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A SOFTWARE APPLICATION TO DEFINE AND RANK ATEX ZONES

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RESUMO

As atividades económicas que envolvam a utilização ou armazenagem de produtos químicos perigosos suscetíveis de provocar acidentes graves, segundo o Artigo 79º da Lei nº 102/2009, de 10 de setembro, com as alterações introduzidas pela Lei nº 3/2014 de 28 de janeiro, estão sujeitas a precauções especiais no que respeita a segurança e saúde dos seus trabalhadores.

Neste contexto, aplica-se o Decreto-Lei nº 236/2003 de 30 de setembro, que transpõe a diretiva europeia nº 1999/92/CE, relativa às prescrições mínimas de proteção e segurança dos trabalhadores expostos a riscos derivados de atmosferas explosivas. Nele estão preconizadas as obrigações do empregador para garantir a segurança dos trabalhadores em áreas onde se possam formar atmosferas explosivas, das quais se destacam a avaliação global dos riscos de explosão e a implementação de medidas técnicas e organizativas para evitar a formação, ignição e propagação de atmosferas explosivas, de forma a proteger a vida, a integridade física e a saúde dos trabalhadores.

A avaliação global dos riscos de explosão passa inevitavelmente pela tarefa de definição e classificação de zonas perigosas devido à existência de atmosferas explosivas. Esta tarefa envolve habitualmente uma equipa multidisciplinar e um trabalho demorado, tanto no que diz respeito à recolha da informação no campo como nos cálculos para chegar aos resultados pretendidos de definição de zonas, categorias de equipamentos e classes de temperatura.

Com a perspetiva de diminuir consideravelmente o tempo de cálculo e os recursos alocados, foi desenvolvido um protótipo de uma aplicação para o cálculo automático das zonas perigosas e sua extensão.

O protótipo foi desenvolvido em Visual Basic for Applications e Microsoft Excel, e traduz-se numa ferramenta de uso amigável, num ambiente conhecido da maioria dos utilizadores.

A metodologia de cálculo baseou-se no referencial IEC/EN 60079-10-1:2015, o que torna a aplicação numa ferramenta fidedigna e de acordo com a normativa em vigor em Portugal e na União Europeia.

Para avaliar a solução proposta, foram criados cenários que simulam situações habitualmente encontradas na indústria. Os dados iniciais foram introduzidos na aplicação e os resultados das simulações comparados com os valores obtidos através de cálculo manual.

Os testes de simulação validaram a solução proposta e realçaram os seguintes aspetos: o tempo de cálculo diminui drasticamente, a falha humana é muito reduzida e a utilização do protótipo de aplicação é simples e intuitiva.

Palavras-chave:

“segurança”, “atmosferas explosivas”, “aplicação”, “Visual Basic for Applications”, “Microsoft Excel”

ABSTRACT

In accordance with Article 79º from Lei nº 102/2009 of September 10th, with the amendments of Lei nº 3/2014 of January 28th, the economic activities involving the use or storage of dangerous chemical substances which are likely to cause severe accidents, are subject to special precautions regarding the safety and health of their workers.

For this context applies the Decreto-Lei nº 236/2003 of September 30th, the Portuguese counterpart of European directive nº 1999/92/CE, relative to the minimum requirements for improving the safety and health protection of workers potentially at risk from explosive atmospheres. This document foresees the employer's obligations to ensure the safety of workers in areas where explosive atmospheres may occur, with relevance to the overall assessment of explosion risks and the implementation of technical and organizational measures to prevent the formation, ignition and propagation of explosive atmospheres, in order to protect the life, physical integrity and health of workers.

The overall assessment of explosion risks involves, inevitably, the definition and classification of hazardous areas due to the presence of explosive atmospheres. This task typically involves a multidisciplinary team and is very time-consuming, either for collecting information in the field, as for calculating the hazardous areas, equipment categories and temperature classes.

With the prospect of reducing considerably the calculation time and resources allocated, a prototype of an application for automatic calculation of dangerous areas and their extension was developed.

The prototype was developed in Visual Basic for Applications and Microsoft Excel, and is a user-friendly tool, in a familiar environment for most users.

The calculation methodology was based on the reference IEC/EN 60079-10-1: 2015, which makes the application a reliable tool and in accordance with the legislation in force in Portugal and in the European Union.

To evaluate the proposed solution, were created scenarios that simulate situations commonly found in the industry. Initial data was introduced in the application and the simulation results compared with the values obtained by manual calculation.

Simulation tests validated the proposed solution and highlighted the following aspects: the calculation time decreases dramatically, human error is greatly reduced and the use of the prototype application is simple and intuitive.

Keywords:

“safety”, “explosive atmospheres”, “application”, “Visual Basic for Applications”, “Microsoft Excel”

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LIST OF ABBREVIATIONS

AIT	Auto-Ignition Temperature
ALOHA®	Areal Locations of Hazardous Atmospheres
ANSI	American National Standards Institute
API	American Petroleum Institute
ATEX	*Atmosphères Explosibles* (Explosive Atmospheres)
CEI	*Comitato Elettrotecnico Italiano* (Italian Electrotechnical Committee)
CENELEC	European Committee for Electrotechnical Standardization
CFD	Computational Fluid Dynamics
DNV GL	Det Norske Veritas Germanischer Lloyd
DSEAR	Dangerous Substances and Explosive Atmospheres Regulations
EC	European Community
EEC	European Economic Community
EFTA	European Free Trade Association
EI	Energy Institute
EN	European Standard
EPA	Environmental Protection Agency
EU	European Union
FEUP	Faculdade de Engenharia da Universidade do Porto
IEC	International Electrotechnical Commission
ISO	International Organization for Standardization
LEL	Lower Explosion Limit
LPG	Liquefied Petroleum Gas
MATLAB	Matrix Laboratory
MESG	Maximum Experimental Safe Gap
MIE	Minimum Ignition Energy
NE	Negligible Extent
NEC	National Electric Code
NFPA	National Fire Protection Association
NOAA	National Oceanic and Atmospheric Administration
PHAST™	Process Hazard Analysis Software Tool
PRISMA	Preferred Reporting Items for Systematic Reviews and Meta-Analyses
UEL	Upper Explosion Limit
UI	User Interface
VBA	Visual Basic for Applications
VBE	Visual Basic Editor

PART 1

1 INTRODUCTION

One of the most challenging subjects in the field of occupational health and safety is the safety (i.e. absence of unacceptable risks) in areas where potentially explosive atmospheres may occur.

The European Union legislation and standards on ATEX (from the French "*ATmosphères EXplosibles*") is very demanding. To comply with it, the companies shall have the support of a multidisciplinary team of experts studying in depth the plant processes and working to guarantee the safety on the potential hazardous areas.

The legislative safety approach, where the occurrence of explosive atmospheres cannot be avoided, is based on the principle that the higher the likelihood for an explosive atmosphere being present, the more severe the requirements on the equipment to be installed in these areas, which means less likely to be able to ignite an explosive atmosphere.

Therefore, the employer must assess the likelihood for an explosive atmosphere being present on his premises which, according to ATEX workplace Directive 1999/92/EC, must be done applying the zone classification system which defines and ranks such hazardous areas in zones.

1.1 Context

Explosive atmospheres may be present in a great variety of industries and production processes. To prevent major accidents with serious human injuries and high financial costs, it's mandatory to classify the hazardous areas and to take preventive measures to assure the safety of the workers exposed to the risks of explosive atmospheres, such as uncontrolled effects of flame and pressure, the presence of noxious reaction products and oxygen shortage.

The zone classification task, albeit being often difficult, is the foundation for all the safety precautions imposed on the employer in the context of prevention and protection against the risk due to the possible occurrence of explosive atmospheres.

ATEX is the name commonly given to the two EU (European Union) directives which intend to control the risks caused by explosive atmospheres: Directive 1999/92/EC (ATEX Workplace Directive) and Directive 2014/34/EU (ATEX Equipment Directive).

Directive 1999/92/EC establishes the minimum requirements (employer obligations) for the protection and safety of the workers potentially at risk from explosive atmospheres, through zone classification of hazardous areas and through explosion risk assessments and appropriate ATEX equipment selection.

Directive 2014/34/EU replaced the previous ATEX equipment Directive 94/9/EC in April 2016. It is an equipment (product) directive which harmonizes the Essential Health and Safety Requirements to be complied with by the manufacturer of ATEX products, including instructions for equipment categorization, conformity assessment procedures and CE- and Ex- marking obligations. In this directive, the equipment is grouped and categorized according to the intended use and level of protection against own possible ignition sources becoming effective. This clearly facilitates the customer's choice of appropriate equipment according to the legal requirements placed on him by ATEX workplace Directive 1999/92/EC.

An "explosive atmosphere", in the scope of the two directives, is defined as "a mixture with air, under atmospheric conditions, of flammable substances in the form of gases, vapours, mists or dust in which, after ignition has occurred, combustion spreads to the entire unburned mixture".

Atmospheric conditions (either indoors or outdoors process equipment) are generally regarded (but not defined in the directives) as places having a pressure between 0.8 bara and 1.1 bara, and a temperature between -20 ºC and +60 ºC. Areas outside atmospheric conditions don’t fall under the scope of these directives.

Although the operating conditions at a factory plant are, in general, are outside “atmospheric conditions” and therefore fall outside the scope of the directives, start-up and shut-down situations may very well belong to “atmospheric conditions” and must therefore comply with the requirements of the directives.

In case of the existence of an explosive atmosphere under non-atmospheric conditions, the employer has the obligation to guarantee the health and safety at work, e.g. under the scope of the Framework Directive 89/391/EEC and the Chemical Agents Directive 98/24/EC, but exact ATEX Directive compliance is not required.

1.2 Motivation

The Portuguese legislative counterpart of Directive 1999/92/EC is Decreto-Lei nº 236/2003 of September 30th, which imposes the adoption of safety and protection measures for the workers exposed to the explosive atmospheres hazards.

Concerning the safety and health of the workers, the Portuguese law is clear: the employer is to draw up an explosion protection manual, which satisfies the minimum requirements established and is to keep it up to date. The explosion protection manual includes the identification of the hazards, the evaluation of risks and the definition of the specific measures to be taken to safeguard the health and safety of workers at risk from explosive atmospheres.

In order to evaluate the risks, it’s necessary to classify the hazardous areas where an explosive atmosphere may exist. The area classification is governed by the standards IEC/EN 60079: Explosive Atmospheres, parts 10-1: “Classification of areas – Explosive gas atmospheres” and 10-2: “Classification of areas – Explosive dust atmospheres”.

In spite of both standards give guidance on the identification and classification of hazardous areas, only IEC/EN 60079-10-1:2015 has an analytical methodology for that end.

The motivation for developing the present thesis arose from the fact that there were not any computational tools developed to calculate automatically the analytical methodology presented in IEC/EN 60079-10-1:2015, which suggests a laborious and time consuming process.

The available tools and software in the market are oriented to specific industries or to specific type of risk, and the majority of them are based on the American standards. It urged the need of a user friendly and expedite mechanism to perform the classification and extent of the hazardous areas in a broader dimension, using the IEC/EN 60079-10-1:2015 methodology.

1.3 Study Goal

The main objective of this study is to develop a prototype of a software application to assist the classification of the hazardous areas and its extent for any type of industry, based on the IEC/EN standards, which is able to:

- Characterize the behaviour of the dangerous substances in a specific environment;
- Define the dimensions of the hazardous areas and its geometry;
- Classify the hazardous areas;
- Indicate the equipment classification and temperature class for the hazardous areas.

1.4 Thesis Structure

As a consequence of the objectives described in the previous section, the structure of the present thesis is divided in six chapters, being this first one devoted to present the scope and the main objectives of the thesis.

In Chapter 2 is presented the state of the art in matter of: standards and legal documents related to the assessment of the hazardous areas, literature review using PRISMA systematic review and a survey of fluid simulation software available in the market.

The Chapter 3 is dedicated to summarize the theory and the physics behind the classification of hazardous areas.

The HALOC GAS application prototype is described in Chapter 4. An overview of the methodology is presented, along with a brief description of each part that composes it.

Chapter 5 is devoted to presenting some implementation details and test of the application prototype. The first part of the chapter comprehends the description of the implementation of the prototype and its usability. The experimental test carried out to validate the prototype is present in the second part of this chapter. The results are compared with the ones obtained with manual calculus.

Finally, in Chapter 6, overall conclusions are drawn and the perspectives for future development of the application prototype as a consequence of this work are suggested.

2 STATE OF THE ART

This chapter analyses the current standards and legal documents applicable to the subject of this study, regarding the national legislation and the European Union directives. It will also have the result of the literature systematic review, based on a research built on the PRISMA systematic review. At last, it’s presented a review of the available software in the market for Computational Fluid Dynamics (CFD) simulations and hazardous areas classification.

2.1 Introduction

The research and study of catastrophic accidents in coal mines began in 18th century. They’ve caused thousands of casualties and the cause was mainly the ignition of fire damp by sparks (often generated by electrical apparatus). The first contributions regarding safety has been made in 1815 by the English chemist, Sir Humphry Davy who developed an oil lamp which prevented the propagation of the flame through a close meshed screen.

Since then, many regulations and laws have been drawn and nowadays, with the technological and scientific advances, the behaviour of the explosions can be predicted with mathematical and simulation models which improve the liability of the risk assessment.

2.2 Standards and Legal Documents

In 1975, the Council of the European Community issued basic directives on explosive protection. The European standards for hazardous areas were worked out by CENELEC, the European Committee for Electrotechnical standardization.

In 1989, the Council of the European Community published the “Framework Directive”, Directive 89/391/EEC of June 12th, on the introduction of measures to encourage improvements in the safety and health of workers at work. The aim of this directive was to introduce measures to encourage improvements in the safety and health of workers at work. It applies to all sectors of activity, both public and private, except for specific public service activities, such as the armed forces, the police or certain civil protection services. This directive is of fundamental importance as it the basic safety and health legal act which lays down general principles concerning the prevention and protection of workers against occupational accidents and diseases.

This “Framework Directive” served as the basis for a series of individual directives. The “Framework Directive” with its general principles continues to apply in full to all the areas covered by the individual directives, but where individual directives contain more stringent and/or specific provisions, these special provisions of individual directives prevail, such as the ATEX Directives.

The Directive 94/9/EC for the harmonization statutory provisions of the member states relating to apparatus and protective systems for use according to the rules in potentially explosive atmospheres, issued on March 23rd, 1994 by the European Parliament and Council, will substitute any directives concerning explosion protection existing on a European level as from July 1st, 2003. The European Parliament determined March 1st, 1996 as the date for transposing this directive into national law. The Portuguese legislative counterpart of this directive is Decreto-Lei nº 112/96 of August 5th and its regulation Portaria nº 341/97 of May 21st.

Five years later was issued the Directive 99/92/EC of December 16th, on the minimum requirements for improving the safety and health protection of workers potentially at risk from explosive atmospheres (15th individual directive within the meaning of Article 16(1) of Directive 89/391/EEC). This directive aims at establishing and harmonising minimum requirements for improving the safety and health of workers potentially at risk from explosive atmospheres. The Portuguese counterpart of this directive is Decreto-Lei nº 236/2003 of September 30th.

The Directive 94/9/EC has been updated and replaced by the Directive 2014/34/EU on April 2016.

Besides the ATEX Equipment Directive 2014/34/EU, there are other directives that may also be relevant for the manufacturer, as for instance the Machinery Directive 2006/42/EC and the Electromagnetic Compatibility Directive 2014/30/EU (equipment for use in potentially explosive atmospheres are explicitly excluded from the scope of the Low Voltage Directive 2014/35/EU). The ATEX Equipment Directive is supported by several harmonised standards offering the manufacturer the possibility to obtain presumption of conformity with the requirements of the directive. The list of harmonised standards is available on the Internet at the European Commission website. (Jespen T., 2016)

Generally, workplace directives aren't directly supported by European standards (EN standards), but the following three standards may be useful for the compliance with the ATEX Workplace Directive 1999/92:

- **EN 1127-1**: Explosive atmospheres – Explosion prevention and protection – Basic concepts and methodology
- **IEC/EN 60079-10-1**: Explosive atmospheres – Classification of areas – Explosive gas atmospheres
- **IEC/EN 60079-10-2**: Explosive atmospheres – Classification of areas – Combustible dust atmospheres

Further guidance for specific areas can be obtained from "codes of good practice", such as:

- **Italian Guide CEI 31-35** – "Explosive atmospheres. Guide for classification of hazardous for the presence of gas in application of CEI EN 60079-10-1". This CEI (*Comitato Elettrotecnico Italiano*) guide gives special features for determination of the type of zone and for the evaluation of its extent. When the type of zone has been determined, this methodology includes a procedure to verify if: i) the likelihood of the explosive atmosphere in one year; ii) the total duration of the explosive atmosphere in one year, are below some critical values. This verification introduces a probabilistic risk-based approach.
- **EI 15** – "Model code of safe practice Part 15: Area classification code for installations handling flammable fluids". EI (Energy Institute) 15 is a well-established, internationally accepted publication that provides methodologies for hazardous area classification around equipment storing or handling flammable fluids in the production, processing, distribution and retail sectors. It constitutes a sector-specific approach to achieving the hazardous area classification requirements for flammable fluids. The scope of EI 15 excludes hazardous area classification arising from dusts.

2.3 Scientific Knowledge: Literature Systematic Review

The bibliographic research was built upon the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) systematic review. It consists of an overview of existing evidence pertinent to a clearly formulated research question, which uses pre-specified and standardized methods to: i) identify and critically appraise relevant research; ii) to collect, report, and analyse data from the studies that are included in the review.

PRISMA method is based on a checklist of 27 items and a flow diagram with 4 stages, which will guide the user along the screening of a database of scientific articles. The 27 items checklist are grouped in 7 sections: title, abstract, introduction, methods, results, discussion and funding. (Moher D. et al., 2009)

The main search resources were the reference databases available from FEUP Library (Academic Search Complete, Scopus and Web of Science). For the research were used the key words "**atex**", "**directive**", "**explosive**", "**atmospheres**", "**hazardous**", "**area**", "**software**" and "**computational fluid dynamics**". These keywords were combined and drove the research by title.

For this specific study, the flow diagram is presented in Figure 2.1.

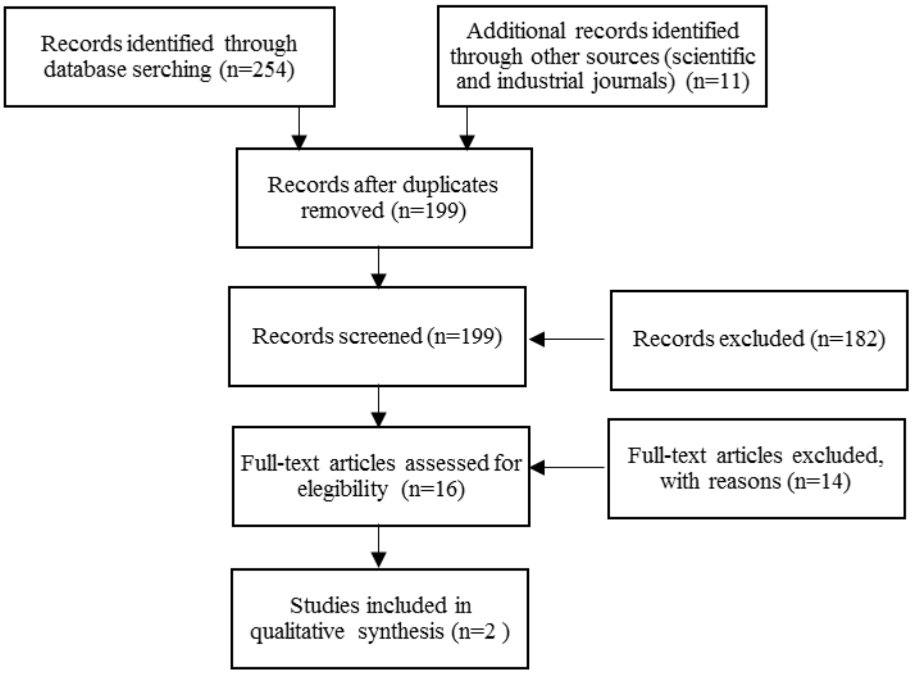


Figure 2.1 – PRISMA methodology application

Of the 265 articles found, 66 were duplicated. After removing them, the following exclusion criteria was applied:

- exclude articles published prior to 2005;
- exclude articles which weren't written in English language;
- exclude articles without access to full text;
- exclude articles related to product certification for hazardous areas.

After applying the exclusion criteria 16 articles remained for full text review. Of those articles, 14 were excluded because were out of the scope.

Table 2.1 summarizes the 2 selected articles relevant for the study.

Table 2.1 – Overview of the articles selected

Nº	1st Author	Year	Country	Article title
1	D.M. Webber	2011	UK	Ventilation theory and dispersion modelling applied to hazardous area classification. (Webber, Ivings et al. 2011)
2	J. Telmo Miranda	2013	Spain	Comparative study of the methodologies based on Standard UNE 60079/10/1 and computational fluid dynamics (CFD) to determine zonal reach of gas-generated Atex explosive atmospheres. (Telmo Miranda, Muñoz Camacho et al. 2013)

2.4 Software to Evaluate Hazardous Areas

The standard IEC/EN 60079-10-1 expressly allows the use of Computational Fluid Dynamics (CFD) to estimate the expected hazardous volume. The majority of the CFD software has commercial licence and isn't available for free download and usage.

