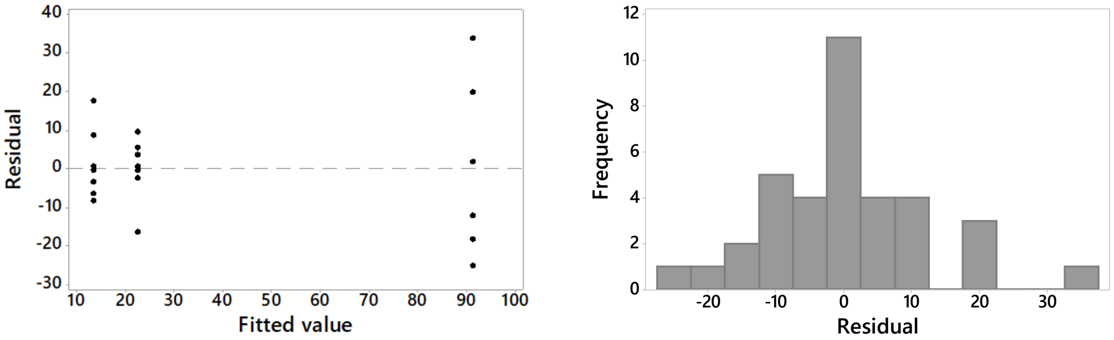

Figure 46. Residual plots for explosion in DE.

5.3. Fires

The last case study within the basic scenario is for the case of fire. In this one, 264 database entries were studied, although 92 were left out of scope due to lack of data. As a result of PCA, it is obtained that with 3 principal components (Table 25), 65.2 % of the variance could be explained. This number of components is chosen because the eigenvalue is higher than 1.

Table 25. Analysis of the eigenvalues and eigenvectors of the correlation matrix for fires.

Eigenvalue	3.0560	1.7842	1.0281	0.9928	0.8470	0.5678	0.4037	0.3061	0.0143
Proportion	0.340	0.198	0.114	0.110	0.094	0.063	0.045	0.034	0.002
Cumulative	0.340	0.538	0.652	0.762	0.856	0.920	0.964	0.998	1.000

Once the number of principal components is determined, their combinations are studied in relation to the initial variables. Table 26 shows the different relations between these components. PC1 consists of temperature, relative humidity, quantity, and source term. PC2 is determined by the combination of the initiator and final frequency. PC3 is the wind velocity and the base frequency.

Table 26. Eigenvalues for fires.

Variable	PC1	PC2	PC3
TEMPERATURE_ºC	-0.462	0.058	0.009
HR_%	-0.390	-0.006	0.148
Uw_m/s	0.099	0.133	-0.640
QUANTITY_kg	-0.520	0.042	-0.222
SOURCE _TERME_kg/s	-0.529	0.068	-0.205
DURATION_TIME_s	0.198	-0.356	-0.166

BASE_FREQUENCY_y-1	0.092	-0.111	-0.669
INICIATOR_FREQUENCY_y-1	0.113	0.649	-0.021
FINAL_FREQUENCY_y-1	0.120	0.642	-0.016

5.3.1. Intervention Zone

For the regression analysis for the IZ, the most important determinants are the categorical variables atmospheric stability and substance. This is decided because their p-value is lower than 0.05, therefore they are considered to be significant variables (Table 27).

Table 27. Analysis of Variance for fires in IZ.

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	35	182758	5221.67	6.40	0.000
PC1	1	17	16.52	0.02	0.887
PC2	1	15	14.60	0.02	0.894
PC3	1	17	16.61	0.02	0.887
STABILITY	2	4434	2216.93	2.72	0.068
SUBSTANCE	24	108770	4532.08	5.55	0.000
TYPE	6	2692	448.66	0.55	0.770
Error	264	215441	816.07		
Absence of adjustment	255	213964	839.07	5.11	0.005
Error due to replications	9	1477	164.15		
Total	299	398200			

As a result of this analysis, an equation is obtained which depends exclusively on substance involved. This equation is able to cover 40.13 % of the variance, using only the one parameter described above. Thus, the result depends on a constant, and on two different coefficients (Table 28), depending on the type of substance (i).

$$IZ = 8.82 + i \quad \text{Eq 6}$$

Table 28. Value of i for each substance in meters and n is the number of inputs.

