Estimations of toxic vapour concentrations, by atmospheric dispersion calculations, in a nuclear power plant control room, following an offsite accidental release in the frame of probabilistic safety assessment.

Main Report

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ABSTRACT

This project is categorized as an atmospheric dispersion study about how a toxic gas external dispersion might reach a nuclear power plant control room with dangerous concentration. In fact, it is contained within a larger project, which studies how likely a train accident, related with hazardous materials transport, could end up in a dangerous toxic vapour concentration in the control room, affecting the plant safety.

The scope of the actual study is to obtain control room toxic vapour concentrations by performing a probabilistic approach of atmospheric dispersion calculations. The goal is to apply a prospective approach, aiming to use the results in the probabilistic safety assessment of the plant. The tasks developed consist of regulations review, atmospheric dispersion codes comparison and selection, scenario design and release points distribution, meteorological analysis and calculations automation, and finally, control room vapour diffusion calculations.

The Nuclear Energy Agency (NEA) has provided the Nuclear Engineering Research Group (NERG) from the Technical University of Catalonia (UPC) with the dispersion and diffusion codes, HABIT and ARCON96, for the development of the present study, under consideration of academic purposes.

The whole project is developed within the frame of a collaborative agreement between NERG group (UPC) and Nuclear Plant Licensee. Since this agreement is confidential, no real names and codification for the plant and its systems, components and materials are used. Therefore, the generic expression "The plant" is written instead.

CONTENTS

PREFACE

The content of this project is distributed in the following documents:

- Main report
- Appendixes
- Environmental impact
- Costs analysis
- Gantt diagram

Furthermore, the content of this project is composed by three main blocks, which are atmospheric dispersion analysis, mathematical methodology for achieving probabilistic approach and programming tools to perform the analysis.

The first two blocks are included in the Main Report document, and the programming tools block is included in the Appendixes.

The binding is organized by the following volumes:

- Volume 1: Main Report
- Volume 2: Appendixes, Environmental impact, Costs analysis and Gantt diagram.

The appendixes contain: codes verification, meteorological concepts, programing methods for instantaneous and continuous release and nuclear technology concepts.

ACKNOWLEDGEMENTS

This work is a culmination of an intense year studying such an amazing science, as to be nuclear engineering. Indeed, I am grateful to all the teachers that made it possible. Furthermore, this is also the beginning of a very interesting project that will be developed at the NERG which I feel fortunate to be a part of. For this reason, I want to thank professor Javier Dies, who gave me this opportunity to collaborate and work in NERG, I also want to thank Alfredo de Blas, who, as the director of this thesis has provide me with guidance in the path to take. Finally, I want to thank my partner Pedro Díaz, who, as an expert in probabilistic safety assessment, has been constantly helping me to better understand this discipline.

GLOSSARY

- ACRS. Advisory Committee on Reactor Safeguards
- AEC. Atomic Energy commission
- DBA. Design Basis Accident
- CFR. Code of Federal Regulations
- CRH. Control room habitability
- GDC. General design criteria
- LOCA. Loss of Coolant Accident
- NIOSH. National Institution for Occupational Safety and Health
- NEA. Nuclear Energy Agency
- NEI. Nuclear Energy Institute
- NERG. Nuclear Engineering Research Group
- NRC. Nuclear Regulatory Commission
- PNL. The Pacific Northwest Laboratory
- PSAR. Preliminary safety analysis report
- UPC. Polytechnic University of Catalonia

LIST OF FIGURES

1. INTRODUCTION

The generation of electricity by nuclear fission reaction consist of an activity with specific associated risks. Due to the importance of maintaining the reactor cooled in front of any transitory situation, derived from either an accident or a transition among operation modes, all the paths that lead the plant to the cold shutdown must be guaranteed with redundancies and quality assurance. These paths consist of any structure, system and/or component, as well as any human action, which allow the reactor to reach cold shutdown from any higher energy state.

This condition makes nuclear fission energy different from any other industrial activity, and requires a rigorous and deep treatment whenever safety assessment and management is to be performed.

Increasingly, the safety studies carried on in nuclear power plants have been taking into account very low probability occurrence scenarios that could cause severe accidents with significant consequences for the plant. Fukushima Daichii accident has been a powerful trigger for this trend change.

Therefore, there is a need of assessing this external risk with a probabilistic approach, which nowadays are performed with a deterministic approach. In this study it is proposed a methodology that provides with a solution for this issue.