The computational fluid dynamics simulates the movement of fluids and sometimes other associated phenomena: heat transfer, chemical reactions, etc.

The CFD packages on the market are powerful enough and easy to use as to make it profitable use at industrial level. Their main advantage is to reduce the number of necessary tests and experimental development time.

For this purpose, the solutions available in the market are discussed in the following paragraphs.

ALOHA®

During the research in governmental environment agencies a free licence of a CDF software was found: "ALOHA® - Areal Locations of Hazardous Atmospheres" 5.4.6, developed by the Office of Emergency Management of EPA (Environmental Protection Agency) and Emergency Response Division of NOAA (National Oceanic and Atmospheric Administration). It is available for download on the website of the United States Environmental Protection Agency.

ALOHA® is a computer program designed to model chemical releases for emergency responders and planners. It can estimate how a toxic cloud might disperse after a chemical release - as well as several fires and explosions scenarios (see Figure 2.2). It contains its own chemical library with physical properties for approximately 1000 common hazardous chemicals so that users do not have to enter that data. (Jones R. et al., 2013)

Includes latitudes, longitudes, altitudes, and time zone data for many cities in the USA. These data are used to compute solar radiation and local ambient pressure. The only available and possible locations are in USA.

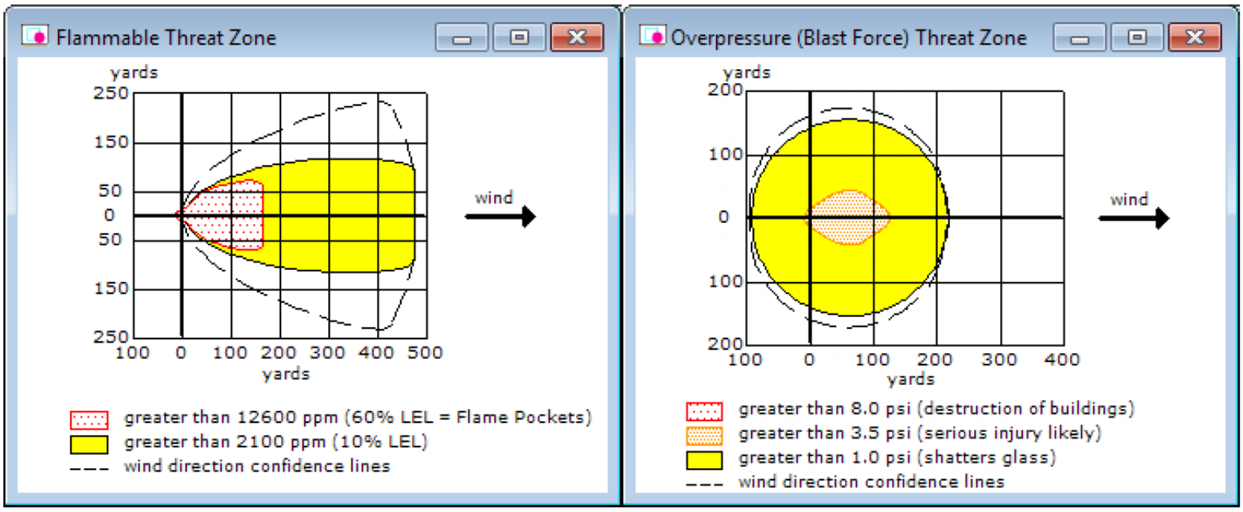


Figure 2.2 – Example of cloud dispersion in the program ALOHA.

A series of dialog boxes prompt users to enter information about the scenario (e.g., chemical, weather conditions, and the type of release). The scenario information and calculation results are summarized in a printable, text-only window. Once ALOHA's calculations are complete, users can choose to display a variety of graphical outputs.

Other forms of assessment, e.g. computational fluid dynamics (CFD), may be used and may provide a good basis for assessment in some situations. Computer modelling is also an appropriate tool when assessing the interaction of multiple factors.

In all cases, the assessment method and tools used should be validated as suitable or used with appropriate caution. Those carrying out the assessment should also understand the limitations or requirements of any tools and adjust the input conditions or results accordingly to ensure appropriate conclusions.

PHAST™

The PHAST™ (Process Hazard Analysis Software Tool) software is developed and commercialised by DNV GL, a company that provides classification and technical assurance along with software and independent expert advisory services to maritime, oil & gas and energy industries. In the software area it provides solutions for critical activities including design and engineering, risk assessment, asset integrity and optimization, QHSE, and ship management.

PHAST™ is used to analyse situations that present potential hazards to life, property and the environment and to quantify their severity. Examines the progress of a potential incident from the initial release to far-field dispersion including modelling of pool spreading and evaporation, and flammable and toxic effects. Includes DNV GL's Unified Dispersion Model for: Jet, heavy and passive dispersion phases, buoyancy, interaction with substrate, plume lift-off, capping at the mixing/inversion layer and droplet formation and rainout.

It's a commercial software without availability of trial version.

HACTool™

BakerRisk company (Head Office in Texas, USA) has developed a proprietary Hazardous Area Classification software, the HACTool™. Although the information available on this tool is very limited, it's possible to know that it calculates boundary distances and displays the contours in both 2-dimensional and 3-dimensional drawings which can allow the user to more easily determine if electrically classified equipment is needed at various elevations.

Further information is only available under commercial contact with the company BakerRisk.

ProgEx4 and ProgExDust4

ProgEx4 and ProgExDust4 are applications for classification of hazardous areas due to the presence of gas and dust, respectively. They're developed and commercialized by the *Comitato Elettrotecnico Italiano (CEI).*

The classification has its bases on the standards:

- ProgEx4 – CEI EN 60079-10-1:2010 and CEI 31-35 (2012);

- ProgExDust4 – CEI EN 60079-10-2:2010 and CEI 31-56 (2007).

ProgEx4 allows the management of multiple emission sources simultaneously and automatically generates a technical report.

ProgExDust4 considers one source of release at each simulation, if the system has multiple sources of release the calculations should be carried out for each one of them and the overall classification is given by the sum of all the results. At the end of the classification of each source of release, ProgExDust4 prepares a classification report in .rtf format, which is easily edited in a common text processing program.

Both include databases of explosive substances and several types of sources of release.

2.5 Conclusions

Computational fluid dynamics may be used and may provide a good basis for assessment in some situations. Computer modelling is also an appropriate tool when assessing the interaction of multiple factors.

In all cases, the assessment method and tools used should be validated as suitable or used with appropriate caution. Those carrying out the assessment should also understand the limitations or requirements of any tools and adjust the input conditions or results accordingly to ensure appropriate conclusions.

PART 2

3 EXPLOSION RISK AND AREA CLASSIFICATION

3.1 Introduction

As the requirement from ATEX Directives,

> *"It is the duty of Member states to protect, on their territory, the safety and health of persons and, where appropriate, domestic animals and property and, in particular, that of workers, especially against the hazards resulting from the use of equipment and systems providing protection against potentially explosive atmospheres."*
>
> *"In view of the nature of the risks involved in the use of equipment in potentially explosive atmospheres it is necessary to establish procedures applying to the assessment of compliance with the basic requirements of the Directives."*
>
> (Citation from: Directive 2014/34/EU, 2014)

ATEX (explosive atmosphere) risk assessment is designed for the workplace safety and is required where any equipment or protective systems are intended for use in potentially explosive atmospheres.

3.2 Definition of Explosion

An explosion is a violent chemical oxidation reaction which generates the combustion of a substance, called a fuel, in the presence of an oxidising agent. The phenomenon is accompanied by a rapid increase of temperature and pressure and by the presence of flames. Supersonic explosions created by high explosives are known as detonations and travel via supersonic shock waves. Subsonic explosions are created by low explosives through a slower burning process known as deflagration (Jespen 2016). In resume:

- Deflagration: subsonic, typically 1 m/s and 7 to 10 bar starting at ambient pressure.
- Detonation:
    - Supersonic.
    - High pressure shock front ahead of the reaction zone (i.e. flame).
    - Adiabatic compression – gas auto ignites.
    - Average pressure 15 to 19 bar, 25 to 30 bar.
    - Typical peak pressure up to 50 bar.
    - Typical velocity 1500 to 3500 m/s.
    - Flame temperature 1600 K to 2300 K.

Nonetheless, the phenomenon of explosion is different from the fire: the fire is a combustion that is spread in an uncontrolled way in time and in space, while the explosion combustion propagation is very rapid with violent release of energy and can only take place in the presence of dust or gas. In order for an explosion to occur, the explosive atmosphere must be in the presence of an effective source of ignition capable of triggering the reaction. This is represented graphically by the fire tetrahedron (Figure 3.1), where its sides indicate the three necessary conditions to cause an explosive reaction. The ignition source must be able to provide the explosive mixture, for a given concentration of the substance in the air, an amount of energy sufficient for the combustion to exceed the critical point beyond which it is capable of self-sustaining, allowing the front of flame to propagate itself without supplying more energy.

Some examples of ignition source are: electrical sparks, spontaneous combustion, friction, impact, hot surfaces, electrostatic discharge, open flames, lightning, chemical reactions and electromagnetic waves.

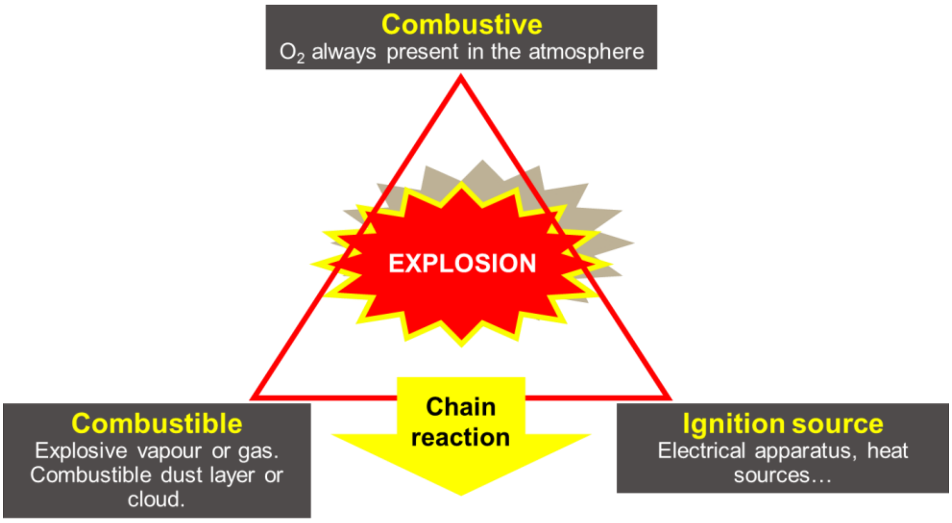


Figure 3.1 – Fire tetrahedron

Once a fire has started, the resulting exothermic chain reaction sustains the fire and allows it to continue unless, at least one of the elements of the fire is supressed.

The consequences of an explosion in a workplace vary and several injury scenarios occur depending on whether they were primarily caused by gas releases, vapour, mist, spray or by combustible dusts, which have different characteristics of explosion, despite the having similar properties in terms of parameters of ignition and combustion.

The hazardousness of mixture with air depends on its concentration of flammable substance but also on the own characteristics of the substance.

Regardless of the differences in behaviour of the various types of substances, the analysis of industrial explosions usually includes the characterization of dangerous substances through quantitative parameters, which allows to classify every aspect related to the stability or reactivity of the substance.

3.3 Fundamental Physical Parameters

Following is a summary of critical parameters used to quantify the risk of explosion in substances/mixtures in form of liquid, vapour, mist, spray or combustible dust.

Explosion Limits

The explosion limits represent the boundaries of the explosion range in which the concentration of the flammable substance in the air can lead to an explosion (deflagration or detonation). The Lower Explosion Limit (LEL) and Upper Explosion Limit (UEL) are defined as follows:

- **LEL**: concentration of flammable substance in air **below which** the atmosphere does not explode;
- **UEL**: concentration of a flammable substance in air **above which** the atmosphere does not explode.

The values of explosion limits for gases and vapours are usually expressed in term of volume-percent [v%] and for dust are usually expressed in mass per volume (such as grams per cubic meter [g/m^3]). Figure 3.2 shows an illustrative example for a gas or vapour.

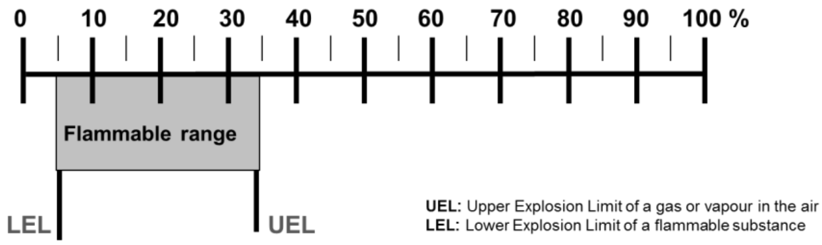


Figure 3.2 – Flammable range: illustrative example.

The explosion limits are measured in mixture with air. These limits are influenced by the test apparatus and determination procedure. For the majority of gas:

- Increasing the concentration of oxygen greatly expands the UEL, and therefore the range of explosion, while it has little influence on the LEL;
- An increase in temperature tends to increase the range of explosion with higher UEL;

The substances with wider flammable range present higher risk than those with smaller flammable range: on a continuous release to the atmosphere, the flammable mixture time span is proportional to the flammable range of the substance. (Jespen T., 2016)

Auto-Ignition Temperature (AIT)

Auto-ignition temperature is the temperature at which a material self-ignites without any obvious sources of ignition, such as a spark or flame.

The evaluation of auto-ignition hazards and safety concerns for a safe operation of any processes requires a comprehensive knowledge of the lowest temperature at which spontaneous ignitions can take place. The auto-ignition temperature data (AITs) found in the literature are usually determined by applying standardized test methods (according to IEC 60079-20-1:2010 - “Material characteristics for gas and vapour classification - Test methods and data”) that are based on small vessels and are performed at atmospheric pressure. However, AITs are not fixed data and largely depend on the equivalence ratio, the pressure as well as the volume since convective transport can influence the tests. Therefore, the AIT values measured at atmospheric pressure and lab scale are often not applicable in industrial environments.

The auto-ignition of a gas mixture is a complex phenomenon that is influenced by many factors, which can be classified into three categories: i) “intrinsic parameters” that are linked to the gas mixture itself (nature and concentration of the reagents, pressure, presence of additives, nature of the oxidizer...), ii) “extrinsic parameters” which are dependent on the test apparatus (volume of the vessel, nature of the wall, flow motion...), and iii) parameters related to the method of detection of the ignition (auto-ignition criterion).

An increase in pressure generally lowers the auto-ignition temperature of a gas mixture. It's also important to remark that while many processes in the chemical industry are conducted at high pressures, experimental data are mainly obtained under atmospheric conditions.

This parameter is crucial for the identification of the maximum surface temperature of the appliances (electric and non-electric) placed and designed to operate in potentially explosive atmospheres.

Minimum Ignition Energy (MIE)

Minimum energy that must be supplied to the mixture, in form of a flame or a spark, to cause the ignition. A source of ignition with an energy equal to MIE is said to be effective.

The MIE in the case of vapours and mists, is dependent on the conditions of temperature and pressure of the mixture. In general, this parameter is proportional to the pressure. For the combustible dust, the MIE is correlated to the particle size; the finest tends to have lower ignition energies than thicker dust. This parameter also tends to decrease with:

- the rise of the temperature of the mixture;
- increasing the percentage of oxygen;
- the reduction of moisture in the dust.

Flash Point Temperature

Flammable and combustible liquids are liquids that can burn and are grouped, as either flammable or combustible by their flashpoints. Generally speaking, flammable liquids will ignite (catch on fire) and burn easily at normal working temperatures. Combustible liquids have the ability to burn at temperatures that are usually above working temperatures.

The flash point is therefore the minimum temperature at which, in the test conditions specified, a liquid releases a sufficient amount of combustible gas or vapour capable of igniting at the moment of the application of an effective ignition source.

In general, the flash point temperature corresponds to the lower limit temperature defined as the temperature at which the liquid will vaporize, in saturation regime, with a concentration of steam corresponding to the LEL.

Maximum Experimental Safe Gap (MESG)

The maximum experimental safe gap for the gas or vapour is determined by adjusting the gap in small steps to find the maximum value of gap which prevents ignition of the external mixture, for any concentration of the gas or vapour in air. It's measured according to IEC 60079-20-1:2010 - "Material characteristics for gas and vapour classification - Test methods and data".

The interior and exterior chambers of the test apparatus (Figure 3.3) are filled with a known mixture of the gas or vapour in air, under normal conditions of temperature and pressure (20 °C, 100 kPa) and with the circumferential gap between the two chambers accurately adjusted to the desired value. The internal mixture is ignited and the flame propagation, if any, is observed through the windows in the external chamber.

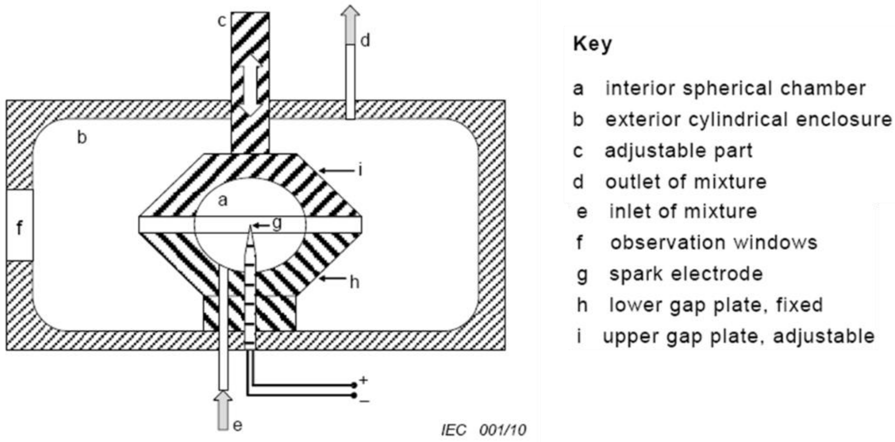


Figure 3.3 – Test apparatus to determine the MESG (source IEC 60079-20-1:2010).

Gases and vapours may be classified according to their maximum experimental safe gaps into the groups I, IIA, IIB and IIC.

The groups for equipment for explosive gas atmospheres are:

- Group I: equipment for mines susceptible to firedamp.
- Group II: equipment for places with an explosive gas atmosphere other than mines susceptible to firedamp.

Group II equipment is subdivided and, for the purpose of classification of gases and vapours, the MESG limits are:

- Group IIA: MESG $\geq$ 0.9 mm.
- Group IIB: 0.5 mm < MESG < 0.9 mm.
- Group IIC: MESG $\leq$ 0.5 mm.

Figure 3.4 resumes the classification of gases and vapours according to the MESG.

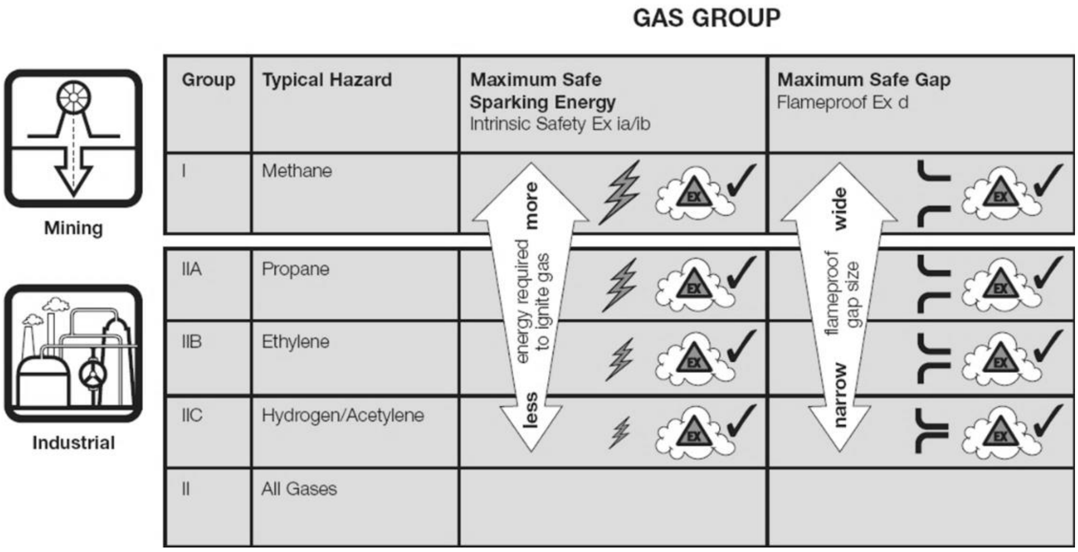


Figure 3.4 – Classification of gas and vapours according to MESG. Source: http://www.wolf-safety.co.uk/atex-explained. Las access on 24/08/2016.

3.4 Equipment Groups and Categories

The ATEX Directive 2014/34/EU (which replaces the ATEX Directive 94/9/EC) defines the minimum technical requirements and conformity assessment procedures for equipment intended for use in potentially explosive atmospheres workplace. Although the ATEX risk assessment is generally applied for a workplace risk assessment, here it is also applied where the industries produce ATEX equipment and prepare for the ATEX Equipment End-user market.