Substance (n)	i	Substance	i
Propylene (20)	90.83	**Butyl Acetate (6)**	2.2
Butane (4)	33.7	**Butadiene (6)**	1.9

Propane (38)	26.68	**Acetic Acid (2)**	0.2
Methane (14)	20.67	**Butanol (2)**	0.2
Kerosene (6)	17.2	**2-propanol (36)**	0
Isopropylamine (4)	13.2	**Methanol (30)**	-0.48
Acrylonitrile (2)	10.2	**Dimethyl disulphide (6)**	-0.5
Xylene (26)	10.18	**Ethanol (30)**	-0.76
THF cyclohexane (4)	6.2	**Methyl chloride (22)**	-1.18
Methyl methacrylate (16)	5.5	**Monomethylamine (10)**	-1.5
Acetone (44)	4.47	**Naphtha (2)**	-3.8
Dichloroethane (16)	3.0	**Hydrogen (4)**	-4.8

Each substance involved will have a different safety distance, ranging from 90 metres as in the case of propylene to -5 metres in the case of hydrogen. Substances with largest coefficients will be those with the longest distances, such as Propylene, Butane, and Propane. While substances such as Monomethylamine, Naphtha or Hydrogen will be the ones with the shortest distances. However, it should be considered that some of the substances due to the fact that there are two entries in the database, the coefficients obtained may not be very accurate.

With the residual analysis (Figure 47), the values obtained according to the above equation are compared with the values described in the DB. It was found that there are atypical values with a residual of around 200 metres. Although, the maximum error density is between -40 and 40 m.

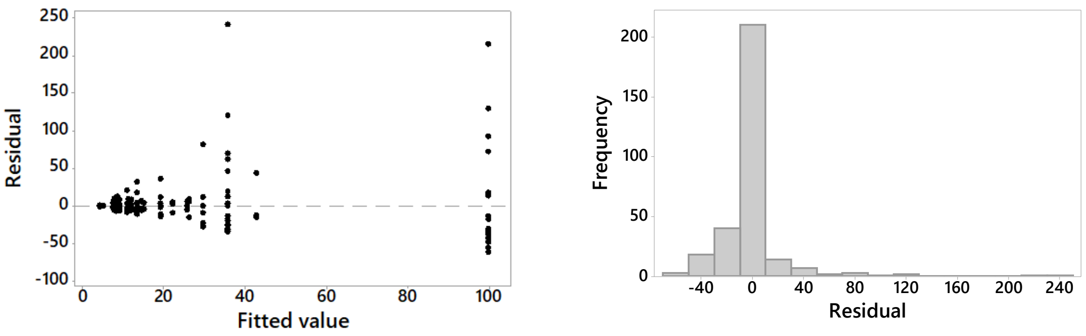

Figure 47. Residual plots for fires in IZ.

In the figure on the right, different zones of dots are visible. However, as determined above, the distance depends exclusively on the substance, therefore, each of these zones can be considered to be a single substance. It can be concluded that in the right-hand area, there are residual values for the substance propylene, and in the left-hand area, for the substance hydrogen.

5.3.2. Alert Zone

By doing the regression fit analysis for AZ, it is concluded that this distance will depend only on the substance too (Table 29).

Table 29. Analysis of Variance for fires in AZ.

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	32	416330	13010.3	6.15	0.000
PC1	1	1642	1641.7	0.78	0.379
PC2	1	1625	1624.7	0.77	0.382
PC3	1	1642	1641.6	0.78	0.379
SUBSTANCE	22	210186	9553.9	4.52	0.000
STABILITY	2	9258	4629.1	2.19	0.114
EQUIPMENT	5	749	149.8	0.07	0.996
Error	226	477737	2113.9		
Absence of adjustment	220	475280	2160.4	5.27	0.020
Error due to replications	6	2457	409.6		
Total	258	894067			

Once the most significant variable for this study is determined, the equation (Eq 7) of the regression line is obtained, with an R^2 of 42.21%. This equation will depend on a constant and one coefficient dependent on the substance (Table 30).

$$AZ = 10.76 + j \qquad \text{Eq 7}$$

Table 30. Value of j for each substance in meters and n is the number of inputs.