The rare events evaluated in this study are classified within external both natural and accidental type, and normally, they are estimated with a punctual frequency of occurrence. In fact, these events consist of a sequence of several little probability events, which might have very different probability density functions.

Specifically, in this project is to be studied how a train accident, with toxic chemical shipment, would affect a nuclear power plant safety, by contaminating the control room with dangerous toxic concentrations and, therefore, preventing the control room personnel to perform their tasks related to the reactor safety.

The methodology applied provides with probability density functions of toxic gas concentration in the control room. And they can be compared with limiting conditions established by regulator body.

2. REGULATIONS HISTORY REVIEW

In February 1971, the Atomic Energy Commission published Appendix A, *General Design Criteria (GDC) for Nuclear Power Plants,* requiring the applicant a preliminary Safety Analysis Report (PSAR) including the description of principal design criteria of the facility. Regarding to **control room safety assessment**, it was established in the criterion 19 (GDC 19), *Control Room,* both alternative shutdown station(s) and habitability requirements. GDC 19, in part, requires:

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

Reference [1][2]

In the early 70's, K. Murphy and K. Campe developed a method for the evaluation of radiological events in control room, ref. [3]. In 1974 and 1975, NRC Regulatory Guides 1.78 and 1.95 were issued to provide guidance on the protection of the control room operator from accidental releases of hazardous chemicals or chlorine gas respectively.

2.1 REGULATORY GUIDE 1.78

The methodology established and applied at that moment, for instance, in the Regulatory Guide 1.78, regarding to shipment **accidental release** of hazardous chemicals, was to obtain the accident probabilities from transportation **frequencies**. Additionally, the atmospheric dispersion was estimated by hand calculations applying Gaussian diffusion equations for an instantaneous ground level release. The input of meteorological conditions, however, was considered to be the worst case scenario. This was accomplished by the application of some assumptions, such as:

a. *Selection of appropriate **stability category** based on the worst five percentile meteorology observed at the site.*
b. *Determination ot the x, y, and z standard deviation values based on the **Pasquill** stability categories.*
c. *Additional credit due to **building wake** or other dispersive phenomena may be allowed, depending on the properties of the released gas, the method of release, and the intervening topology or structures.*

> d. **Windspeed** *should be selected to maximize the two-minute concentration within the control room.*

<div align="right">Reference [4]</div>

In that guide, ref. [4], were also described **methodologies** to identify which chemicals were to be studied. One of the substances was chlorine, and a separate guide (Regulatory Guide 1.95, ref. [5]) was provided to give direction of proper protection for control room operators from an onsite chlorine release. Finally, the **substances selection** would be done utilizing the tables of hazardous materials contained in the guide. This tables linked **toxicity limits** of main hazardous materials, distance from the source to the intake and type of control room, regarding to volume and air exchange rate.

2.2 THREE MILE ISLAND AND CRH REQUIREMENTS

The accident of Three Mile Island caused changes on the Regulatory Body policy, which made, among other actions, a revision of the Standard Review Plan in July 1981, NUREG 0800, ref. [6]. The SRP identified Loss of Coolant Accident (LOCA) as the **limiting design basis accident** (DBA) for CRH. Nevertheless, other DBAs had to be reviewed to determine whether they could be more limiting. Licensees were to provide assurance that the **habitability systems** will operate under all postulated conditions (DBA) to permit the control room operators to remain in the control room to take appropriate actions required by GDC 19.

2.3 REVIEWS OF CONTROL ROOM HABITABILITY

In the 1980s the Advisory Committee on Reactor Safeguards (ACRS) identified some issues related to CRH, such as:

- *Control room **infiltration measurements**, which identified that a key parameter affecting control room habitability is the magnitude of control room air infiltration rates.*
- *Control Room **Habitability**, which identified that loss of control room habitability following an accidental release of external airborne toxic or radioactive material or smoke can impair or cause loss of the control room operators capability to safely control the reactor.*

<div align="right">NUREG-0933, ref. [7]</div>

The main concern of ACRS was that they found deficiencies in the maintenance and testing of engineered safety features designed to maintain control room habitability.

Consequently, a Control Room Habitability **Working Group** was created, with NRC and ACRS constituents, with the purpose of identifying any recommended actions that would **correct** significant deficiencies in control room habitability design, installation, test or maintenance.