This directive gives the criteria to determine the classification of equipment-groups into categories. This information is resumed in Tables 3.1 and 3.2.

The notion of intended use of the equipment is of prime importance for the explosion-proofing of equipment and protective systems. It is essential that manufacturers supply exhaustive information. Specific, clear marking of equipment and protective systems, stating their use in a potentially explosive atmosphere, is also necessary.

The conformity assessment procedures set out in this directive for the categories M1, 1 and 2, require the intervention of conformity assessment bodies, which are notified by the Member States to the Commission. If a conformity assessment body demonstrates conformity with the criteria laid down in harmonised standards, it's presumed to comply with the corresponding requirements set out in this directive.

Table 3.1 – Equipment Category for Group I. Adapted from Directive 2014/34/EU.

Group I Equipment intended for use in mines or on those parts of surface installations of such mines endangered by firedamp and/or combustible dust		
Level of protection	Very high level of protection. Additional special means of protection to be capable of functioning in conformity with the operational parameters established by the manufacturer.	High level of protection. The equipment assures the requisite level of protection during normal operation and also in the case of more severe operating conditions, in particular those arising from rough handling and changing environmental conditions.
Level of safety	Remain functional, even in the event of rare incidents relating to equipment with an explosive atmosphere present.	Intended to be de-energized in the event of an explosive atmosphere
Equipment category	M1	M2

Besides the certification of the equipment, the manufacturers are also obliged to maintain the quality assurance of the production process. The quality system shall ensure that the products are in conformity with the type described in the EU-type examination certificate of the equipment and comply with the requirements of this directive that apply to them.

The notified body shall assess the quality system to determine whether it satisfies the requirements of this directive. It shall presume conformity with those requirements in respect of the elements of the quality system that comply with the corresponding specifications of the harmonised standard ISO/IEC 80079-34: 2011. This part of ISO/IEC 80079 specifies particular requirements and information for establishing and maintaining a quality system to manufacture Ex equipment including protective systems in accordance with the Ex certificate. It does not preclude the use of other quality systems that are compatible with the objectives of ISO 9001 and which provide equivalent results.

Table 3.2 – Equipment Category for Group II. Adapted from Directive 2014/34/EU.

Group II Equipment intended for use in surface industry						
Zone	0	20	1	21	2	22
Type of explosive atmosphere	G Gas	D Dust	G Gas	D Dust	G Gas	D Dust
Likelihood of an explosive atmosphere	Always present		Occasionally present		Infrequently and only for a short period	
Level of protection	Very high		High		Normal	
Level of safety	Remain functional even in the event of rare incidents relating to equipment. Is characterized by additional means of protection.		Remain functional even in the event of frequently occurring disturbances or equipment faults.		Ensures the requisite level of protection only during normal operation	
Equipment category	**1**		**2**		**3**	

3.5 Area Classification

Area classification is a method of analysing and classifying the environment where explosive atmospheres may occur, so as to facilitate the proper selection, installation and operation of equipment to be used safely in that environment.

The ATEX Directive 1999/92/EC classifies the hazardous places in terms of zones on the basis of the frequency and duration of the occurrence of an explosive atmosphere:

- **Zone 0** - A place in which an explosive atmosphere consisting of a mixture with air of flammable substances in the form of gas, vapour or mist is present continuously or for long periods or frequently.
- **Zone 1** - A place in which an explosive atmosphere consisting of a mixture with air or flammable substances in the form of gas, vapour or mist is likely to occur occasionally in normal operation.
- **Zone 2** - A place in which an explosive atmosphere consisting of a mixture with air of flammable substances in the form of gas, vapour or mist is not likely to occur in normal operation but, if it does occur, will persist for a short period only.
- **Zone 20** - A place in which an explosive atmosphere in the form of a cloud of combustible dust in air is present continuously, or for long periods or frequently.
- **Zone 21** - A place in which an explosive atmosphere in the form of a cloud of combustible dust in air is likely to occur occasionally in normal operation.
- **Zone 22** - A place in which an explosive atmosphere in the form of a cloud of combustible dust in air is not likely to occur in normal operation but, if it does occur, will persist for a short period only.

This directive defines "Normal operation" as the situation when installations are used within their design parameters.

The employer is obliged to classify places where explosive atmospheres may occur into zones and ensure the minimum requirements for improving the safety and health protection of the workers potentially at risk from explosive atmospheres.

The classified zones must be marked with signs at their points of entry as illustrated in Figure 3.5.

Figure 3.5 – Warning sign for places where explosive atmospheres may occur. Adapted from Directive 1999/92/EC.

3.5.1 Criteria for the Selection of Equipment and Protective Systems

If the explosion protection document based on a risk assessment does not state otherwise, equipment and protective systems for all places in which explosive atmospheres may occur must be selected according to the categories set out in Directive 2014/34/EU.

In particular, the following categories of equipment must be used in the zones indicated, provided they are suitable for gases, vapours or mists and/or dusts as appropriate:

- in zone 0 or zone 20, category 1 equipment marked as II1G or II1D;
- in zone 1 or zone 21, category 1 or 2 equipment marked as II1G, II1D, II2G or II2D;
- in zone 2 or zone 22, category 1, 2 or 3 equipment marked as II1G, II1D, II2G, II2D, II3G or II3D.

4 HALOC GAS PROTOTYPE

This chapter presentes a brief review of suitable development frameworks, as well as available standards to guide the application prototype development.

The application prototype developed is an auxiliary tool for the professional and doesn’t intend to replace him at any moment. As any other application, the results obtained from it must be analysed and judged with fully knowledge of the context, and the decisions are responsibility of the user.

4.1 Study Goals

The main purpose of this thesis was to develop an application prototype to help support the decision of area classification where explosive gas atmosphere may occur and to characterize it in accordance with the methodologies of the selected standard. The main advantages of this application are:

- reduce the human error by automate the repetitive tasks;
- perform the calculations in accordance with the standard;
- allow the storage of flammable substances parameters;
- save all the critical data for the simulations.

4.2 Applicable Standards

The theory of hazardous area classification has been independently developed by different organizations till nowadays which led to standards and industrial codes with singular characteristics.

The main international organizations issuing standards for explosive atmospheres are: IEC – International Electrotechnical Commission, API – American Petroleum Institute and NFPA – National Fire Protection Association. As for the industrial codes, the emphasis goes to CEI – Comitato elettrotecnico italiano (Italy) and EI – Energy Institute (United Kingdom).

IEC – International Electrotechnical Commission

IEC is a non-governmental international organization responsible for issuing standards for all electrical and electronic technologies. IEC standards cover a vast range of technologies from power generation, transmission and distribution to home appliances and office equipment, semiconductors, fibre optics, batteries, solar energy, nanotechnology and marine energy as well as many others. The IEC also manages three global conformity assessment systems that certify whether equipment, system or components conform to its International Standards.

The IEC held its inaugural meeting on 26 June 1906. Currently, 82 countries are members while another 82 participate in the Affiliate Country Programme, which is not a form of membership but is designed to help industrializing countries get involved with the IEC. Originally located in London, the commission moved to its current headquarters in Geneva in 1948. It has regional centres in Asia-Pacific (Singapore), Latin America (São Paulo, Brazil) and North America (Boston, United States).

Today, the IEC is the world's leading international organization in its field, and its standards are adopted as national standards by its members. The work is done by some 10,000 electrical and electronics experts from industry, government, academia, test labs and others with an interest in the subject.

CEN, CENELEC and ETSI

The European Committee for Standardization (CEN, French: Comité Européen de Normalisation) is a public standards organization whose mission is to foster the economy of the European Union (EU) in global trading, the welfare of European citizens and the environment by providing an efficient infrastructure to interested parties for the development, maintenance and distribution of coherent sets of standards and specifications.

The CEN was founded in 1961. Its 33 national members work together to develop European Standards (EN) in various sectors to build a European internal market for goods and services and to position Europe in the global economy. CEN is officially recognised as a European standards body by the European Union; the other official European standards bodies are the European Committee for Electrotechnical Standardization (CENELEC) and the European Telecommunications Standards Institute (ETSI).

The standardisation bodies of the thirty national members represent the 27 member states of the European Union, three countries of the European Free Trade Association (EFTA) and countries which are likely to join the EU or EFTA in the future. CEN is contributing to the objectives of the European Union and European Economic Area with technical standards (EN standards) which promote free trade, the safety of workers and consumers, interoperability of networks, environmental protection, exploitation of research and development programmes, and public procurement.

CEN and CENELEC closely cooperate with their international counterparts, respectively the International Organization for Standardization (ISO) and the International Electrotechnical Commission (IEC). This close cooperation has been materialised by the signature of the Vienna Agreement (ISO-CEN) and the Dresden Agreement (IEC-CENELEC). The main objectives of these agreements are to provide a: (i) Framework for the optimal use of resources and expertise available for standardization work; (ii) Mechanism for information exchange between international and European Standardization Organizations (ESOs) to increase the transparency of ongoing work at international and European levels. These two cooperation agreements led to the adoption of many International Standards as regional standards.

The adoption of an International Standard is defined as:

"The publication of a regional or national normative document based on a relevant International Standard, or endorsement of the International Standard as having the same status as a national normative document, with any deviations from the International Standard identified." (from ISO/IEC Guide 21-1)

CEN/CENELEC Guide 12 - "The concept of Affiliation with CEN and CENELEC provides rights and obligations of affiliates" defines the rules for European Standards implementation as national standards. Each national member shall have a national designation for its national implementation of the European Standard.

Portugal, being an affiliate country of CEN/CENELEC, has the obligation to implement European standards, in its own language or in one of the official languages, as national standards in accordance with the “CEN/CENELEC Internal Regulations – Part 2”, and to withdraw conflicting national standards.

API – American Petroleum Institute

The American Petroleum Institute (API) is the largest United States trade association for the oil and natural gas industry. It represents about 650 corporations involved in production, refining, distribution, and many other aspects of the petroleum industry.

Its mission is to influence public policy in support of a strong and viable United States oil and natural gas industry. Its chief functions on behalf of the industry include advocacy, negotiation and lobbying with governmental, legal, and regulatory agencies; research into economic, toxicological, and environmental effects; establishment and certification of industry standards; and education outreach. API both funds and conducts research related to many aspects of the petroleum industry.

API RP 500 and RP 505 classify the locations for electrical equipment in hazardous areas.

NFPA - National Fire Protection Association

The National Fire Protection Association (NFPA) is a United States trade association, though with some international members, that creates and maintains private, copyrighted, standards and codes for usage and adoption by local governments. It was formed in 1896 by a group of insurance firms with the stated purpose of standardizing the new and growing market of fire sprinkler systems.

NFPA defines its mission as follows: "We help save lives and reduce loss with information, knowledge and passion."

NFPA is responsible for 380 codes and standards that are designed to minimize the risk and effects of fire by establishing criteria for building, processing, design, service, and installation in the United States, as well as many other countries. Its more than 200 technical code and standard development committees have over 6000 volunteer seats. Volunteers vote on proposals and revisions in a process that is accredited by the American National Standards Institute (ANSI).

NFPA 70 – National Electric Code (NEC) is a regionally adoptable standard for the safe installation of electrical wiring and equipment in the United States. Despite the use of the term "national", it is not a federal law. It is typically adopted by states and municipalities in an effort to standardize their enforcement of safe electrical practices. NEC 500 and NEC 505 classify the locations for electrical equipment in hazardous areas.

CEI – Comitato Elettrotecnico Italiano

Italian Electrotechnical Committee (acronym CEI) is a private association, responsible at national level for technical standardisation in the electrotechnical, electronic and telecommunications fields. It participates as a member, with a mandate by the Italian State, on the activities of the corresponding European standardisation organisation CENELEC and international IEC.

Founded in 1909 and formally recognized by the Italian Government and by the European Union, CEI proposes, elaborates, publishes and disseminates technical standards that, according to the Italian Law 186/1968, provide the presumption of conformity to the "state of the art" of electrical products, systems, installations and processes.

CEI standardisation documents define the best practices, i.e. the set of normative requirements enabling the design and construction of electric and electronic components, equipment, machines and systems, as well as installations, on the basis of well-defined safety principles and performance criteria, evolving in parallel with technological progress.

The standardisation activity is carried out by the experts nominated by the CEI membership, within Technical Committees and Subcommittees that are in charge of the development of normative documents in the different sectors.

Beside the preparation of normative documents, CEI produces other publications such as books, application software, informative documents in order to support the correct interpretation and application of technical standards to favour an effective disclosure of the technical culture of operators in the electrical/electronic sectors.

In the special case of ATEX applications, CEI has developed dedicated guidelines: CEI 31-35: “Atmosfere esplosive Guida alla classificazione dei luoghi con pericolo di esplosione per la presenza di gas in applicazione della Norma CEI EN 60079-10-1” and CEI 31-56: “Atmosfere esplosive Guida alla classificazione dei luoghi con pericolo di esplosione per la presenza di polveri combustibili in applicazione della Norma CEI EN 60079-10-2”. These standards and guidelines provide procedures to evaluate the likelihood to have explosive atmosphere in the workplace.

EI – Energy Institute

The Energy Institute (EI) is the professional body for the energy industry in the United Kingdom (UK). Is the leading chartered professional membership body for the energy industry, supporting over 19000 individuals working in or studying energy and 250 companies worldwide. The EI provides learning and networking opportunities to support professional development, as well as professional recognition and technical and scientific knowledge resources on energy in all its forms and applications.

It was formed in 2003 from a merger between the Institute of Petroleum and the Institute of Energy. The formation of the EI reflects the increasing convergence of various sectors of the UK energy industry.

The EI produces an extensive range of technical guidance, standards, and research reports for the energy sector.

The EI’s Area Classification Working Group is responsible for the development of technical content contained in Model code of safe practice Part 15: Area classification code for installations handling flammable fluids (EI 15, formerly referred to as IP 15). EI 15 is a well-established, internationally accepted publication that provides methodologies for hazardous area classification around equipment storing or handling flammable fluids in the production, processing, distribution and retail sectors. It constitutes a sector-specific approach to achieving the hazardous area classification requirements for flammable fluids required in the UK by the Dangerous Substances and Explosive Atmospheres Regulations (DSEAR) 2002 and in doing so, provides much more detail than BS EN 60079-10 – Electrical apparatus for explosive gas atmospheres: Classification of hazardous areas. The scope of EI 15 excludes hazardous area classification arising from dusts.

4.3 Selected Standards

The concept of a globalized single market is one of the great achievements of the European Union (EU). To make it happen, conducive conditions needed to be created such that the goods, services, capital and labour would circulate freely.

The standardization development in EU brought original and innovative instruments to remove the barriers to free circulation of goods and amongst them the New Approach to product regulation and the Global Approach (IECEx Scheme) to conformity assessment in the field of hazardous area.

The common thread amongst these complementary approaches is that they limit public intervention to what is essential and leave business and industry the greatest possible choice on how to meet their public obligations.

Progressive globalization obviously also includes industries such as large-scale chemicals, pharmaceuticals, petroleum, and gas extraction and processing, and many other industries directly or indirectly involved with hazardous areas. Hence, in the long term, it will be unacceptable for globally active companies to have to conform to different safety standards in different areas of the world. The development of internationally valid Explosion-Protection Directives and Standards will therefore continue to accelerate.

Adding to the previous, the fact that this study was developed in a EU country member, the obvious choice of standards relays on the IEC/EN harmonized standards.

The industrial codes issued by Energy Institute and Italian Electrotechnical Committee are very useful in the hazardous area classification process, especially where similar processes can be found in similar industries. But the main goal of this study is to be applicable to any industry, so the choice of not using those industrial codes had to do with the universal nature of the application.

It’s also important to be aware that the hazardous area classification varies when it comes to compare the IEC/EN standards with the North American (including Canada) NEC/API standards. In the Table 4.1. it’s stated a summary of the major differences between them.

Finally, the expense of the standards is also an important matter when the studies are developed on an academic environment. Thus the access to the IEC/EN standards is facilitated.

Table 4.1 – Discrepancy in the classification of hazardous areas depending on the choosen satndards

Standard		Flammable Material	Present Continuously	Present Intermittently	Present Abnormally
IEC / CENELEC	IEC / EN 60079-10-1	Gas / Vapour	Zone 0	Zone 1	Zone 2
	IEC / EN 60079-10-2	Combustible Dust or Ignitable Fibers	Zone 20	Zone 21	Zone 22
ATEX	Directive 99/92/EC	Gas / Vapour	Zone 0	Zone 1	Zone 2
		Combustible Dust or Ignitable Fibers	Zone 20	Zone 21	Zone 22
NEC 501	ANSI/NFPA 70 National Electrical Code Article 501	Gas / Vapour	Class I, Division 1	Class I, Division 1	Class I, Division 2
NEC 505	ANSI/NFPA 70 National Electrical Code Article 505	Gas / Vapour	Class I, Zone 0	Class I, Zone 1	Class I, Zone 2
NEC 502	ANSI/NFPA 70 National Electrical Code Article 502	Combustible Dust or Ignitable Fibers	Class II, Division 1	Class II, Division 1	Class II, Division 2
NEC 506	ANSI/NFPA 70 National Electrical Code Article 506	Combustible Dust or Ignitable Fibers	Zone 20	Zone 21	Zone 22

4.4 Frameworks Survey

The choice of technology for the development of an application implies several choices: the learning curve of the programming language, cost, reliability, stability and maturity of the of the software for development.

Regarding the available technologies, it was necessary to establish a reasonable compromise that would allow the selection of the most adequate software for the development of the application prototype.

The research of technologies was built on the following premises: (i) the application prototype should be able to perform numerous mathematical operations; (ii) the user interface should be simple and intuitive; iii) fast learning curve due to available time constraints; iv) easy deployment.

WOLFRAM Mathematica

Wolfram Mathematica (usually referred to as Mathematica) is a symbolic mathematical computation program, used in many scientific, engineering, mathematical, and computing fields. It is developed by Wolfram Research of Champaign, Illinois. The Wolfram Language is the programming language used in Mathematica.

Mathematica has a protocol which allows communication with other applications using the programming languages C, Java, .NET, Haskell, AppleScript, Racket, Visual Basic, Python and Clojure. It also allows the communication with SQL databases through a built-in support.

Data connecters are available to many mathematical software packages including OpenOffice.org Calc, Microsoft Excel, MATLAB, Sage, SINGULAR, Wolfram SystemModeler, and Origin. Mathematical equations can be exchanged with other computational or typesetting software via MathML.

SageMath

SageMath (System for Algebra and Geometry Experimentation) is a mathematical software with features covering many aspects of mathematics, including algebra, combinatorics, numerical mathematics, number theory, and calculus.

The first version of SageMath was released on 24 February 2005 as free and open source software under the terms of the GNU General Public License, with the initial goals of creating an "open source alternative to Magma, Maple, Mathematica, and MATLAB". The creator and leader of the SageMath project, William Stein, is a mathematician at the University of Washington.

SageMath "uses a Python-like syntax", supporting procedural, functional and object-oriented constructs.

DataMelt

DataMelt is a free software for scientists, engineers and students. It can be used for numeric computation, statistics, symbolic calculations, data analysis and data visualization.

DataMelt has its roots in particle physics where data mining is a primary task. It was created as jHepWork project in 2005 and it was initially written for data analysis for particle physics. Later versions of jHepWork were modified for general public use (for scientists, engineers, students for educational purpose). In 2013, jHepWork was renamed to DataMelt and become a general-purpose community-supported project. The main source of reference is the book "Scientific Data analysis using Jython Scripting and Java" which discuss in depth data analysis methods using Java and Jython scripting.

DataMelt is hosted by jWork.ORG portal.

It can be used with several scripting languages for the JAVA platform: Jython (Python programming language), Groovy, JRuby (Ruby programming language) and BeanShell. All scripting languages use common DMelt JAVA API. Data analyses and statistical computations can be done in JAVA. Finally, symbolic calculations can be done using Matlab/Octave high-level interpreted language integrated with JAVA.

DataMelt runs on Windows, Linux, Mac and Android operating systems. It's a portable application. No installation is needed: simply download and unzip the package, and it's ready to run. One can run it from a hard drive, from a USB flash drive or from any media. DataMelt exists as an open-source portable application, and as JAVA libraries under a commercial friendly license.

MATLAB®

MATLAB (matrix laboratory) is a multi-paradigm numerical computing environment and fourth-generation programming language. A proprietary programming language developed by The MathWorks, Inc., MATLAB allows matrix manipulations, plotting of functions and data, implementation of algorithms, creation of user interfaces, and interfacing with programs written in other languages, including C, C++, Java, Fortran and Python. Although MATLAB Builder products can deploy MATLAB functions as library files which can be used with .NET or Java application building environment, future development will still be tied to the MATLAB language.

The MATLAB application is built around the MATLAB scripting language. Common usage of the MATLAB application involves using the Command Window as an interactive mathematical shell or executing text files containing MATLAB code.

The framework is organised as toolboxes which can be purchased separately. If an evaluation license is requested, the MathWorks sales department requires detailed information about the project for which MATLAB is to be evaluated. If granted (which it often is), the evaluation license is valid for two to four weeks. A student version of MATLAB is available as is a home-use license for MATLAB, Simulink, and a subset of Mathwork's Toolboxes at substantially reduced prices.