Substance (n)	j	Substance (n)	j
Propylene (20)	135.5	**Methyl chloride (22)**	3.8
Propane (38)	60.4	**Butyl Acetate (6)**	2.2

Butane (4)	47.7	**Acetic Acid (2)**	0.2
Kerosene (14)	19.2	**Butanol (2)**	0.2
Isopropylamine (4)	17.5	**2-propanol (36)**	0
Xylene (26)	12.8	**Dimethyl disulphide (6)**	-1.1
Acrylonitrile (2)	11.2	**Methanol (30)**	-1.4
THF cyclohexane (4)	6.2	**Ethanol (30)**	-1.5
Butadiene (6)	4.8	**Monomethylamine (10)**	-1.8
Methyl methacrylate (16)	4.5	**Acetone (44)**	-2.6
Dichloroethane (16)	3.9	**Naphtha (2)**	-4.8

From the values obtained for the coefficients of the substances, it is possible to deduce that this range of distances will be from about 150 metres to about 5 metres. Each substance will have a different impact on the AZ calculation. In the case of substances such as propylene, propane and butane, these distances will be longer, although for Monomethylamine, acetone, naphtha they will be shorter distances, as the coefficients are negative. Although, it must be considered that as some substances only have two inputs in the DB, the coefficients obtained may not be very accurate.

Comparing these values with those obtained in the case of the intervention area, similarities are found. The substances with high coefficients correspond to the substances for both cases, while in the case of the substances with low coefficients, they are very almost the same.

Finally, the values obtained theoretically, according to the equation described above, and the database values were compared. The residuals of these values were obtained by comparing them, concluding that they are within a range between -100 and 400 metres. The maximum density of error cases is between 0 and 20 metres (Figure 48).

Based on the graph on the left, it is seen that there are different zones of very distinguishable points between them. There are values near 20-30 metres, also in the 50m, and finally around 150m. So, based on the above coefficients, the points with values around 150m refer to propylene and the points around 50 could be referred to propane and butane.

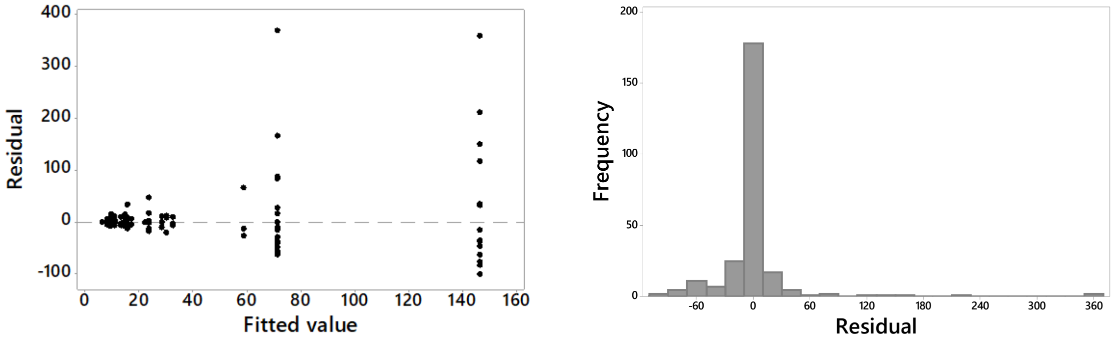

Figure 48. Residual plots for fires in AZ.

5.3.3. Domino Effect Zone

The last zone to be analysed is DE for fire, in which the regression adjustment shows that the quantitative variables and the stability, substance and type of LOC are significant factors (Table 31). This selection is due to the fact that the p-values are lower than 0.05 and are thereby considered determinant factors.

Table 31. Analysis of Variance for fires in DE.

Source	DE	Adj SS	Adj MS	F-Value	P-Value
Regression	35	27018.0	771.94	11.52	0.000
PC1	1	572.2	572.21	8.54	0.004
PC2	1	570.2	570.19	8.51	0.004
PC3	1	572.2	572.19	8.54	0.004
STABILITY	24	15838.4	659.93	9.85	0.000
SUBSTANCE	2	1176.4	588.21	8.78	0.000
TYPE	6	1331.5	221.92	3.31	0.004
Error	192	12863.7	67.00		
Absence of adjustment	186	11686.4	62.83	0.32	0.994
Error due to replications	6	1177.3	196.22		
Total	227	39881.7			

Therefore, considering only these variables, a regression equation is obtained, which allows explaining 57.19 % of the variance. This equation (Eq 8) is determined by a constant, three coefficients assigned to each PC, and three other coefficients which refer to substance (Table 32), type of initiator event (Table 33) and stability (Table 34).

$$DE = -79 - 1.446*PC1 - 2.186*PC2 + 2.97*PC3 + k + l + m \qquad \text{Eq 8}$$

Table 32. Value of k for each substance in meters and n is the number of inputs.