The working Group concluded that, some improvements were needed in the control room habitability system evaluation. Accordingly, the staff (NRC) initiated activities to develop:

- Improved methods for calculating control room dose and **exposure levels**,
- Improved **meteorological models** for use in control room habitability calculations and
- Revised **exposure limits** to toxic gases for control room operators.

The results of the improved methods were documented in NUREG/CR-5669, ref. [8] and NUREG/CR-62, ref. [9]. The first one was conducted to evaluated five toxic substances concentrations in order to determine limiting conditions for operators in a dynamic scenario. The substances were ammonia, chlorine, Halon 1211, Halon 1301, and sulfur dioxide, of which both Halons are forbidden nowadays, due to their implication in the greenhouse effect.

The second one, NUREG/CR-62, ref. [9] is related to **computer codes** for evaluation of control room habitability. These codes constitute a package called **HABIT**, and they allow calculations of both hazardous and radioactive materials concentrations.

Furthermore, as it was expected from the ACRS, the NRC staff took into consideration the recommendations of the National Institution for Occupational Safety and Health (NIOSH) regarding to hazardous chemicals.

2.4 COMPUTER CODES FOR ATMOSPHERIC DISPERSION CALCULATIONS

These codes included in HABIT, however, were developed to evaluate only **instantaneous release** within a two minutes effect in the control room, which, accordingly to RG-1.78, ref. [4], corresponds to a maximum concentration chemical accident. Hence, they did not cover the whole evaluation recommended by the regulatory guide, since it differenced between maximum concentration chemical accident and maximum concentration-duration chemical accident. The second evaluation type is related to continuous release accident.

On the other hand, after the work done in the 1980s regarding to atmospheric dispersion field tests, which were conducted within building complexes, it was safe to say that Murphy-Campe methodology ref. [3], had a tendency to overestimate concentrations during low wind speed conditions. Thus, a more complete methodology for better describe the dispersion phenomena became desirable.

The Pacific Northwest National Laboratory, under contract with the NRC, got to work on the development of a more robust code. The result was the ARCON96 code, which stands for Atmospheric Relative CONcentrations in building wakes, and which was published in May 9, 1997 in revision 1 to NUREG/CR-6331, ref. [10].

The **ARCON96** code uses hourly meteorological data to calculate relative concentrations at control room air intakes that would be exceeded no more than five percent of the time. These concentrations are calculated for **averaging periods** ranging from one hour to 30 days in duration. Additionally, ARCON96 gather the improvements resulting from atmospheric dispersion studies in presence of buildings whenever meteorological conditions indicate calm winds. Consequently, the concentration data obtained correspond to a **continuous release** chemical accident scenario, which coincides with the second evaluation type recommended by RG-1.78, ref. [4].

In July 2000 it was published a review of the GDC-19 as the RG-1.183, with the title "*Alternative Radiological Source Terms For Evaluating Design Basis Accidents At Nuclear Power Reactors* ". Since it was about the improvements of effective dose criterion for control room operator, it will not be treated in this study.

In June 2001, Nuclear Energy Institute (NEI) published a guide document to assess control room habitability. It was published as NEI 99-03, ref. [2], and by which, this summary is considerably inspired.

Finally, in June 2003, NRC staff issued a regulatory guide which provides **guidance** on determining atmospheric relative concentration values, which will be used in radiological habitability assessments of the control room. This is RG-1.194, ref. [11] and it clarifies the use of **ARCON96** code in relative concentration calculations, as well as alternative procedures for calculating ground level and instantaneous releases.

2.5 RECOMMENDED METHODOLOGY IN FORCE

Although ARCON96 was an improvement in dispersion models, it is important to take into account that, this code was developed for control room radiological habitability assessments. Therefore, it should not be assumed that it is acceptable for any other purpose than that. Hence, whenever relative concentrations for toxic gas dispersion are to be estimated, the regulatory positions are provided in Regulatory Guide 1.78, ref. [4].

3. OBJECTIVE OF THIS STUDY. "FROM DETERMINISTIC TO PROBABILISTIC".

The procedure established in RG 1.78 to preform risk assessment associated to an accidental toxic chemicals release, consist of a sequence of conservative assumptions about the weather conditions, as well as filtering criteria to enter the input initial conditions, such as accident distance, chemical quantities and release rates. The only statistical frequencies introduced would be train accident and the amount of chemical shipped.