MATLAB has a number of competitors: commercial competitors include Mathematica, TK Solver, Maple, and IDL and the free open source alternatives are GNU Octave, Scilab, FreeMat, Julia, and Sage which are intended to be mostly compatible with the MATLAB language.

Microsoft® Excel + Visual Basic for Applications

Microsoft Excel is a software developed by Microsoft for Windows, Mac OS X, Android and iOS. It features calculation, graphing tools, pivot tables, and a macro programming language called VBA (Visual Basic for Applications). It has been widely adopted, especially since version 5 in 1993, and it has replaced Lotus 1-2-3 as the industry standard for this kind of software. Excel is part of Microsoft Office suite of applications.

VBA, allows the user to employ a wide variety of numerical methods and report the results back to the spreadsheet. It also has a variety of interactive features allowing user interfaces that can completely hide the business logic from the user, so that the spreadsheet presents itself as a so-called application, or decision support system, via a custom-designed user interface that asks the user questions and provides answers and reports.

The Windows version of Excel supports programming through Microsoft's Visual Basic for Applications (VBA), which is a dialect of Visual Basic. Programmers may write code directly using the Visual Basic Editor (VBE), which includes a window for writing code, debugging code, and code module organization environment. The user can implement numerical methods as well as automating tasks such as formatting or data saving in VBA.

4.5 Selected Framework

The choice of using a spreadsheet with Microsoft® Visual Basic for Applications programming had to do with the extensive use of that type of software among the national companies and previous experience of the author in the development of some tools with this language along with Microsoft® Office Access.

Although it has a paid licence, the extended usage of Microsoft Office applications has provided the skill to start the development immediately without spending time learning a new programming languages. In other hand, if any of the open source development frameworks were used, the learning curve of the programming language would preclude the accomplishment of the task in the expected time.

4.6 Application Requisites

For the development of the prototype application the following steps will be taken:

- Definition of typical sources of release in the industry.
- Calculation of the hazardous areas based on the IEC/EN 60079-10-1:2015 standard.
- Definition of the variables that need to be obtained from the process.
- Creation of dangerous substances database.
- Creation of the prototype application using spreadsheets and VBA.
- Testing the prototype.

4.6.1 Industrial Process Survey

In determining where a release of flammable gas or vapour may occur, the likelihood and duration of the release should be assessed in accordance with the definitions of continuous, primary and secondary grades of release. The IEC/EN 60079-10-1:2015 defines the grades of release as:

- **continuous:** release which is continuous or is expected to occur frequently or for long periods;
- **primary:** release which can be expected to occur periodically or occasionally during normal operation;
- **secondary:** release which is not expected to occur in normal operation and, if it does occur, is likely to do so only infrequently and for short periods.

Therefore, the most common sources of release found in the majority of the industries may be classified according to their grade of release. The main sources arise from the following equipment:

- **Continuous grade of release:**
  - surface of a flammable liquid in a fixed roof tank, with a permanent vent to the atmosphere;
  - surface of a flammable liquid which is open to the atmosphere continuously or for long periods (for example an oil/water separator).
- **Primary grade of release:**
  - seals of pumps, compressors or valves if release of flammable material during normal operation is expected;
  - water drainage points on vessels which contain flammable liquids, which may release flammable material into the atmosphere while draining off water during normal operation;
  - sample points which are expected to release flammable material into the atmosphere during normal operation;
  - relief valves, vents and other openings which are expected to release flammable material into the atmosphere during normal operation.
- **Secondary grade of release:**
  - seals of pumps, compressors and valves where release of flammable material during normal operation of the equipment is not expected;
  - flanges, connections and pipe fittings, where release of flammable material is not expected during normal operation;
  - sample points which are not expected to release flammable material during normal operation;
  - relief valves, vents and other openings which are not expected to release flammable materials into the atmosphere during normal operation.

The terms “normal” and its expressed or implied opposite “abnormal” require some explanation. “Normal” means actual or real applied to the conditions, as they exist in any given plant: actual standard of design used, achieved state of maintenance, expected environmental limitations, usual operations and operating practices employed, etc. In modern plants handling flammable materials, it is of course the main objective of design, maintenance and operating philosophy to ensure that there are few ways in which a flammable atmosphere can occur. This is to be achieved by proper choice of process equipment, safe removal of escaped products, provision of special ventilation arrangements, good maintenance and good production supervision and other similar precautions.

The “abnormal” condition refers to circumstances recognizable as abnormal events, which though they may occur at some time will do so infrequently. Examples would be the collapse of a pump gland, the failure of a pipe gasket, the loss of control of the manual draining operation of a tank, the fracture of a small branch pipe or the accidental spillage of small quantities of flammable liquid. They are usually the unintended, unpredictable, non-catastrophic events in a plant. They are in most instances the kinds of faults, which it is expected, will be avoided by good design and preventive maintenance; if despite this they do occur, matters will have been so arranged that they will be rapidly rectified. With conditions so well controlled these events will therefore be both infrequent and have short duration. (Bottrill G. et al., 2005)

Once the grade of release, the release rate, concentration, velocity, ventilation and other factors are assessed there is then a firm foundation to assess the likely presence of an explosive gas atmosphere in the surrounding areas and determine the type and/or extent of the hazardous zones.

This approach requires detailed consideration to be given to each item of process equipment which contains a flammable substance by itself or due to process conditions, and which could be a source of release.

4.6.2 Developed Process Outline (Building Blocks)

A three-dimensional region or space is defined as an "area". Area classification is a method of analysing and classifying the environment where explosive gas atmospheres may occur so as to facilitate the proper selection and installation of apparatus to be safely used in that environment, taking into account gas groups and temperature classes.

It may not be possible to classify areas into Zone 0, 1 or 2 by a simple examination of a plant or plant design. Hence, a systematic analysis and detailed approach is required to determine the possibility of an explosive gas atmosphere occurring.

Classification may be achieved by calculation, considering appropriate statistical and numerical assessments for the factors concerned, for each source of release. The source of release approach can be summarized as: i) identify sources of release; ii) determine the release rate and grade of release for each source based on likely frequency and duration of release; iii) assess ventilation or dilution conditions and effectiveness; iv) determine zone type based on grade of release and ventilation or dilution effectiveness; v) determine extent of zone.

The classification of hazardous areas using the standard IEC/EN 60079-10-1:2015 is a procedure involving the generic steps show in the scheme of Table 4.2.

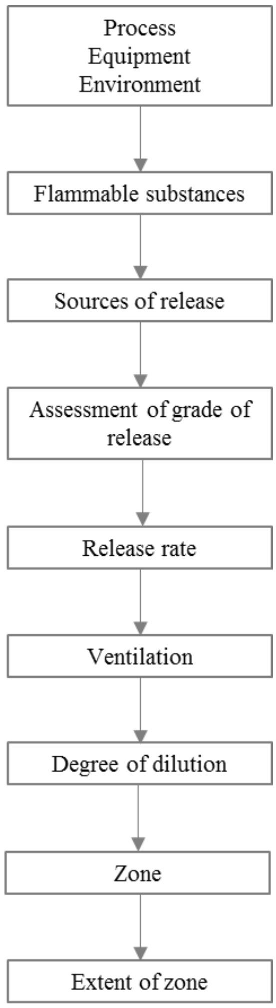
Classification by Sources of Release Method

The basic elements for establishing the hazardous zone types are the identification of the source of release and the determination of the grade of release. If it's established that the item may release flammable material into the atmosphere, it's necessary, first of all, to determine the grade of release by establishing the likely frequency and duration of the release.

The characteristic of any release depends upon the physical state of the flammable substance, its temperature and pressure. The physical states include:

- a gas, which may be at an elevated temperature or pressure;
- a gas liquefied by the application of pressure, e.g. LPG;
- a gas which can only be liquefied by refrigeration, e.g. methane;
- a liquid with an associated release of flammable vapour.

Table 4.2 – Scheme of the generic process of area classification



1) Register environmental conditions: pressure, temperature and wind.
2) Identify process and the equipment involved.
3) Identify flammable substances in the process.
4) Register process conditions of pressure and temperature.
5) Identify sources of release.
6) Assess the grade of release for each source of release.
7) Calculate the release rate for each source of release.
8) Characterize the location: indoor/outdoor, presence of physical barriers to the ventilation.
9) Calculate the degree of dilution (for indoor locations must be considered the background concentration).
10) Determine the availability of ventilation.
11) Determine the type of zone
12) Calculate the extent of zone

A release of flammable substance above its flashpoint will give rise to a flammable vapour or gas cloud which may initially be less or denser than the surrounding air or may be neutrally buoyant. The forms of release and the pattern of behaviour at various conditions are displayed as a flow chart in Figure 4.1.

Every form of release will eventually end as a gaseous or vapour release and the gas or vapour may appear as buoyant, neutrally buoyant or heavy (see Figure 4.1). These characteristics will affect the extent of the zone generated by a particular form of release.

The horizontal extent of the zone at ground level will generally increase with increasing relative density and the vertical extent above the source will generally increase with decreasing relative density.

In Figures 4.2, 4.3 and 4.4, are shown detailed schematic approaches of the classification procedure whether the release is respectively continuous, primary or secondary.

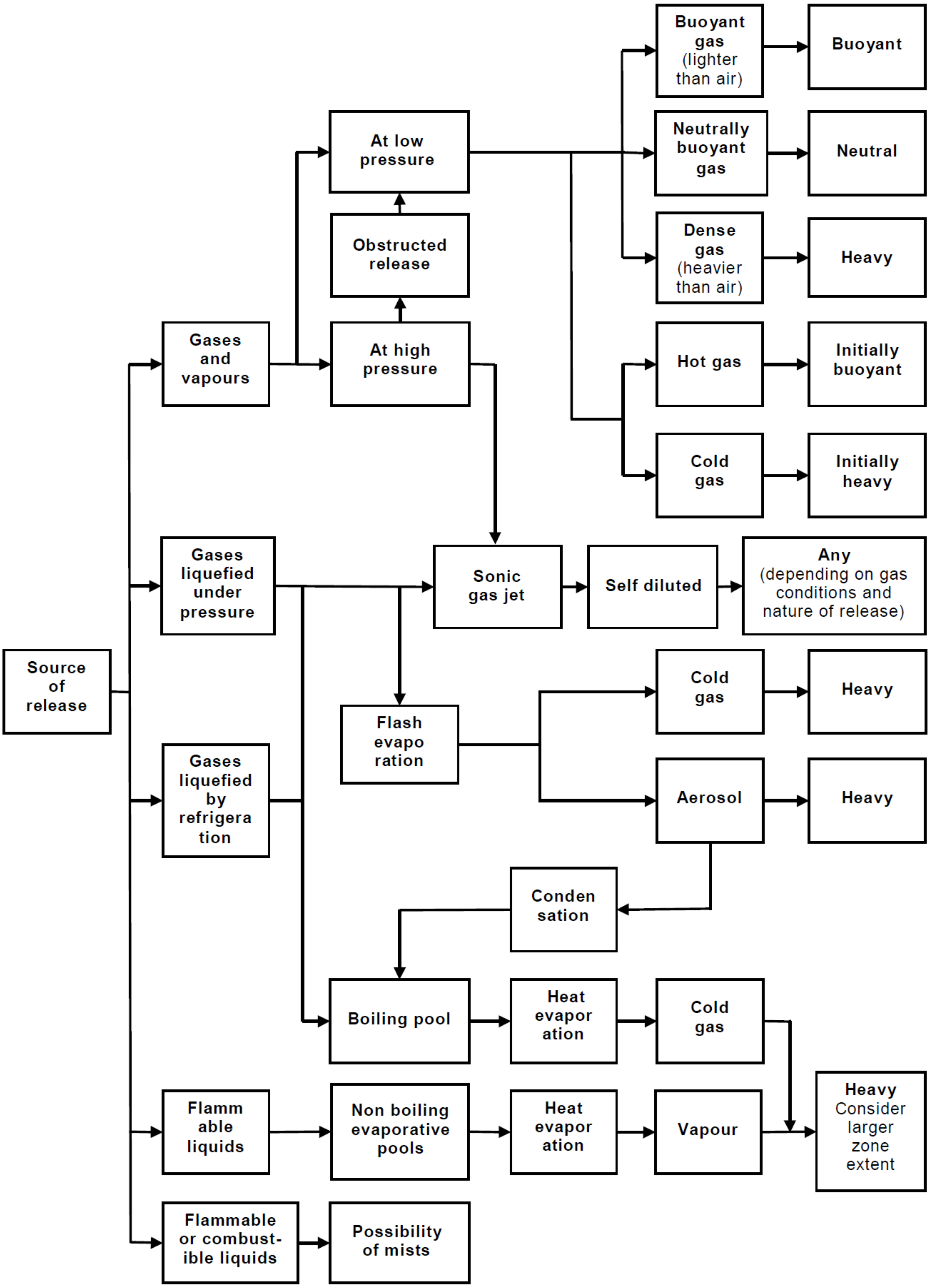


Figure 4.1 – Schematic flow illustrating the general nature of different forms of release. Adapted from IEC/EN 60079-10-1:2015.

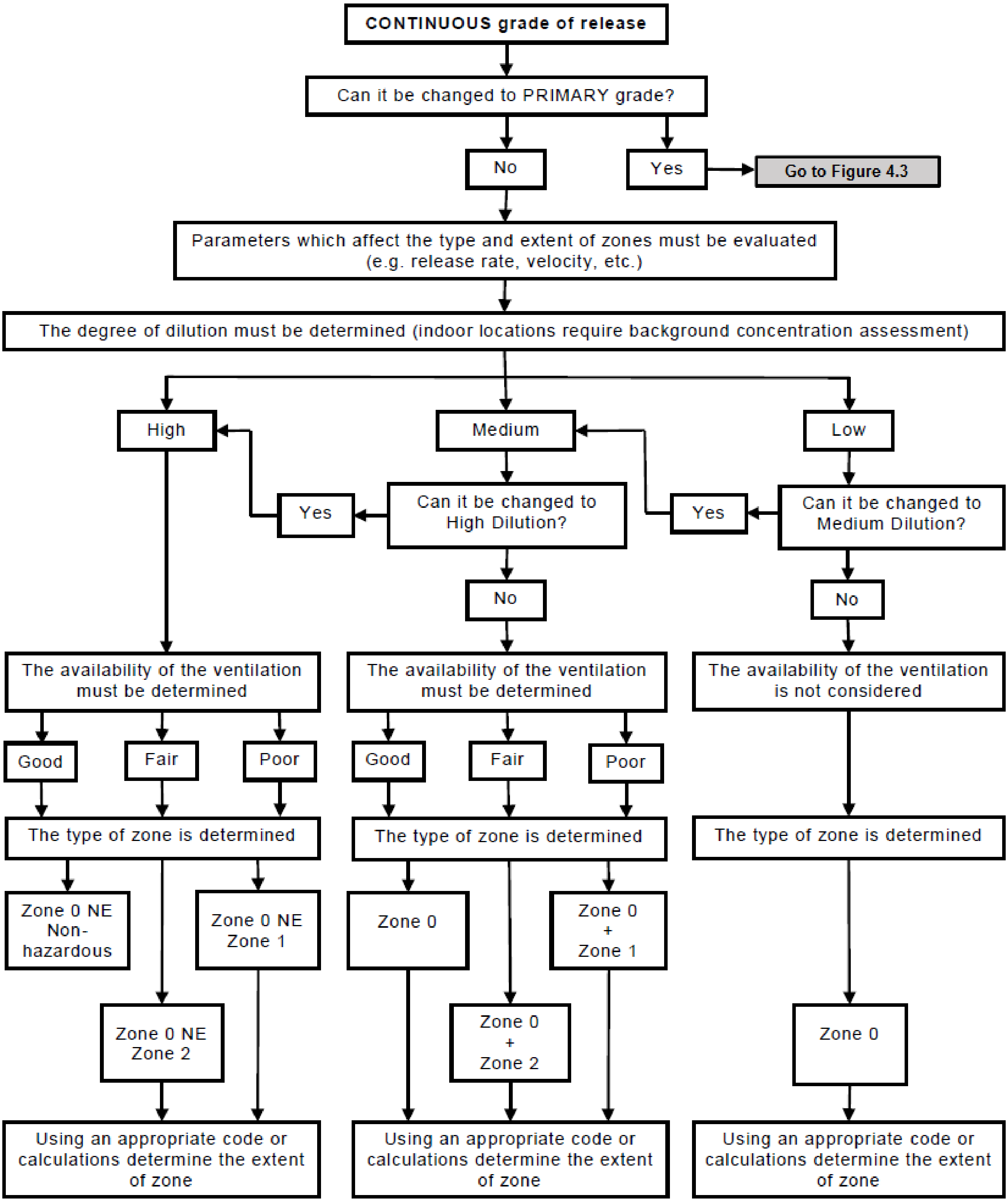


Figure 4.2 – Scheme of classification for continuous grade releases. Adapted from IEC/EN 60079-10-1:2015.

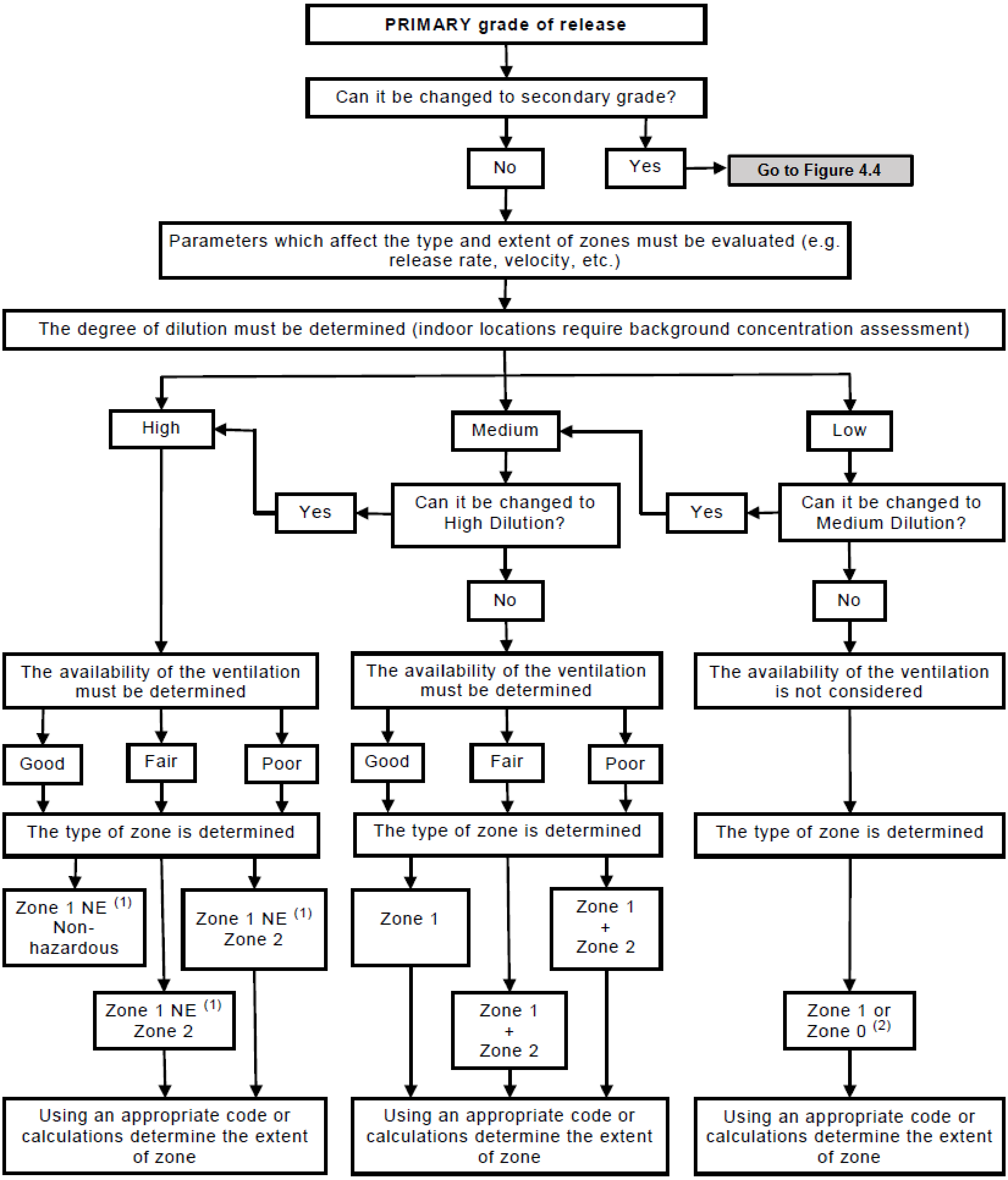


Figure 4.3 – Scheme of classification for primary grade releases. Adapted from IEC/EN 60079-10-1:2015.