Substance (n)	k	Substance (n)	k
Propylene (20)	31.52	**Acetic Acid (2)**	2.02
Isopropylamine (4)	16.53	**2-propanol (36)**	0
Kerosene (6)	16.44	**Ethanol (30)**	-0.04
THF cyclohexane ()	14.92	**Methanol (30)**	-0.76
Acrylonitrile (2)	11.52	**Butanol (2)**	-1.25
Butane (4)	5.88	**Methyl chloride (22)**	-2.72
Xylene (26)	5.84	**Acetone (44)**	-3.64
Methyl methacrylate (16)	4.67	**Dimethyl disulphide (6)**	-6.78
Propane (38)	4.19	**Naphtha (2)**	-7.68
Monomethylamine (10)	2.88	**Methane (14)**	-8.82
Dichloroethane (16)	2.87	**Butadiene (6)**	-13.28
Butyl Acetate (6)	2.48	**Hydrogen (4)**	-13.79

For the case of the substances, the coefficients obtained vary between a range of 32 metres and -50. Therefore, the substances that will extend this distance the most are propylene, Isopropylamine and Kerosene. In contrast to butadiene and hydrogen, which will have shorter distances. However, it should be also considered there are some substances (n=2) that only have two entries in the DB so the coefficients obtained may not be very accurate.

Table 33. Value of l for each type in meters.

	Above Ground	Batch	Continuous	In-ground	Single Containment	Underground
l	11.51	5.88	7.07	16.54	0.43	7.72

Following on from the analysis, in the case of type, these will cause the distances to vary between 12 and 0 metres depending on the location of the potential major accident.

Table 34. Value of m for each stability in meters.

	B	D	F
m	0	13.42	3.52

Analysing the stability in the case of DE for fire, it is seen that if a stability class B is determined, it will have no impact on the distance. However, in the case of classes D and F, these would increase the distance.

Finally, by analysing the residuals between the value calculated by the above equation and the database value, Figure 49 is obtained. It is possible to observe that the error range of the equation is between-20 and 90 metres. The maximum error density is between 0 and 10 metres.

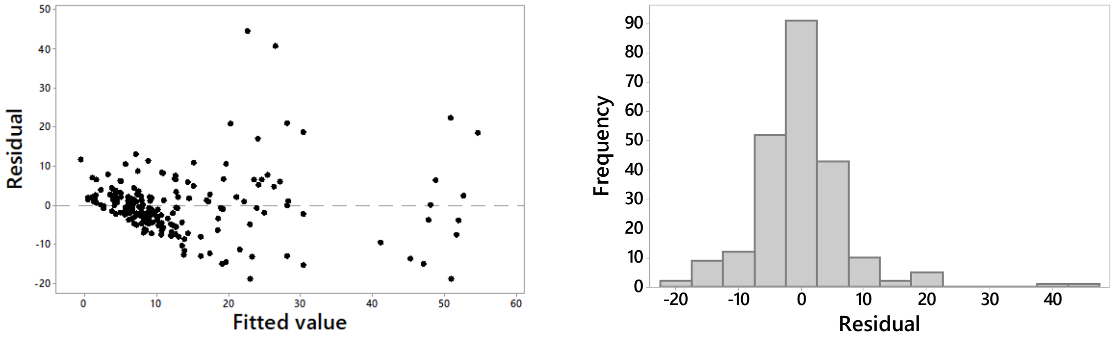

Figure 49. Residual plots for fires in DE.

6. Environmental impact analysis

The environmental impact deriving from the implementation of this project lies in the electrical energy consumed during the use of the computer, and therefore the amount of CO_2 generated that has been emitted into the atmosphere.

For the calculation of the electrical consumption, a power of 80 W must be considered, and 520 hours of computer use divided between bibliographic research, the writing of the report and data processing.

$$electricity\ consumption = 80\ W * 520\ h = 41.600\ Wh = 41{,}6\ kWh$$

For calculating the amount of CO_2 emitted to the atmosphere, it is necessary to use a factor of $0{,}392\frac{kg\ de\ CO_2}{kWh}$ published by Generalitat de Catalunya [57].

$$CO_2\ consumption = 41{,}6\ kWh * 0{,}392\frac{kg\ de\ CO_2}{kWh} = 16,31\ kg\ de\ CO_2$$

The positive environmental impact of this project must also be considered. This is related to the analysis carried out in order to be able to reduce the risks caused by some possible major accident. Consequently, through the analysis and the implementation of the database, patterns of behaviour can be identified for each of the possible events, in order to prevent the risks associated with possible major accidents.