The result of applying this methodology is the determination of whether the resultant frequency is acceptable or not, for the plant safety.

Nowadays, however, the odd external events, that could cause severe consequences, are growing in importance, especially after the Fukushima Daiichi accident. Hence, there is an increasing need of understanding the likelihood of these events, in a way that would allow them to be integrated in the safety assessment of the plant.

On account of the fact that the plants apply a probabilistic approach in their risk assessment studies, by performing Probabilistic Safety Assessments, it is concluded that the better way of integrating external events risk evaluations, would be to determine their probabilistic density function.

Consequently, the goal of this study is to perform a risk analysis about external event of toxic chemical release using a probabilistic approach, ergo, to find the probability density function of the event that leads to significant consequences for the plant.

In order to achieve it, solid statistic studies about meteorological conditions and train accidents must be carried on.

As a part of a bigger project, this study focuses on how meteorological conditions can be introduced in the calculations in a probabilistic way, instead of applying the worst case scenario, which is the procedure described in RG-1.78.

4. METHODOLOGY APPLIED

The methodology applied, to achieve the project objectives, consist of the following steps:

- Validated dispersion models analysis, (already introduced in previous chapters)
- Alternative dispersion models exploration and assessment.
- Meteorological data analysis
- Computational methodology selection and solution proposal
- Case study development
- Analysis of the Results and comparisons

Let us introduce the atmospheric dispersion phenomenology before developing the objectives.

There are several ways to estimate **atmospheric dispersion**. The dispersion models can be classified according to the approach on how they represent the system to be modeled, that is, physical approach or mathematical approach. They also can be classified according to the scale they try to represent, that is, micro scale or meso-scale or global scale.

Meso-scale models represent atmospheric dispersion in areas from 20 km to 500 km. Finally, global scale models represent the whole atmosphere. Lagrangian puff models are an example of the mathematical approach for this scale.

The **micro-scale** models represent atmospheric dispersion that takes into account the terrain and buildings effects. They can be realistic, as to be CFD models, or simpler and more conservative, like Box models, Gaussian models or Eulerian models.

On the account that validated models are programmed with Gaussian plume models, it is added a brief description about it. Gaussian model equation is the solution a mass balance transport equation when the standard deviations are function of distance and atmospheric stability.

As advantages, they are esay to use and program, very intuitive, fast and consistent with the random nature of turbulence. Furthermore, they are officially accepted, since many regulatory organisms use it.

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The drawbacks are mainly related to accuracy. Flow is idealized, emission rates are constant and the mean wind speed is assumed to be larger than the standard deviations of turbulent velocities. Ref. [21]. Additionally, they need corrections for terrain or building effects, as for instance, the building wake effects, that are explained on the following lines.