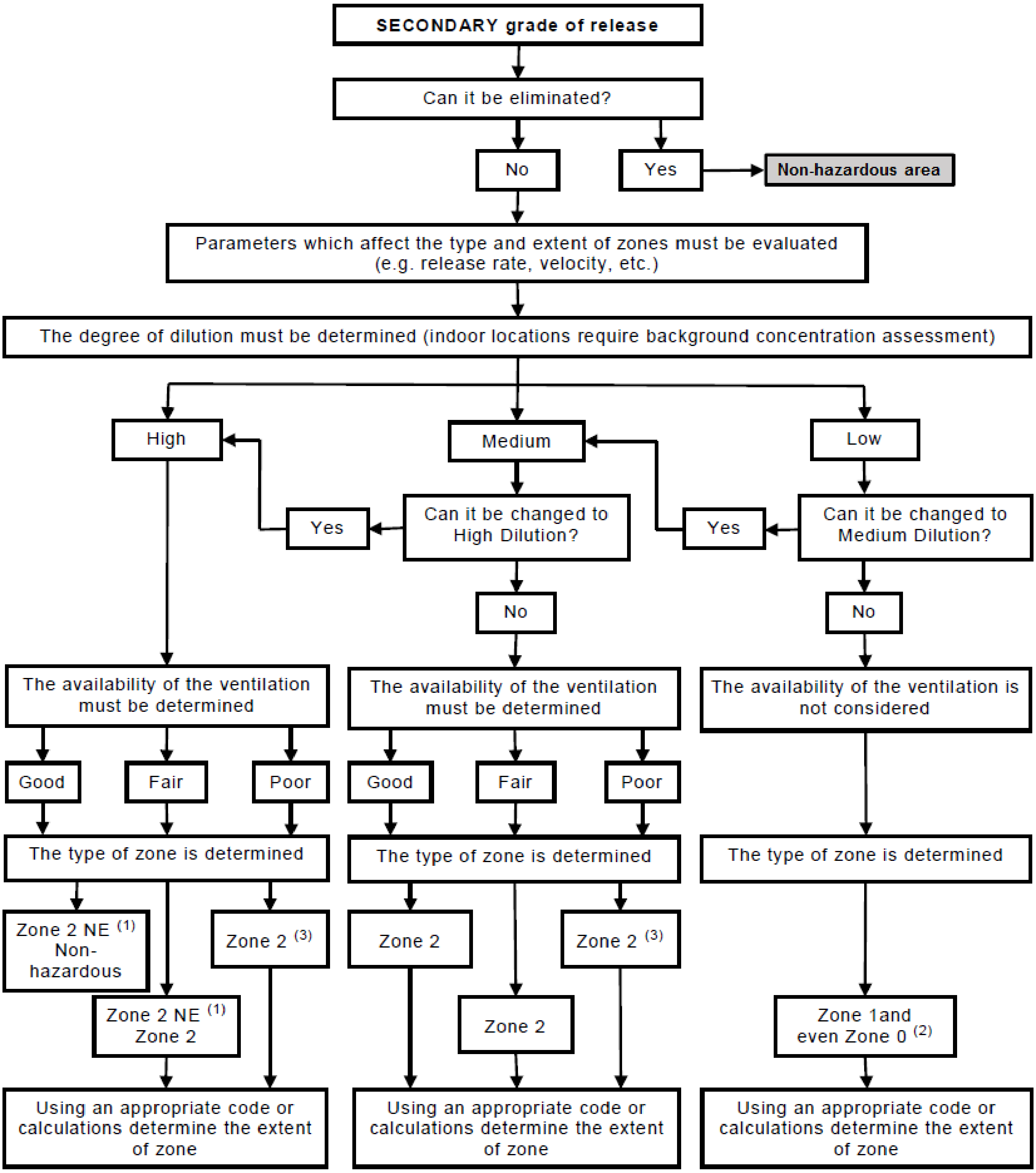


Figure 4.4 – Scheme of classification for secondary grade releases. Adapted from IEC/EN 60079-10-1:2015.

Type of Zone

The likelihood of the presence of an explosive gas atmosphere and hence the type of zone depends mainly on the grade of release and the ventilation. A continuous grade of release normally leads to Zone 0, a primary grade to Zone 1 and a secondary grade to Zone 2.

Extent of Zone

The extent of the zone is mainly affected by chemical and physical parameters, some of which are intrinsic properties of the flammable material, others are specific to the process.

Consideration should always be given to the possibility that a gas which is heavier than air may flow into areas below ground level, for example, pits or depressions and that a gas which is lighter than air may be retained at high level, for example, in a roof space.

Where the source of release is situated outside an area or in an adjoining area, the penetration of a significant quantity of flammable gas or vapour into the area can be prevented by suitable means such as:

- Physical barriers.
- Maintaining a static overpressure in the area relative to the adjacent hazardous areas, so preventing the ingress of the hazardous atmosphere.
- Purging the area with a significant flow of air, so ensuring that the air escapes from all openings where the hazardous gas or vapour may enter.

Thus, the main parameters affecting the extent of zones are:

1) Release rate of gas or vapour: the greater the release rates the larger the extent of the zone. The release rate itself depends on other parameters, such as: geometry of the source of release, release velocity, concentration, vapour pressure, flashpoint, boiling point and liquid temperature.

2) Lower explosive limit (LEL): for a given release volume, the lower the LEL the greater will be the extent of the zone.

3) Ventilation: With increased ventilation, the extent of the zone will be reduced. Obstacles, which impede the ventilation, may increase the extent of the zone. On the other hand, some obstacles, for example dykes, walls or ceilings, may limit the extent.

4) Relative density of the gas or vapour when it is released: If the gas or vapour is significantly lighter than air, it will tend to move upward. If significantly heavier, it will tend to accumulate at ground level. The horizontal extent of the zone at ground level will increase with increasing relative density, and the vertical extent above the source will increase with decreasing relative density.

5) Climatic conditions.

6) Topography.

Openings

Openings between areas should be considered as possible sources of release. The grade of release will depend upon:

- the zone type of the adjoining area;
- the frequency and duration of opening periods;
- the effectiveness of seals or joints;
- the difference in pressure between the areas involved.

Openings are classified as A, B, C and D with the following characteristics:

- **Type A:** Openings not conforming to the characteristics specified for types B, C or D.

  Examples:

- Open passages for access or utilities, for example, ducts, pipes through walls, ceilings and floors.
- Fixed ventilation outlets in rooms, buildings and similar openings of types B, C and D which are opened frequently or for long periods.

- **Type B:** Openings that are normally closed (for example, automatic closing) and infrequently opened, and which are close fitting.
- **Type C:** Openings normally closed and infrequently opened, conforming to Type B, which are also fitted with sealing devices (for example, a gasket) along the whole perimeter; or two openings Type B in series, having independent automatic closing devices.
- **Type D:** Openings normally closed conforming to Type C, which can only be opened by special means or in an emergency. Type D openings are effectively sealed, such as in utility passages (for example, ducts, pipes) or can be a combination of one opening Type C adjacent to a hazardous area and one opening Type B in series.

Table 4.3 describes the effect of openings on grade of release.

Table 4.3 – Effect of hazardous zones on openings as possible sources of release

Zone Upstream of Opening	Opening Type	Grade of Release of Openings Considered as Sources of Release
Zone 0	A	Continuous
	B	(Continuous)/primary
	C	Secondary
	D	No release
Zone 1	A	Primary
	B	(Primary)/secondary
	C	(Secondary)/no release
	D	No release
Zone 2	A	Secondary
	B	(Secondary)/no release
	C	No release
	D	No release

Source: IEC/EN 60079-10-1:2015

Note: For grades of release shown in brackets, the frequency of operation of the openings should be considered in the design.

Ventilation

Gas or vapour released into the atmosphere can be diluted by dispersion or diffusion into the air until its concentration is below the lower explosion limit. Hence, the designs of artificial ventilation systems are of paramount importance in the control of the dispersion of releases of flammable gases and vapours. Ventilation, i.e. air movement leading to replacement of the atmosphere in a (hypothetical) volume around the source of release by fresh air will promote dispersion. Suitable ventilation rates can also avoid persistence of an explosive gas atmosphere, thus influencing the type of zone.

Ventilation can be accomplished by the movement of air due to the wind and/or by temperature gradients or by artificial means such as fans. So two main types of ventilation are thus recognized:

a) Natural ventilation
b) Artificial ventilation, general or local.

The **natural ventilation** is a type of ventilation that is accomplished by the movement of air caused by the wind and/or by temperature gradients. In open-air situations, natural ventilation will often be sufficient to ensure dispersal of any explosive atmosphere, which arises in the area. Natural ventilation may also be effective in certain indoor situations (for example, where a building has openings in its walls and/or roof). For outdoor areas, the evaluation of ventilation should normally be based on an assumed minimum wind speed of 0.5 m/s, which will be present virtually continuously, although the wind speed will frequently be above 2 m/s.

Artificial ventilation is generally applied inside a room or enclosed space but it can also be applied to situations in the open air to compensate for restricted or impeded natural ventilation due to obstacles.

The artificial ventilation of an area may be either general or local and, for both of these, differing degrees of air movement and replacement can be appropriate.

With the use of artificial ventilation, it is possible to achieve:

- reduction in the extent of zones;
- shortening of the time of persistence of an explosive atmosphere;
- prevention of the generation of an explosive atmosphere.

Artificial ventilation makes it possible to provide an effective and reliable ventilation system in an indoor situation. An artificial ventilation system, which is designed for explosion protection, should meet the following requirements:

- Its effectiveness should be controlled and monitored.
- Consideration should be given to the classification immediately outside the extract system discharge point.
- For ventilation of a hazardous area the ventilation air should usually be drawn from a non-hazardous area.
- Before determining the dimensions and design of the ventilation system, the location, grade of release and release rate should be defined.

In addition, the following factors will influence the quality of an artificial ventilation system:

- Flammable gases and vapours usually have densities other than that of air, thus they will tend to accumulate near to either the floor or ceiling of an enclosed area, where air movement is likely to be reduced.
- Changes in gas density with temperature.
- Impediments and obstacles may cause reduced, or even no air movement, i.e. no ventilation in certain parts of the area.

Degree of Ventilation

The effectiveness of the ventilation in controlling dispersion and persistence of the explosive atmosphere will depend upon the degree and availability of ventilation and the design of the system.

The most important factor is that the degree or amount of ventilation is directly related to the types of sources of release and their corresponding release rates.

Optimal ventilation conditions in the hazardous area can be achieved and the higher the amount of ventilation in respect of the possible release rates, the smaller will be the extent of the zones (hazardous areas), in some cases reducing them to a negligible extent (non-hazardous area).

Estimation of Hazardous Zone

The effectiveness of ventilation, the availability of ventilation and the grade of release are combined in a qualitative method for the evaluation of the zone type. Table 4.4. shows this relation and is to be used both on indoor and on open areas.

Table 4.4 – Zones for grade of release and effectiveness of ventilation. Adapted from IEC/EN 60079-10-1:2015.

Grade of release	Effectiveness of Ventilation						
	High Dilution			Medium Dilution			Low Dilution
	Availability of ventilation						
	Good	Fair	Poor	Good	Fair	Poor	Good, Fair, Poor
Continuous	Non-hazardous (Zone 0 NE) 1)	Zone 2 (Zone 0 NE) 1)	Zone 1 (Zone 0 NE) 1)	Zone 0	Zone 0 + Zone 2	Zone 0 + Zone 1	Zone 0
Primary	Non-hazardous (Zone 1 NE) 1)	Zone 2 (Zone 1 NE) 1)	Zone 2 (Zone 1 NE) 1)	Zone 1	Zone 1 + Zone 2	Zone 1 + Zone 2	Zone 1 or Zone 0 3)
Secondary	Non-hazardous (Zone 2 NE) 1)	Non-hazardous (Zone 2 NE) 1)	Zone 2	Zone 2	Zone 2	Zone 2	Zone 1 and even Zone 0 3)

Notes:

1) Zone 0 NE, 1 NE or 2 NE indicates a theoretical zone which would be of negligible extent under normal conditions.

2) The zone 2 area created by a secondary grade of release may exceed that attributable to a primary or continuous grade of release; in this case, the greater distance should be taken.

3) Will be zone 0 if the ventilation is so weak and the release is such that in practice an explosive gas atmosphere exists virtually continuously (i.e. approaching a “no ventilation” condition).

“+” means “surrounded by”

Availability of ventilation in naturally ventilated enclosed spaces shall never be considered as good.

Estimation of the Extent of the Hazardous Zone

The extent of the hazardous zone or region where flammable gas may occur depends on the release rate and several other factors such as gas properties and release geometry and surrounding geometry. Figure 4.5 can be used as a guide to determine the extent of hazardous zones for various forms of release.

The appropriate line should be selected based on the type of release as either:

a) an unimpeded jet release with high velocity;
b) a diffusive jet release with low velocity or a jet that loses its momentum due to the geometry of the release or impingement on nearby surfaces;
c) heavy gases or vapours that spread along horizontal surfaces (e.g. the ground).

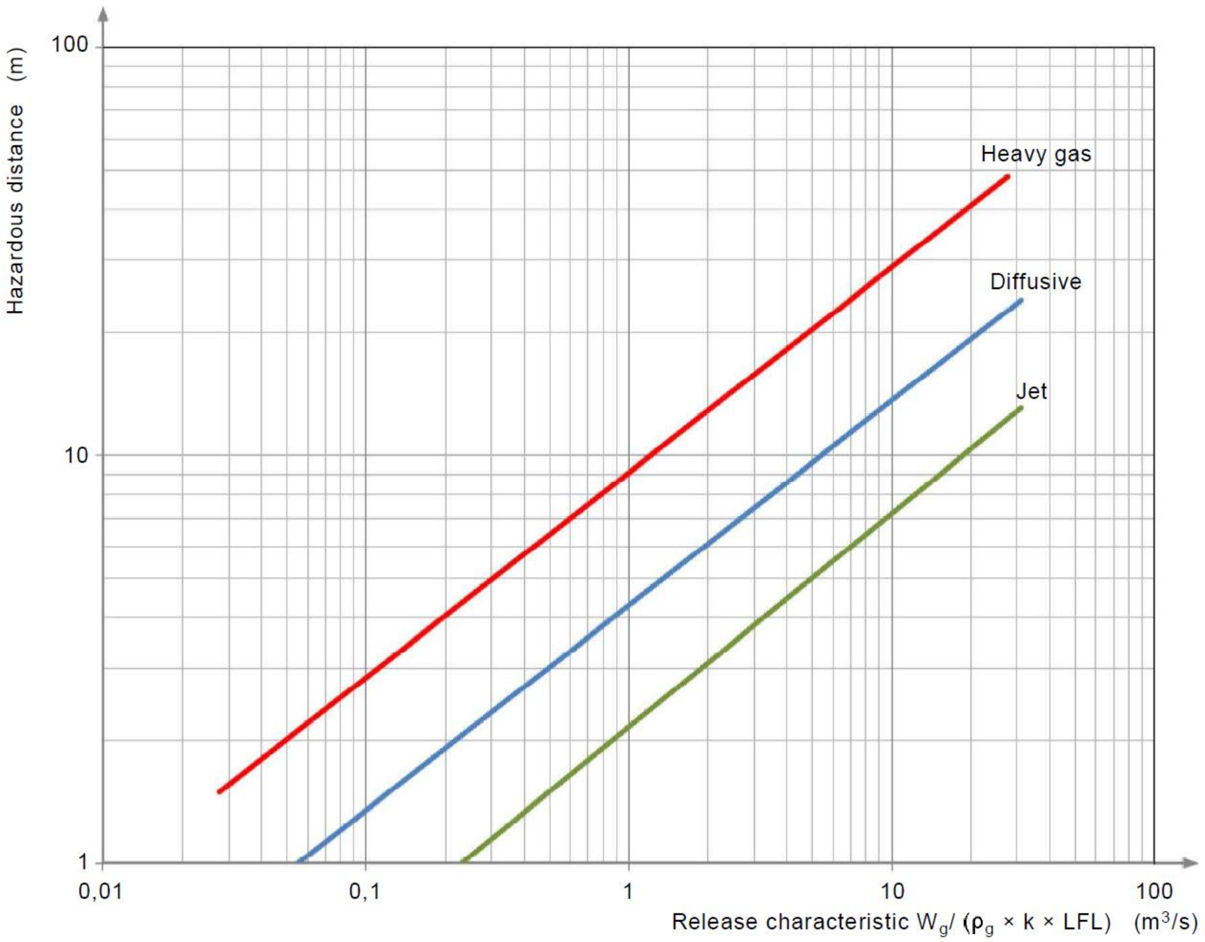


Figure 4.5 – Chart for estimating hazardous area distances. Source IEC/EN 60079-10-1:2015.

Where a zone of negligible extent (NE) is suggested then the use of this chart is not applicable.

The curves are based on a zero background concentration and are not applicable for indoor low dilution situations.

5 HALOC GAS IMPLEMENTATION AND CASE STUDIES

This chapter presents the main aspects of the implementation of the application, namely the conceptual model, the user interface and the linkage between the forms and the spreadsheets.

5.1 Implementation Details

To aid the development and debugging, from start there was a clear separation between code related to present information to the user (User Interface) and the code relating to the calculation (Business Logic).

In this section will be presented the implementation details regarding this two application layers.

5.1.1 Conceptual Model

The conceptual model has been developed in accordance with the following premises:

- For each simulation there is one or more sources of release;
- Each source of release only releases one flammable substance;
- For each simulation there is only one configurable type of ventilation;
- All sources of release are affected by the same type of ventilation;
- Each source of release only has one nature of release (liquid, gas or evaporative pool);
- The methodology for evaluating the effects of the source of release is based on its nature (gas, liquid, evaporative pool).

As a result of the previous premises, the conceptual model is represented in Figure 5.1.

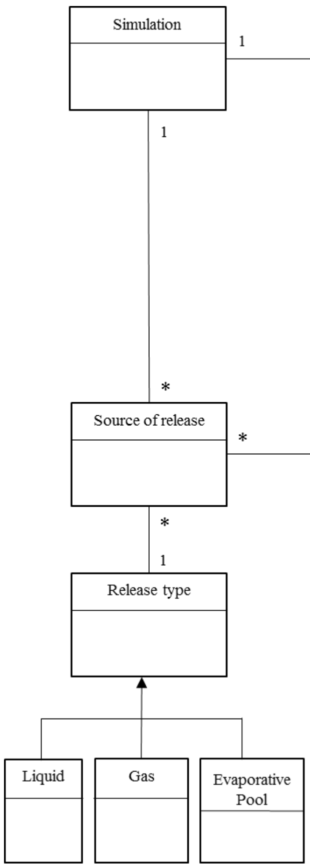


Figure 5.1 – Conceptual Model of the prototype

5.1.2 User Interface (UI)

The user interface (UI) sequence is detailed in Figure 5.2.

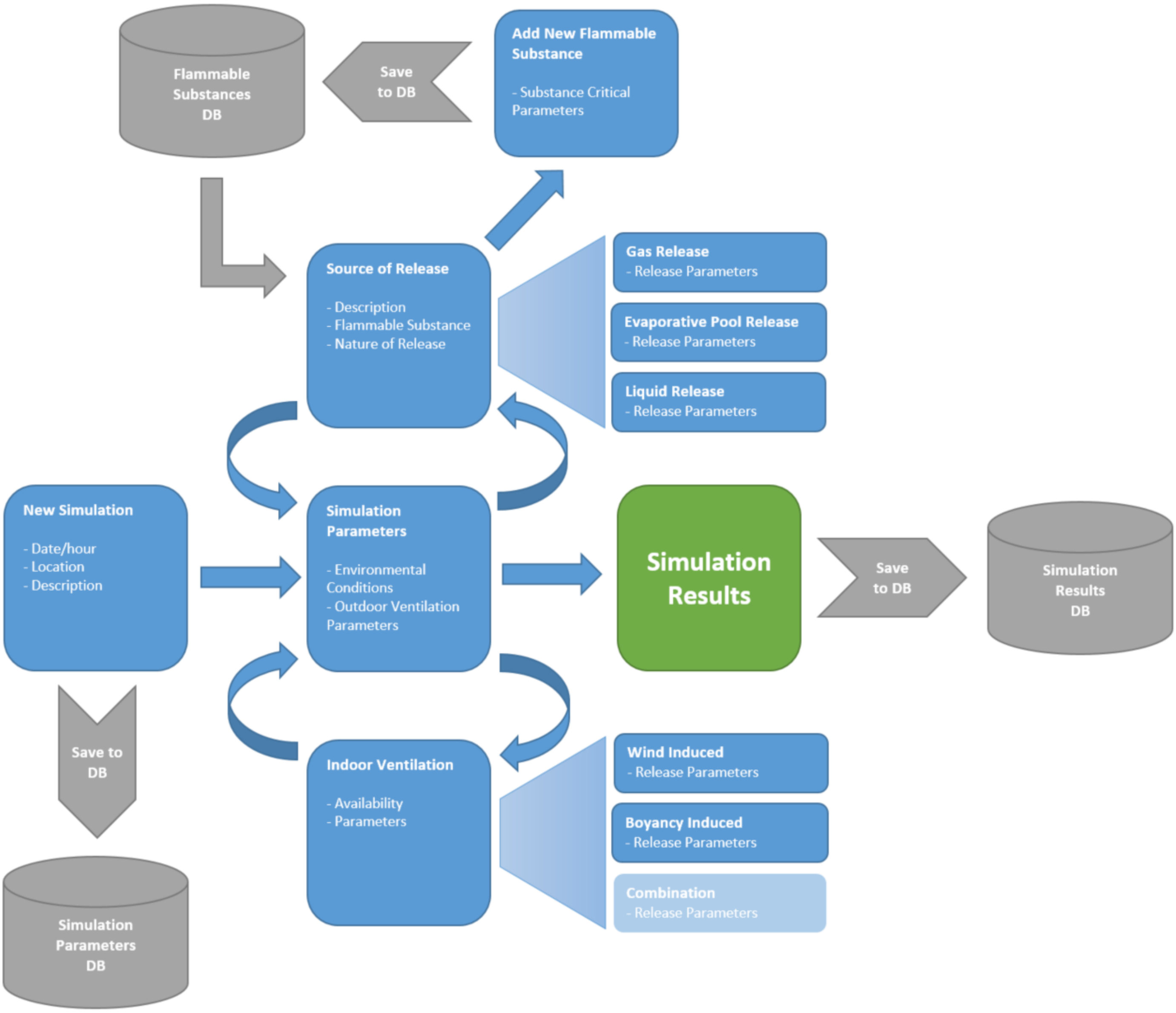


Figure 5.2 – User Interface sequence

The design of the UI follows the natural sequence of the methodology for calculation and classification of hazardous areas.