Conclusions

This project presents a bibliographic search on the legislation (European, Spanish, and Catalan level) applied to the establishments affected by the SEVESO regulation. It is concluded that for the establishments affected at Autonomous level by the Decree 3/2021, an AQR and/or a safety report must be presented, depending on their classification. However, this project is focused on high-level affected establishments, which are obliged to submit a safety report.

A database is designed for the compilation of data from the safety reports. Its structure is based on the *Generalitat de Catalunya's* accident hypothesis coding table, although its information is extended. Thus, data of the location of the company, of the meteorological conditions and of the hazardous substances involved was collected. Also, the loss of containment parameter and the possible options for the final accident scenario were considered. Consequently, the information on accident frequencies and safety distances was listed. Basically, a database of hazardous scenarios is created in which the emergency planning distances are described, fed from QRAs included in safety reports.

An exploratory analysis of the database data according to its location, meteorological conditions (temperature, RH, stability class, wind direction and wind velocity), substances, final accident, and the magnitude of the safety distances, has been performed. It is concluded that the highest density of entries determined for major accidents are located in Barcelona, having a temperature between [14,16), a relative humidity of [73,76), a stability of class F, a wind direction N, and a wind velocity between [1,2). Regarding the substances involved, it has been possible to classify them according to the GHS categories, determining which of them present physical, health or environmental hazards. Concerning the final accident case, fire has the highest density of possible basic scenarios (pool, flash, jet, and warehouse), followed by dispersion (toxic, flammable, and oxidising) and the least abundant cases are explosions (CVE, BLEVE, and UVCE).

Finally, the safety distances offered by these accidents were analysed, concluding that dispersion is the scenario providing the longest distances, followed by fire and explosions. Lastly, the effect of these factors on the safety distances was studied. In relation to the possible specific accident, the order of these distances from the largest to the shortest is dispersion, followed by fires (pool > flash > jet > warehouse) and finally explosions (BLEVE > UVCE > CVE for IZ and AZ and UVCE > BLEVE & VCE for DE zone).

A pattern recognition analysis based on PCA considering quantitative variables and regression adjustment coupled with categorical variables has been carried out to study the relation between these parameters and safety distances, distinguishing for each of the basic scenarios presented. For dispersion, it is found that in order to calculate IZ and AZ, the quantitative variables (temperature, RH, quantity, source term, duration time, and frequencies), substance, and stability are significant parameters. For explosions, it is found that the wind velocity, the quantity, the source term, the final frequency, the stability, and the substance involved will be needed to calculate the IZ. For the AZ it will depend only on the substance and the final accident. For the DE calculation the associated final accident will be required. Lastly, in the case of the IZ and AZ of fires, it will be mainly dependent on the substance, while for the DE, qualitative variables (temperature, RH, quantity, source term, duration time, and frequencies) will be needed together with the substance, the stability, and the type of event initiator. To finish with, an equation for modelling the different safety distances has been obtained for each of those scenarios.

Economic evaluation

In order to calculate the total cost of the project, all the required resources are considered, including the cost of office material, the cost of personnel and the cost of energy. All these prices are calculated considering the VAT included.

Cost of office equipment

In relation to the costs associated with office material (Table 35), the project is carried out with an ASUS model laptop computer which has a cost of 1050€, taking into account that it has a depreciation period and will continue to be useful for future projects, so a 10% of its price is the cost assigned to this project, as a proportion of the time dedicated.

Table 35. Cost of office equipment

Concept	Unit Price	Amortisation	Total
Computer	1050€	10%	**105€**

Cost of personnel

The personnel cost (Table 36) is obtained by considering the price per hour of the work done. In this case, these are the hours worked by the author of the project and the hours of dedication of the project directors. According to the BOE, a value of 30 €/h is set since this project is done by a graduate engineer. In the case of project direction, the price established by the BOE oscillates around 40 €/h [58].

Table 36. Cost of personnel

Concept	Price/hour	Hours	Total
Bibliographic research	30€/h	150	4.500€
Memory writing	30€/h	300	9.000€
Project management	40€/h	70	2.800€
Total cost		520	**16.300€**

Cost of energy consumption

In relation to the energy cost (Table 37), an approximation of the cost of this project is made taking into account only the electricity.

Table 37. Cost of energy consumption

Concept	Price/hour	Hours	Total
Electricity	0,04 €/h	520	**20,80 €**

Total cost

Finally, the total cost of this project is as listed in Table 38.

Table 38. Total cost

Cost	Price
Office equipment	105
Personnel	16.300
Energy consumption	20,8
Total	**16.470,8 €**

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