4.1 BUILDING WAKE EFFECTS

Building wake effects are turbulences that modify the pollutant trajectory calculated with dispersion models. The validated codes below correct this effects by coefficients obtained from experimental data. The way this correction is added to main program is by Cross-sectional Area parameter, and it is explained with the next three figures.
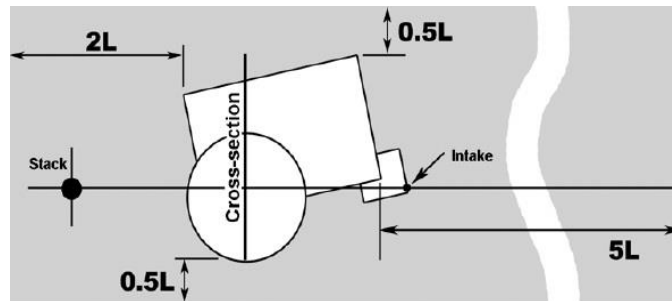
1 Figure 5.1. Overhead view of the cross-section. Source: ref. [11]
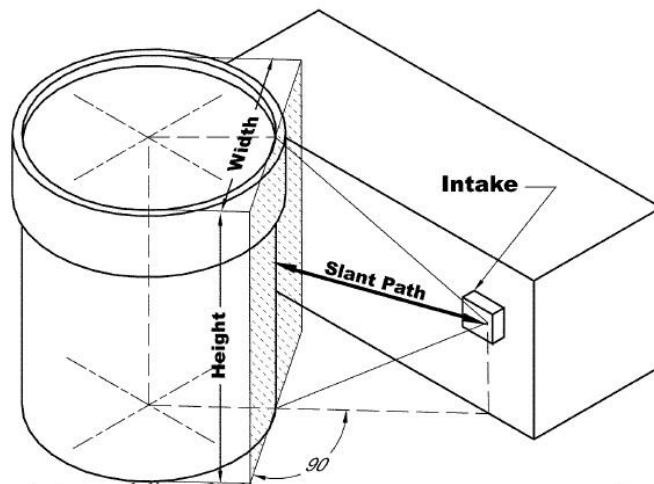
2 Figure 5.2. How to apply angularity when obtaining cross-sectional area. Source: RG-1.194, ref. [11]
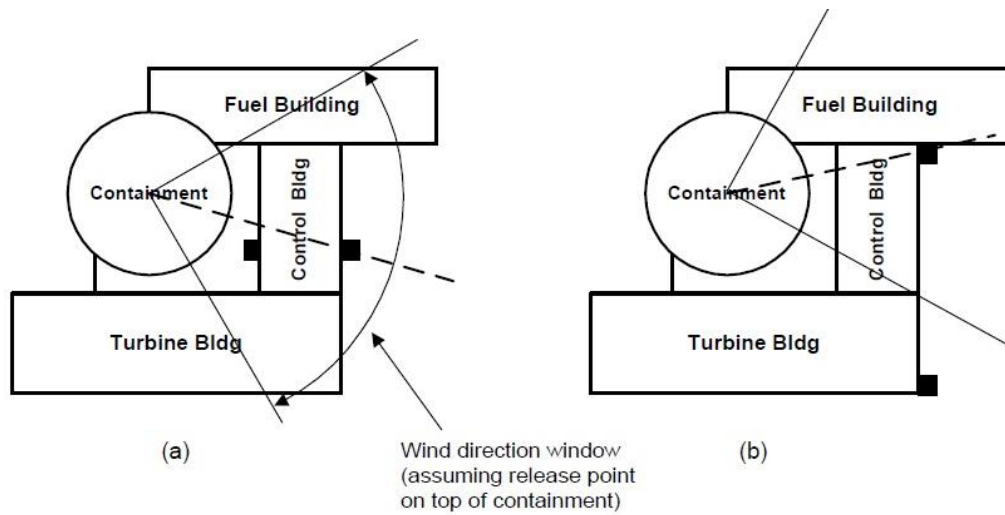
3Figure 5.3. How to calculate the wind direction window to apply wake effects. Source: ref. [11]

The figure 5.3 illustrates how to estimate wind direction window in the cases the release comes from the containment building. In contrast, the wake effect for a release on the rail zone has opposite wind direction window. It can be appreciated at solution proposal chapter below.

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5. VALIDATED DISPERSION COMPUTER CODES

NEA has provided the NERG group with HABIT and ARCON96 codes with the purpose of allowing this academic analysis. In the following chapters there is a brief description of both codes. These codes are validated by NRC for the dispersion estimations and control room habitability, in the case of HABIT, and for the maximum concentration-duration release of radionuclides in the case of ARCON96.

5.1 HABIT

As it has been commented, HABIT consist of an integrated package of several programs validated by NRC ref. [2][9], that can estimate both radionuclides and toxic chemicals concentration in the control room by dispersion coming from both in-site and off-site sources.

The package is composed of five modules, of which two are used to calculate toxic chemicals concentration in the control room. The first one is EXTRAN, which returns the release rate of a chemical in the event of accidental release due to leaks or ruptures of liquid or gas tanks. It uses a model that computes atmospheric dilution, including the effects of building wakes, to determine the relative concentration arriving at the intake to the control room. The second code, CHEM, models the dilution of the chemical by mass balance calculations in the control room allowing the assessment of the habitability related to the exposure of the personnel.

The other three modules TACT5, FPFP_2 and CONHAB estimate dose in the control room due to an accidental release of radionuclides.

The Pacific Northwest Laboratory (PNL) unified the five modules and gave the package a user-friendly interface. Data entry routines use windows designed to guide the user through the correct sequence of steps and to allow easy review and editing of the data. However, the modules can be processed separately with no interaction with the interface.

5.1.1 EXTRAN dispersion code

EXTRAN was developed by PNL aiming to improve atmospheric transport and diffusion models existing and validated by U.S.NRC (Murphy and Campe 1974) ref.[6]. The EXTRAN code combines procedures for estimating the amount of airborne material, a Gaussian puff model, and finer building-wake diffusion coefficient algorithms (Ramsdell, 1995), ref. [12].