The application begins with the form **Simulations** (see Figure 5.3). This form allows to:

- open a previously saved simulation by selecting the corresponding line;
- delete a previously saved simulation by selecting the corresponding line;
- start a new simulation.

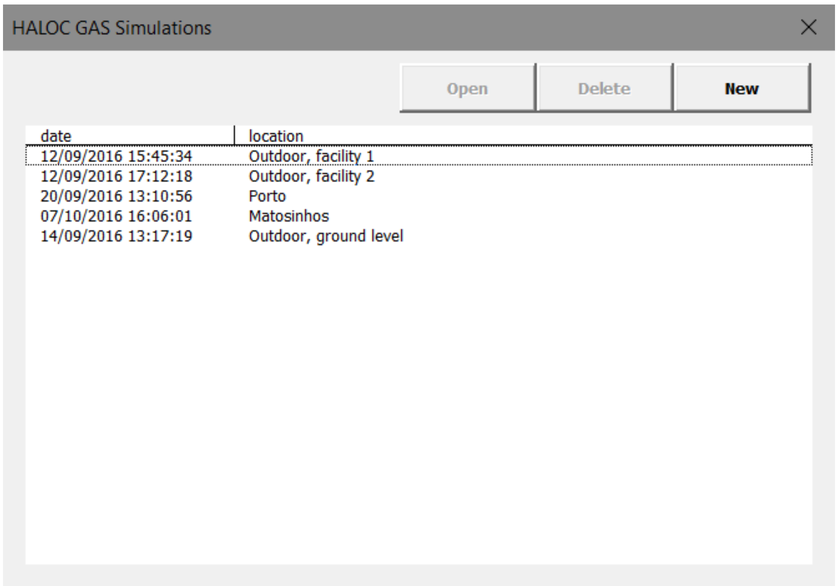


Figure 5.3 – Simulations form

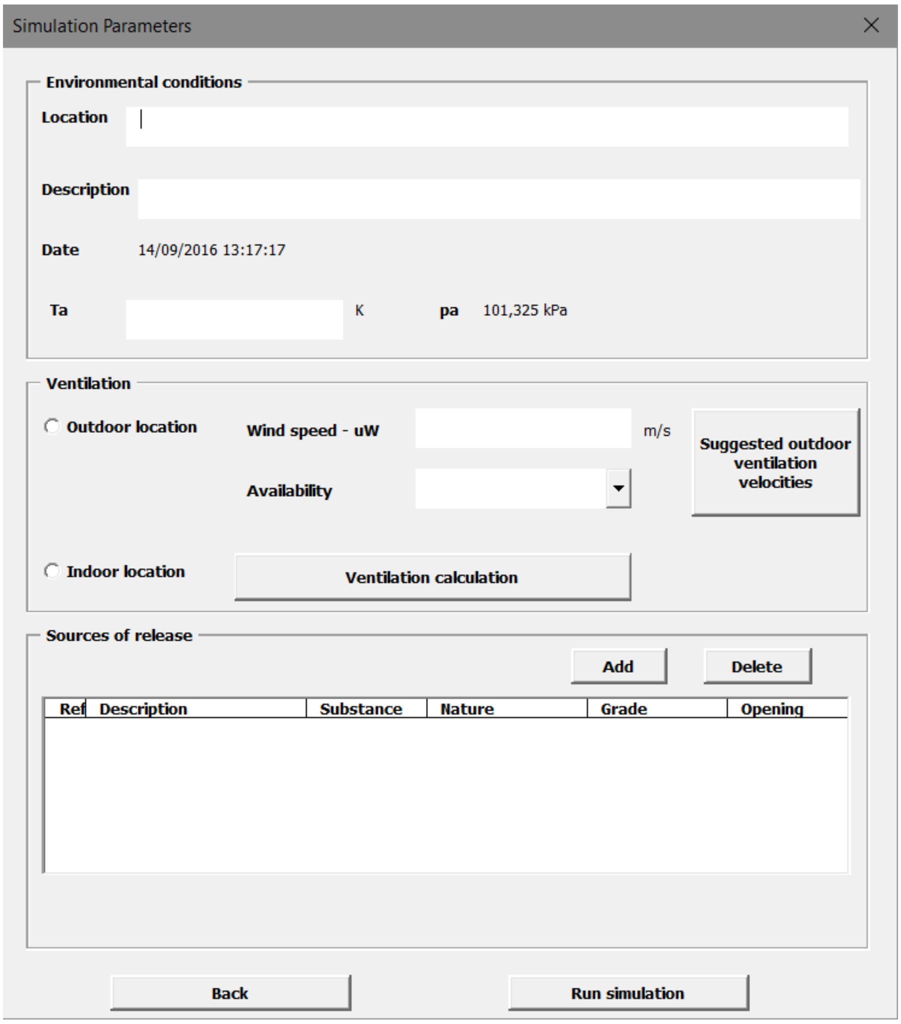


Figure 5.4 – Simulation Parameters form

Simulation Parameters form

Once chosen a new simulation, a new form appears: **Simulation Parameters** (see Figure 5.4). It is subdivided in three sections:

Environmental conditions

The fields *Date/hour*, *Location* and *Description*, will be saved to the **Simulation Parameters DB** (Database). The field *Ta*, meaning ambient temperature, is an input for the calculations and will be saved in the **Simulation Results DB**.

Ventilation

In the section *Ventilation* the user selects *Outdoor location* or *Indoor location*, depending on the situation. When the location is outdoor, the application has a help button with the suggested outdoor ventilation velocities (from the standard IEC/EN 60079-10-1:2015). The objects related to the *Indoor location* become disabled. The input data of outdoor ventilation will be used for calculation and saved in the **Simulation Results DB**.

If the source of release is located indoor, the button *Ventilation calculation* becomes enabled and, when pressed, opens a new form: **Indoor Ventilation**.

Sources of release

In this section the user can add or delete sources of release. The same simulation supports several sources of release.

To delete one source of release, the user selects the corresponding line of the source of release to be deleted.

When the user intends to add a source of release, the button *Add* will open a new form: **Source of Release**.

Source of Release form

Sources of release must be added for each simulation. The **Source of Release** form is used to characterize each of the sources of release (see Figure 5.5).

The upper section of the form is dedicated to the source of release identification, with the fields *Ref* (abbreviation for reference) and *Description*. Each source of release must have a unique reference.

The *Flammable substance* can be chosen from the application database or it can be added a new one. By pressing the button “+” the form **Flammable substance** opens and a new flammable substance can be added to the database.

In the section *Nature of the release*, the user can select if the release is due to a liquid, a gas or an evaporative pool. This will be a key selection to the next steps in the application – depending on the nature of release selected, the respective form will appear. The release parameters of each one vary in accordance with the nature of release.

The section *Release characteristics* will give fundamental inputs for the calculation of the release rate and zone classification.

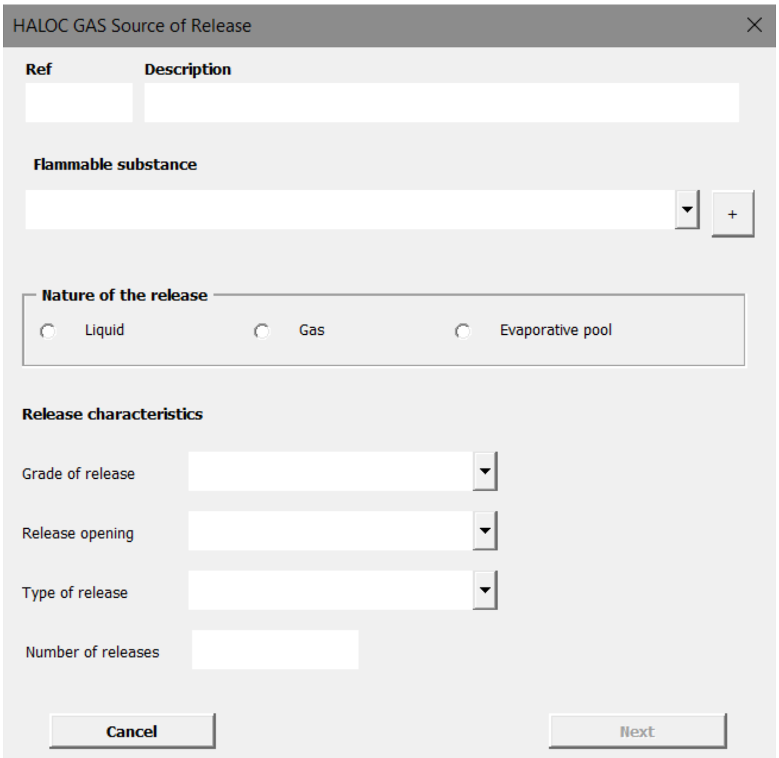


Figure 5.5 – Source of Release form

Indoor Ventilation form

The **Indoor Ventilation** form (see Figure 5.6) has, in its first section, the input data for the availability of ventilation, the input for the calculation of the air change frequency in a room, volumetric flow rate and background concentration.

In the section *Assessment of the natural ventilation in buildings* the user has to select if the ventilation is *Wind induced*, *Buoyancy induced* or *Combination*. Each one of this possibilities will open a form to introduce the input data to perform the calculations.

In the standard IEC/EN 60079-10-1:2015, the artificial ventilation in buildings isn't assessed by means of calculation. Some illustrative examples are shown but the degree of dilution should be done by other means such as, for example, CFD software.

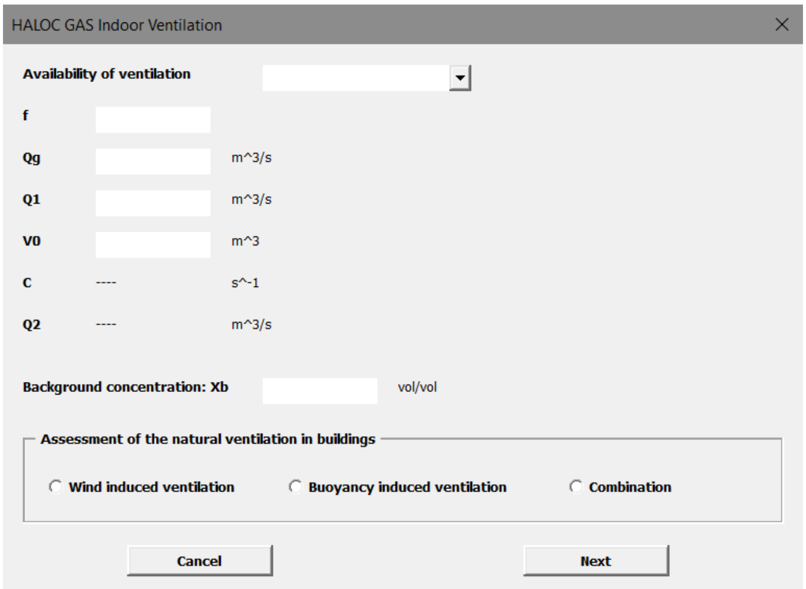


Figure 5.6 – Indoor Ventilation form

Flammable Substance form

This form (see Figure 5.7) gives the opportunity to add a new flammable substance to the application. The inputs are the critical properties of the substances that will be used for the upcoming calculations. Usually the material safety data sheets (MSDS) have all the information required.

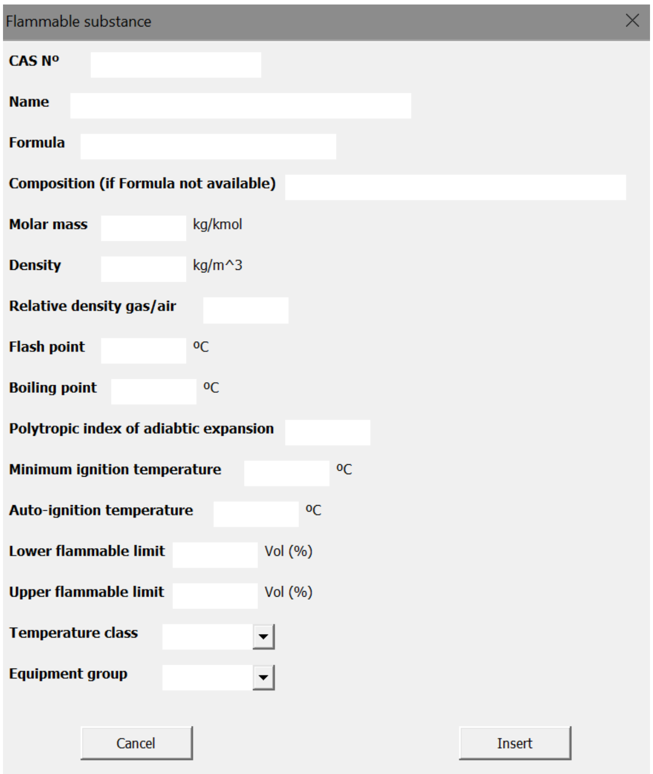


Figure 5.7 – Flammable Substance form

When adding a new flammable substance to the simulation, its data will be saved in **Flammable Substances DB** and will be available for future simulations.

The application prototype has in its database the most common flammable substances, but as already said, it's always possible to add new ones. This database was adapted from the standard IEC 60079-20-1:2010.

At the end of the data introduction in the relevant forms, the user must press the button to *Run simulation* in the Simulation Parameters form (see Figure 5.4). The simulation results are shown on a spreadsheet and are saved, for future reference, on the **Simulation Results DB**.

5.1.3 Business Logic

The Business Logic was implemented in classes separate from the ones responsible for building the forms. To this objective, the following VBA modules were created:

- mdlCommon – functions common to all release types;
- mdlDataAccess – data access procedures;
- mdlGas – gas release related mathematical functions;
- mdlLiquid – liquid release related mathematical functions;
- mdlEvaporative – evaporative pool release related functions.

5.2 Application Evaluation Through Case Studies

The following case studies are meant to validate the HALOC GAS prototype. The simulation parameters were introduced in the application and the results were validated with manual calculation using the methodology of the IEC/EN 60079-10-1:2015. The case studies are based on examples available on the standard.

Test Scenario 1

A normal industrial pump with mechanical seal, mounted at ground level, located outdoor, pumping a flammable liquid.

The initial conditions are:

Flammable substance	Benzene (CAS nº 71-43-2)
M - molar mass	78,11 kg/kmol
LFL	1,2 % vol. (0,012 vol./vol.)
AIT	498 °C
ρ_{gas} - density of the gas or vapour	3,25 kg/m^3
Ambient temperature	293,15 K
u_W - Wind speed	0,3 m/s
Ventilation availability	Good
Source of release	Mechanical seal
Grade of release	Secondary
Cd - discharge coefficient	0,75

S - cross section of the opening (hole)	5 mm^2
ρ_{liquid} **- liquid density**	876,5 kg/m^3
Δp - pressure difference across the opening that leaks	1500 kPa
k - safety factor attributed to LFL	1,0
% vaporised	2%

After starting a new simulation, the **Simulation Parameters** form gets to be filled as shown in Figure 5.8.

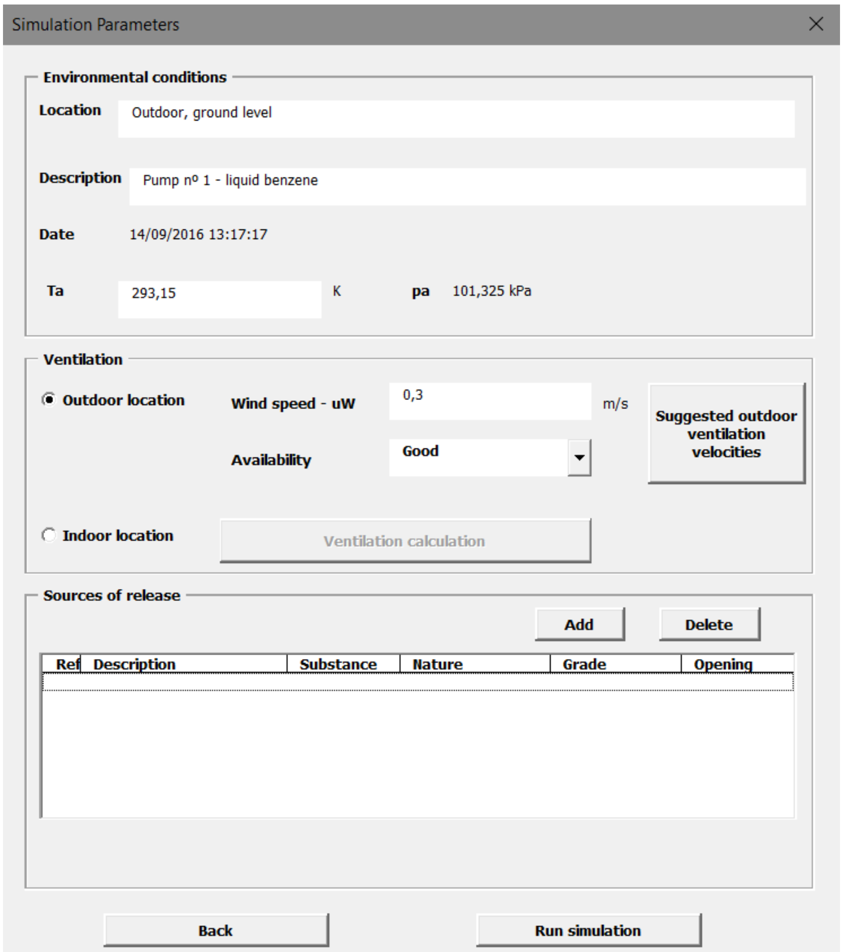


Figure 5.8 – Simulation Parameters form for Test 1

For the source of release data, the form **Source of Release** is filled as shown in Figure 5.9.

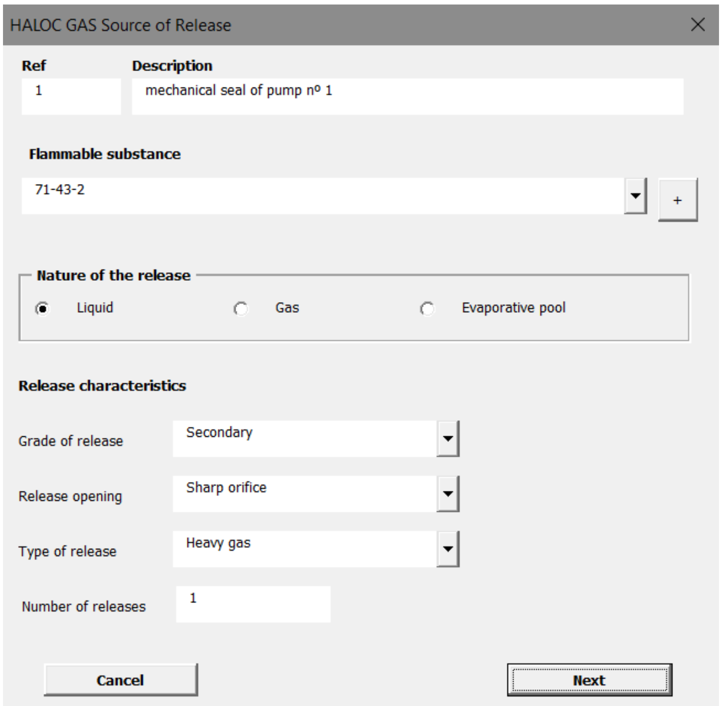


Figure 5.9 – Source of Release form for Test 1

Considering the liquid release, the form **Release of Liquid** is filled as shown in Figure 5.10.

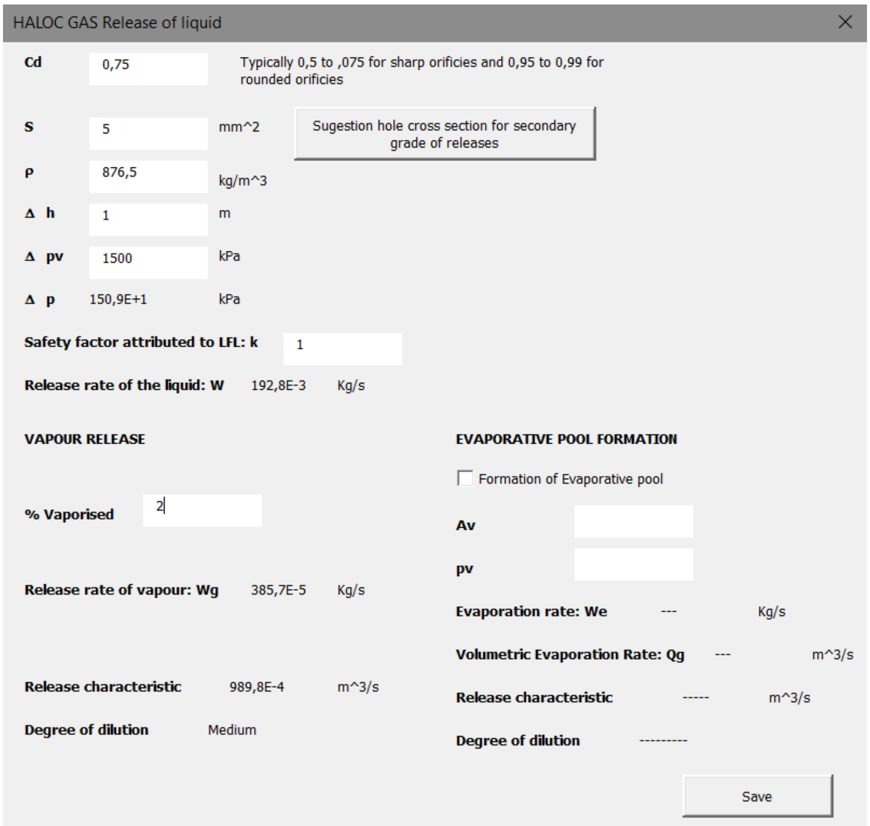


Figure 5.10 – Release of Liquid form for Test 1

The release rate of liquid, W, can be estimated by means of the following equation:

$$W = C_d S\sqrt{2\rho\Delta p} \quad (kg/s)$$

where,

C_d – discharge coefficient (dimensionless)

S – cross section of the opening (hole), through which the fluid is released (m^2);

ρ – liquid density (kg/m^3);

Δp – pressure difference across the opening that leaks in (Pa).

And the release rate of vapour, Wg, is:

$$W_g = W \times \%vaporised \quad (kg/s).$$

The release characteristic is given by the expression: $W_g/(\rho \times k \times LFL)$. It allows the evaluation of the degree of dilution in accordance with the Figure 5.11.

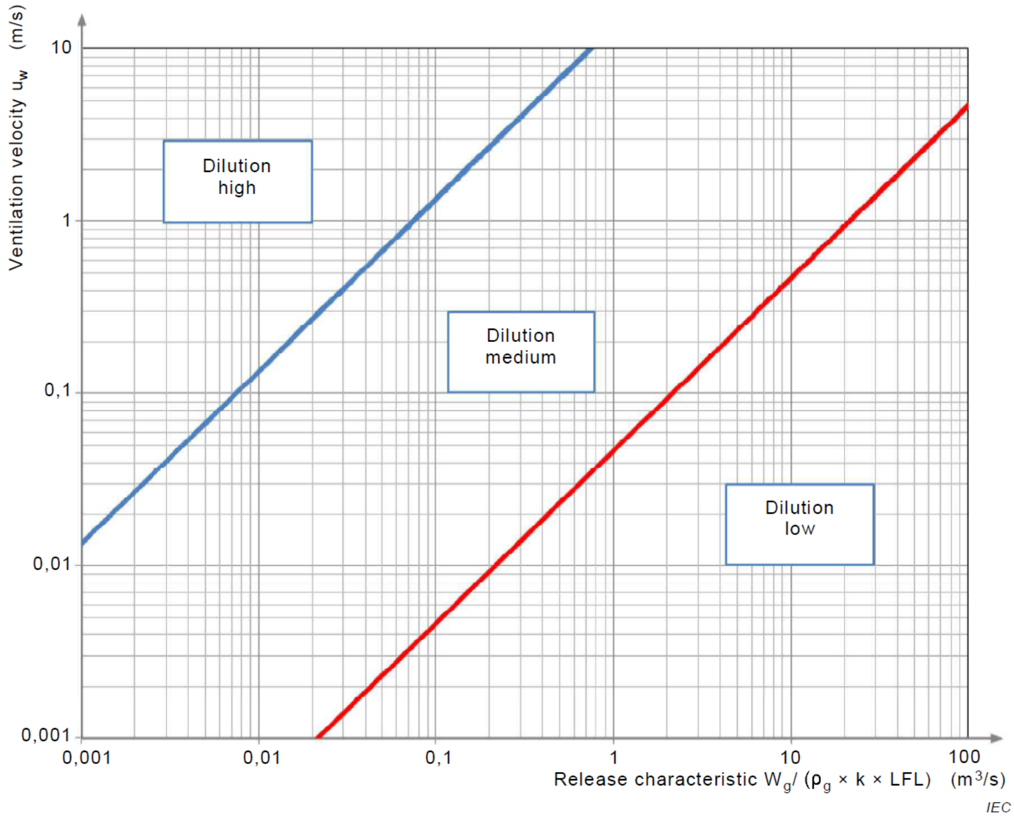


Figure 5.11 – Degree of dilution. Source IEC/EN 60079-10-1:2015

The final results of the simulation appear in the form **Simulation Results**, as shown in Figure 5.12.

From the manual calculation for this test, the following results were obtained:

W – liquid release rate	192,8 x 10^{-3} kg/s
Wg – gas release rate	3,85 x 10^{-3} kg/s
Release characteristic	0,1 m^3/s
Degree of dilution	Medium

Zone	2
Equipment Group (from flammable substance parameters)	IIA
Temperature Class (from flammable substance parameters)	T1
Horizontal Extent of Zone (From Figure 4.5)	3 m
Vertical Extent of Zone	1,5 m

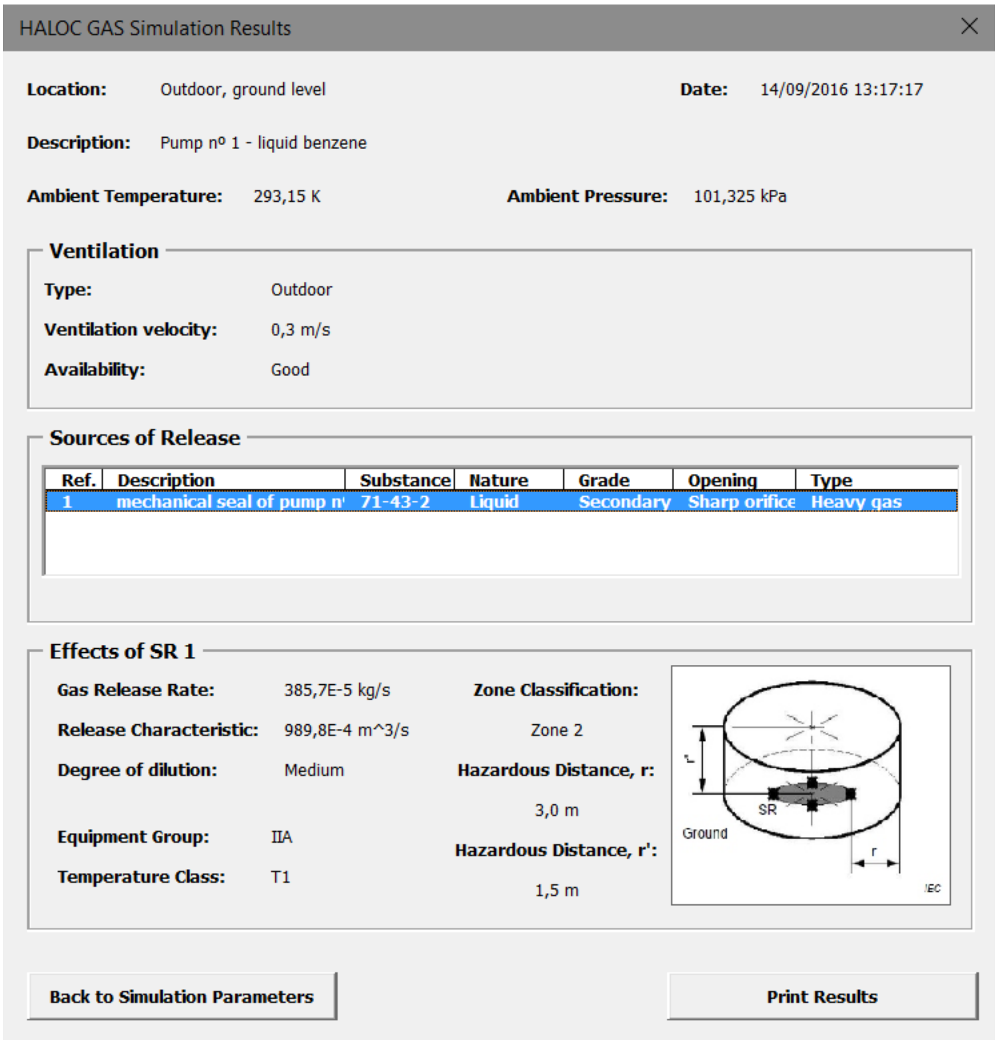


Figure 5.12 – Results form for Test 1

By comparing the results it's possible to validate the HALOC GAS prototype for this test scenario.

Test Scenario 2

A normal industrial pump with mechanical seal, mounted at ground level, located indoor, pumping a flammable liquid.

The initial conditions are:

Flammable substance	Benzene (CAS nº 71-43-2)
M – molar mass	78,11 kg/kmol
LFL	1,2 % vol. (0,012 vol./vol.)

AIT	498 °C
ρ_{gas} – density of the gas or vapour	3,25 kg/m^3
Ambient temperature	293,15 K
Ventilation situation	Building ventilated by wind
Ventilation availability	Good
Source of release	Mechanical seal
Grade of release	Secondary
Cd - discharge coefficient	0,75
S – cross section of the opening (hole)	5 mm^2
ρ_{liquid} – liquid density	876,5 kg/m^3
Δp – pressure difference across the opening that leaks	1500 kPa
k – safety factor attributed to LFL	1,0
% vaporised	2%
V_0 – Enclosure size	150 m^3
f – ventilation efficiency factor	5
Q_a – volumetric flow rate of air	0,085 m^3/s
X_b – background concentration	0,07 vol./vol.

The procedure begins starting a new simulation and then the **Simulation Parameters** form is filled in accordance with Figure 5.13:

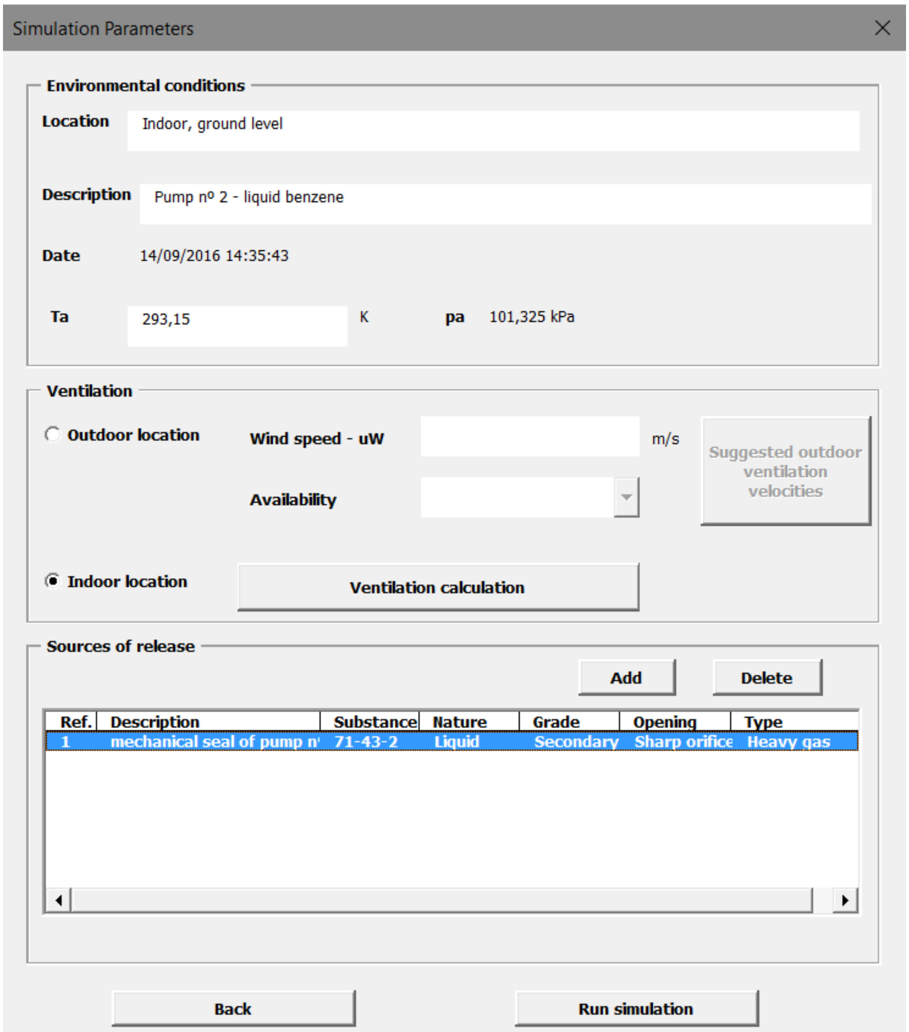


Figure 5.13 – Simulation Parameters form for Test 2

The calculation of the release is similar to the one described in Test 1, as Figure 5.14 shows.

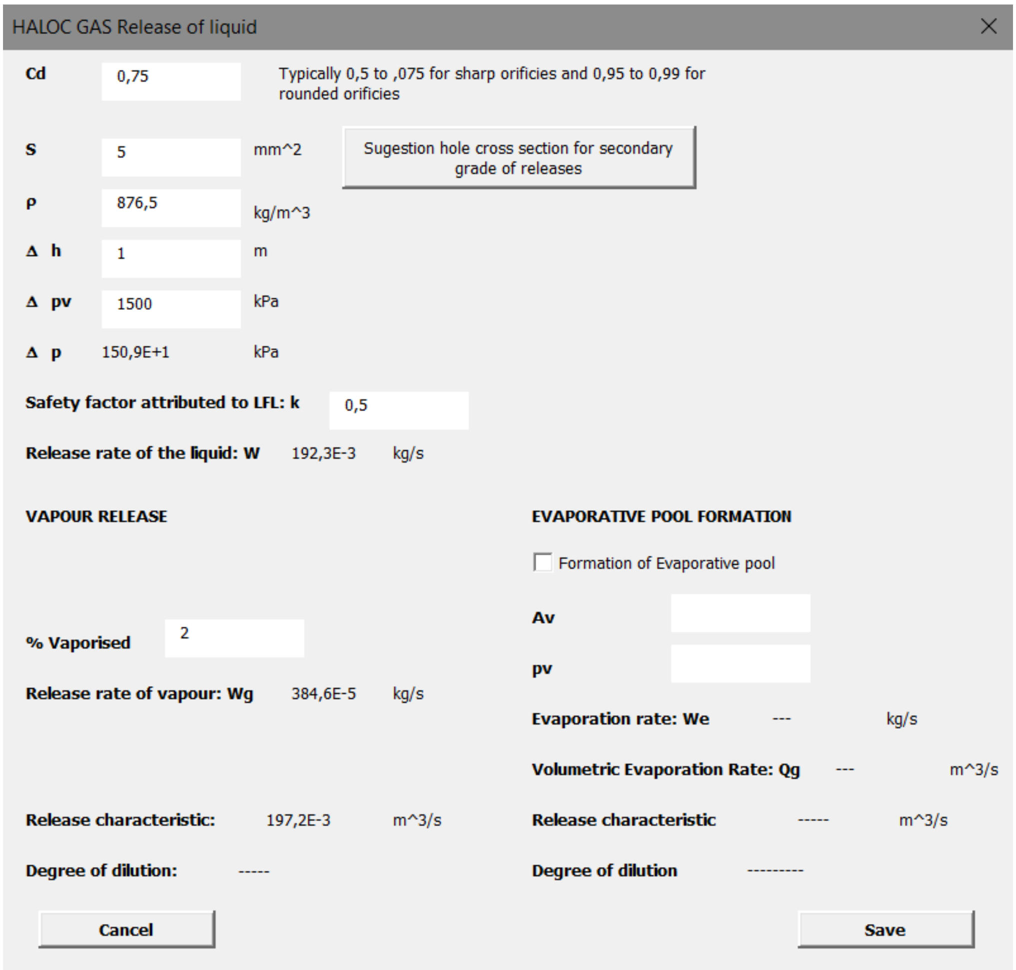


Figure 5.14 – Release of Liquid form for Test 2

As for the ventilation calculation, in this scenario the ventilation is indoor, so it's necessary to perform several operations to determine its influence in the dispersion of the vapour.

To start, the volume of the room under consideration shall be assessed. Afterwards, the ventilation velocity, u_W, is estimated by the equation:

$$u_W = \frac{Q_a}{L \times H} \quad (m/s)$$

where

- Q_a – volumetric flow rate (m^3/s);
- L – length of the room (m);
- H – height of the room (m).

The next step is to determine the critical concentration, X_{crit}. The critical concentration with which the background concentration is compared is a proportion of the LFL (typically 25%).

The theoretical time t_d required to dilute the concentration of flammable substance from a certain steady state background concentration X_b to a required critical concentration X_{crit}, in a specific volume, can be estimated from:

$$t_d = \frac{1}{C} \ln\left(\frac{X_b}{X_{crit}}\right) \quad (s)$$

where

- t_d – theoretical time required to dilute a defined value of flammable substance concentration to another one lesser than first (s);
- C – number of air changes per unit of time in the specific volume (s^{-1});
- X_b – flammable substance background concentration at steady-state conditions (vol/vol);
- X_{crit} – desired/critical value of the flammable substance concentration (vol/vol).

In Figure 5.15 are shown the results of the ventilation assessment.

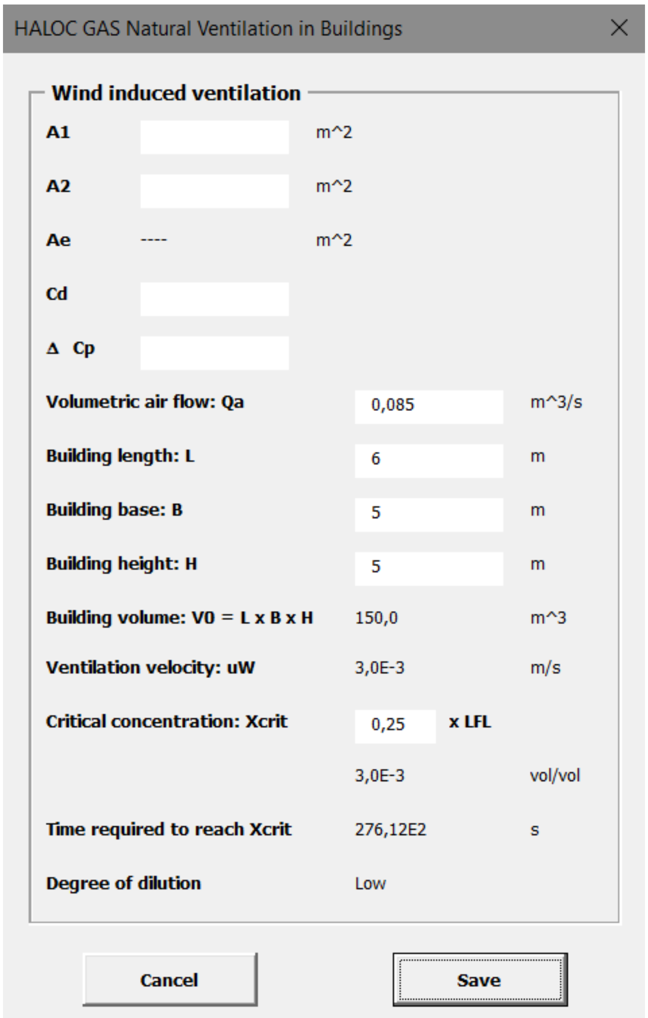


Figure 5.15 Natural ventilation in buildings form for Test 2

The final results of the simulation appear in the form **Simulation Results**, as shown in Figure 5.16.

From the manual calculation for this test, the following results were obtained:

W – liquid release rate	0,19 kg/s
Wg – gas release rate	3,85 x 10^{-3} kg/s
Release characteristic	0,2 m^3/s
Degree of dilution	Low
Zone	1
Equipment Group (from flammable substance parameters)	IIA

Temperature Class (from flammable substance parameters)	T1
Horizontal Extent of Zone (From Figure 4.5)	4 m
Vertical Extent of Zone	2 m

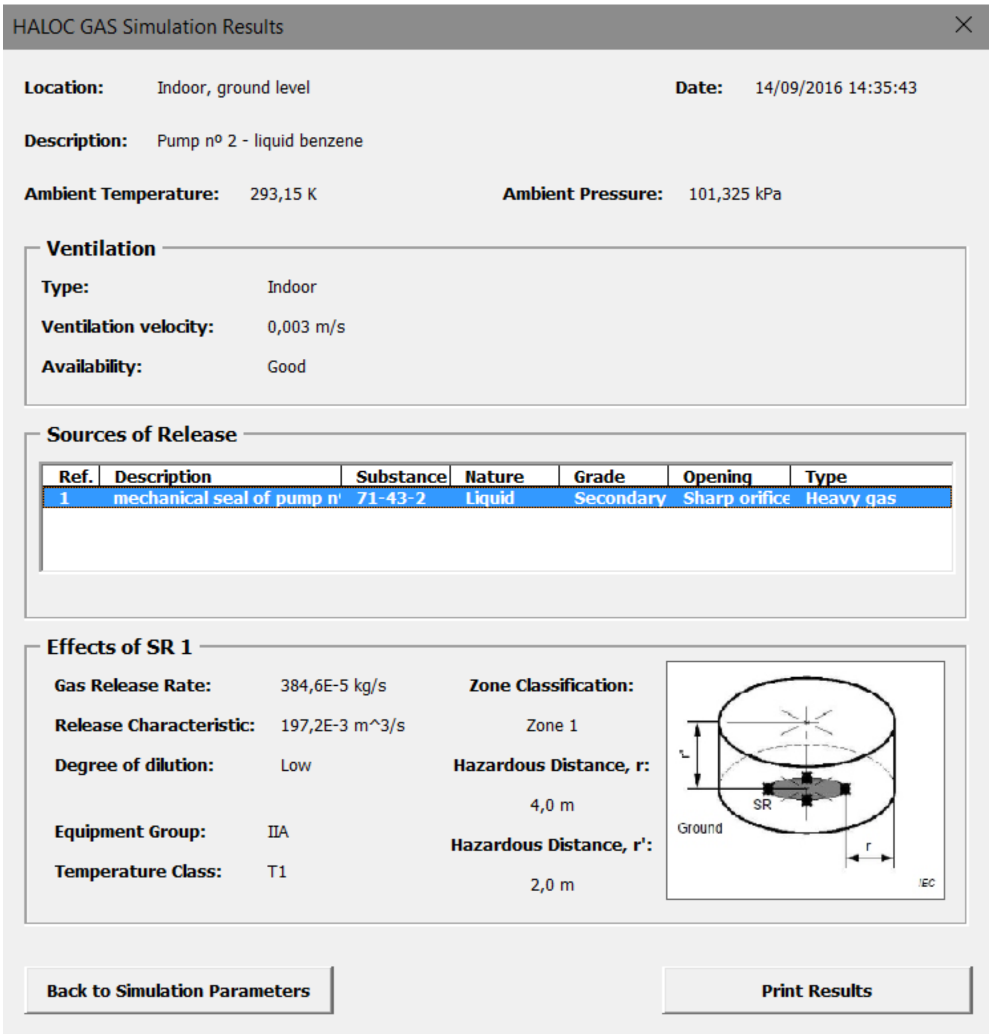


Figure 5.16 – Results form for Test 2

Also in this scenario, the results comparison validates the HALOC GAS prototype.

Test Scenario 3

Closed process pipework system, located indoor, conveying flammable gas with multiple sources of release.

The initial conditions are:

Flammable substance	Wet, oil well natural gas
M – molar mass	20 kg/kmol
LFL	4 % vol. (0,012 vol./vol.)

AIT	500 °C
ρ_{gas} – density of the gas	0,83 kg/m^3 (diffusive jet release)
Equipment Group	IIA
Temperature class	T1
Ambient temperature	293,15 K
Ventilation situation	Building ventilated by wind
Ventilation availability	Good
Sources of release	
1) Type	Pipe fittings with discontinuities along piping
Grade of release	Continuous
W_g – Release rate per unit	1x10^{-9} kg/s
Number of releases	10
X_b – background concentration	4,88x10^{-7} vol./vol.
2) Type	Sealing elements on moving parts at low speed
Grade of release	Primary
W_g – Release rate per unit	1x10^{-6} kg/s
Number of releases	3
X_b – background concentration	2,2x10^{-4} vol./vol.
3) Type	Sealing elements on fixed parts
Grade of release	Secondary
p – operating pressure	500 kPa
T – operating temperature	288,15 K
S – cross section of the opening (hole)	2,5 mm^2
C_d – discharge coefficient	0,75
Z – compressibility factor	1
γ – polytropic index of adiabatic expansion	1,1
Number of releases	1
X_b – background concentration	0,103 vol./vol.
k – safety factor attributed to LFL	0,5
V_0 – Enclosure size	21,88 m^3
f – ventilation efficiency factor	3
Q_a – volumetric flow rate of air	0,074 m^3/s

After starting a new simulation in HALOC GAS application, the next step is to add a new flammable substance, the natural gas mixture, with the known data.

The next step is to add one type of source of release at the time and assess the release rate for each one of them. As an example, Figure 5.17 shows the first type of sources of release and Figure 5.18 illustrates the assessment of the release rate for third type of sources of release.

For the assessment of the release rate of a gas, it's necessary to verify if the release is sonic or subsonic. The velocity of released gas is choked (sonic) if the pressure inside the gas container is higher than the critical pressure p_c.

Critical pressure, p_c, is determined by the following equation:

$$p_c = p_a \times \left(\frac{\gamma + 1}{2}\right)^{\frac{\gamma}{(\gamma - 1)}} \quad (Pa)$$

where

- p_a – atmospheric pressure (101325 Pa);
- γ – polytropic index of adiabatic expansion (dimensionless).

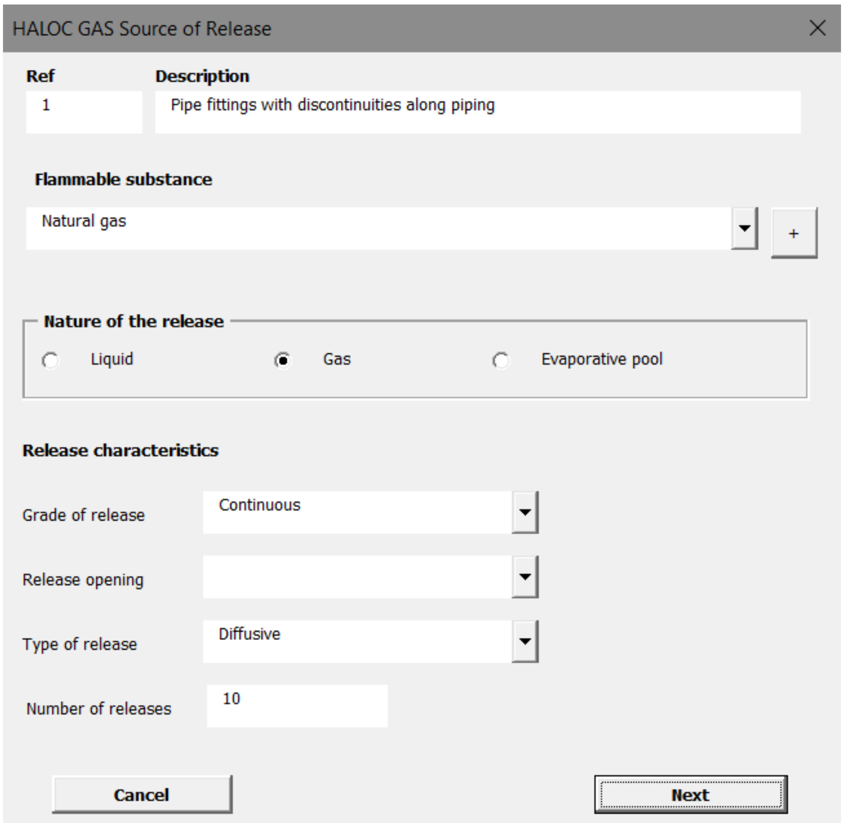


Figure 5.17 – Source of Release form for the first type of sources of release of Test 3

Release rate of gas with non-choked gas velocity (subsonic releases) is a discharge velocity below the speed of sound for the particular gas.

The release rate of gas from a container, if the gas velocity is non-choked, can be estimated by means of the following approximation:

$$W_g = C_d \times S \times p \times \sqrt{\frac{M}{ZRT} \times \frac{2\gamma}{\gamma - 1} \times \left[1 - \left(\frac{p_a}{p}\right)^{\frac{(\gamma-1)}{\gamma}}\right] \times \left(\frac{p_a}{p}\right)^{\frac{1}{\gamma}}} \quad (kg/s)$$

where

- C_d – discharge coefficient (dimensionless);
- S – cross section of the opening (hole), through which the fluid is released (m^2)
- p – pressure inside the container (Pa);
- M – molar mass of gas or vapour (kg/kmol);
- Z – compressibility factor (dimensionless);
- R – universal gas constant (8314 J/kmol K);
- T – absolute temperature of the fluid, gas or liquid (K);
- γ – polytropic index of adiabatic expansion (dimensionless);
- p_a – atmospheric pressure (101325 Pa).

Choked gas velocity is equal to the speed of sound for the gas. This is the maximum theoretical discharge velocity.

The release rate of gas from a container, if the gas velocity is choked, can be estimated by means of the following approximation:

$$W_g = C_d \times S \times p \times \sqrt{\frac{M}{ZRT} \times \gamma \times \left(\frac{2}{\gamma + 1}\right)^{\frac{(\gamma+1)}{(\gamma-1)}}} \quad (kg/s)$$

where

- C_d – discharge coefficient (dimensionless);
- S – cross section of the opening (hole), through which the fluid is released (m^2)
- p – pressure inside the container (Pa);
- M – molar mass of gas or vapour (kg/kmol);
- Z – compressibility factor (dimensionless);
- R – universal gas constant (8314 J/kmol K);
- T – absolute temperature of the fluid, gas or liquid (K);
- γ – polytropic index of adiabatic expansion (dimensionless).

The volumetric flow rate of gas in (m^3/s) is equal to:

$$Q_g = \frac{W_g}{\rho_g} \quad (m^3/s)$$

where,

$$\rho_g = \frac{p_a \times M}{R \times T_a} \quad (kg/m^3)$$

is the density of the gas at atmospheric pressure (p_a = 101325 Pa) and absolute ambient temperature (T_a).

Figure 5.18 illustrates the assessment of the release rate for the third type of sources of release of Test 3. This release is sonic, because the pressure inside the gas container is higher than the critical pressure p_c. It considers the summation of the sources of release as detailed in the following paragraphs.

In indoor areas with more than one source of release, the releases need to be summated before the degree of dilution and background concentration is determined. Since continuous grade releases, by definition, can be expected to be releasing most if not all of the time, then all continuous grade releases should be included.

Primary grade releases occur in normal operation but it is unlikely that all of these sources will be releasing at the same time. Knowledge and experience of the installation should be used to determine the maximum number of primary grade releases that may release simultaneously under worst case scenarios.

Secondary grade releases are not expected to happen in normal operation so, given that, it is unlikely that more than one secondary source would release at the same time. Only the largest secondary release should be considered.

The summation of sources of release with predictable activity should be based on detailed analysis of operating conditions. In the determination of the summated releases (both mass and volumetric):

- the overall continuous release is the sum of all the individual continuous releases;
- the overall primary release is the sum of some of the individual primary releases combined with the overall continuous release;
- the overall secondary release is the largest individual secondary release combined with the overall primary release.

Where the same flammable substance is released from all of the release sources then the release rates (both mass and volumetric) can be summated directly.

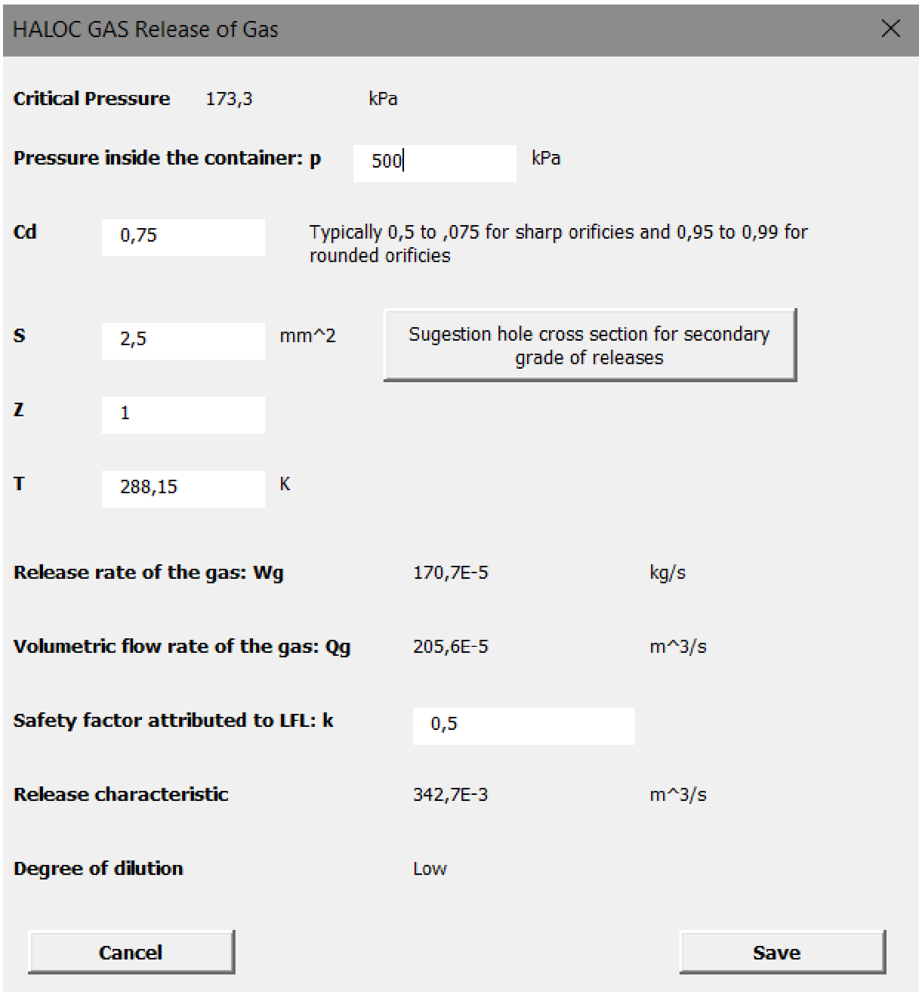


Figure 5.18 – Release of Gas form for the 3rd source of release of Test 3

In Figure 5.19 are the results obtained at the end of the simulation.

In this case, because the background concentration in the enclosed space is higher than the critical ($X_b > X_{crit}$), the degree of dilution is **low**. The procedure of estimating the degree of dilution by using the chart is a confirmation of that fact.

By means of manual calculation for this test, the following results were obtained:

Sources of release	
1) Type	Pipe fittings with discontinuities along piping
Grade of release	Continuous
ΣW_g – summation of release rates	$1x10^{-8}$ kg/s
ΣQ_g – summation of volumetric release rates	$1,2x10^{-8}$ m^3/s
Release characteristic	$6,01x10^{-8}$ m^3/s
Degree of dilution	High ($X_b << X_{crit}$)
Zone	Zone 0 with negligible extent
2) Type	Sealing elements on moving parts at low speed
Grade of release	Primary plus continuous

ΣW_g – summation of release rates	$4{,}51\text{x}10^{-6}$ kg/s
ΣQ_g – summation of volumetric release rates	$5{,}412\text{x}10^{-6}$ m^3/s
Release characteristic	$9{,}02\text{x}10^{-5}$ m^3/s
Degree of dilution	High ($X_b << X_{crit}$)
Zone	Zone 1 with negligible extent
3) Type	Sealing elements on fixed parts
Grade of release	Secondary plus primary plus continuous
ΣW_g – summation of release rates	$1{,}707\text{x}10^{-3}$ kg/s
ΣQ_g – summation of volumetric release rates	$2{,}056\text{x}10^{-3}$ m^3/s
Release characteristic	0,34 m^3/s
Degree of dilution	Low ($X_b > X_{crit}$)
Zone	Zone 1
t_d – time required to reach X_{crit}	$2{,}052\text{x}10^3$ s
Equipment Group (from flammable substance parameters)	IIA
Temperature Class (from flammable substance parameters)	T1
Extent of Zone (From Figure 4.5)	2,5 m

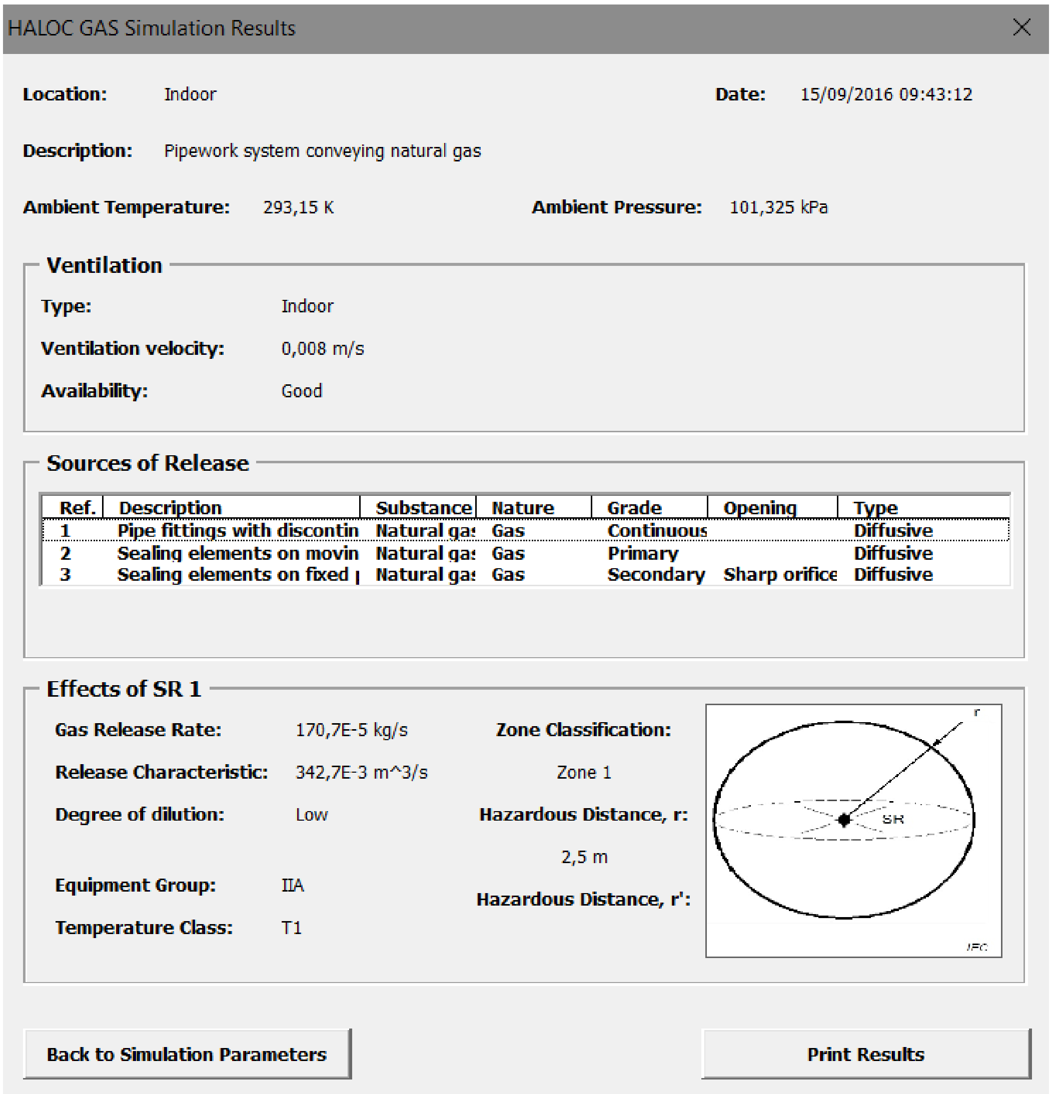


Figure 5.19 – Results form for Test 3

The resulting hazardous area comprehends the whole volume of the indoor location because:

1) the background concentration (X_b) exceeds the critical concentration (X_{crit});
2) the time t_d, for the concentration to fall to the critical concentration after the release has stopped, is significant.

Comparing the above results with the ones from the HALOC GAS prototype, one can validate the application performance in a scenario where multiple sources of release may arise.

6 CONCLUSIONS AND FUTURE WORK

6.1 Conclusions

The hazardous are classification methodology presented in IEC/EN 60079-10-1:2015 is extremely time consuming and requires a high level of expertise in physics and chemistry sciences.

Usually, the hazardous areas classification is made with manual calculation, some exceptions are major companies that have dedicated software for risk analysis.

The HALOC GAS prototype developed in this study, is designed to classify and rank the hazardous areas due to gas releases on any kind of industry, supporting the technicians on the risk analysis decisions and removing the laborious and time consuming manual calculations.

The proposed solution has satisfied the initial objectives, which were the definition, ranking and extent of hazardous areas according to the standard IEC/EN 60079-10.1:2015. Although HALOC GAS has the complexity of the methodology on its programming structure, provides a user friendly and intuitive interface without the complexity of the standard.

The HALOC GAS prototype was tested with a series of different case studies combining: liquid releases, gas releases, single source of release, multiple sources of release, indoor location and outdoor location.

The results of the case studies have validated the proposed solution, mainly in the following aspect: scientific accuracy of the results regarding the standard methodology, fast results achievement, fast usability and low probability of human error.

6.2 Future Work

Regarding the predetermined objectives for the application, there are several aspects that need improvement and a considerable set of upgrades must be implemented before scaling it into real life usage.

As future work, the following improvements will be critical:

- Integrated field checklist to support the technicians when collecting the input data at the industrial plant;
- Import data from CFD simulation;
- Compare the CFD simulation data with the results obtained from the IEC/EN 60079-10-1:2015 methodology;
- Integrate the drawings of the facilities in CAD to have an accurate visualization of the hazardous areas and its extension;
- Release an instructions manual for the application.

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