With a scenario postulated by the user, specifying meteorological and release conditions, EXTRAN computes a concentration time history at the control room air intake. Specifically, it estimates concentrations from the time the substance first arrives at the air intake until actions can be taken to protect control room occupants.

Moreover, EXTRAN estimates the transfer of the substance from the tank to the atmosphere. This transfer can be executed either in one time step, as might be in an instantaneous gas release, or in a sequence of a liquid pool evaporation.

The toxic substance processed by the code may be gas, a liquefied gas, a volatile liquid, or fine particulate material suspended in a gas. It processes as well the tank material, environmental conditions and the relationship between the tank and the intake. However, it does NOT include a model for the rise of a plume from a stack. For a situation in which a toxic substance is released at a temperature significantly warmer than the ambient air or with a significant vertical velocity, it is necessary to first calculate the effective stack height of the plume and use that value for the "Release Height" in EXTRAN.

EXTRAN estimates **short-term** concentrations at a single location **downwind** of a release of toxic or radioactive material. Additionally, it deals with releases of two types of material: gasses and liquids.

Gas burst and leaks
The source term and the mass must be specified. The mass balance is simple. All of the material leaving the tank enters the atmosphere directly. The energy balance is not maintained for gases releases. Hence, when an accident of a tank containing gas is postulated, **all** of the **gas** enters the **atmosphere** at the time of the failure.

Liquid Tank Bursts and Leaks.
In the case of release of material stored as a liquid, specifying the amount of liquid in the tank and the release rate does not completely determine the source term for atmospheric dispersion. Material in the pool evaporates in response to the **vapor pressure** of the liquid, and the temperature of the pool is adjusted to maintain an **energy balance** between the pool and the environment.

The phenomena, such as Flashing, Liquid pool, Evaporation, solar radiation, long-wave radiation, etc, that take place in mass balance of materials that are stored as liquids, are detailed in the code guidelines. Before any of the material can enter a plume, it must become vapor. This state change involves energy transfers and

transformations. Thus, the mass balance depends on a scenario dependent energy budget.

Puff Model

The method applied is a three-dimensional puff diffusion model produced by superposition of solutions to the one-dimensional equation. The concentration at position x,y,z is given by:

$$C(x,y,z) = \frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} exp\left[\frac{-0.5(x-x_0)^2}{\sigma_x^2}\right] exp\left[\frac{-0.5(y-y_0)^2}{\sigma_y^2}\right] exp\left[\frac{-0.5(z-z_0)^2}{\sigma_z^2}\right] \qquad (5.1)$$

Where:

- $C(x,y,z)$ = the concentration at x,y,z
- Q = the mass of material in the puff
- $\sigma_x\sigma_y\sigma_z$ = diffusion coefficients in the longitudinal, lateral and vertical directions.

The diffusion coefficients are characteristic dimensions of the puff. They are functions of the distance (or time) from the release point, the atmospheric stability, and the surface roughness.

By defining Cartesian coordinate system, with the X-axis parallel to the wind direction, being Z-axis vertical, the center of the puff may be allowed to move with the wind. At a given moment from the release, the center of the plume can be located in the coordinates: $x_0 = Ut$; $y_0 = 0$; $z_0 = h$ where U stands for wind speed, and h would be the release height.

5.1.2   CHEM

CHEM is a simplified version of CONHAB (included in HABIT), which is used to perform radionuclides control room exposure assessment. Thus, in CHEM, all features pertaining to radioactive decay and daughter formation have been removed.

Concentrations at the control room intakes are computed by EXTRAN. The modeled process consist of the conservation of chemical mass associated with inflow and outflow.

Let us establish the outflow as the inflow plus the bottled clean air flow:

$$F_{out} = F_{in} + F_{clean} \qquad (5.2)$$

Then, the concentration in the control room may be expressed by the following equation:

$$\frac{dC}{dt} + \frac{C \cdot F_{out} - C_{in} F_{in}}{V} = 0 \tag{5.3}$$

Where:

- $\frac{dC}{dt}$ = stands for the concentration variation in a time step
- V = is the control room volume
- C_{in} = stands for the concentration at the intake of the control room.

Thus, given a concentration at the time step C(t), the concentration at the next time step would be:

$$C(t + \delta t) = C(t) \exp(-\alpha \delta t) + \frac{C_{in} F_{in}}{\alpha V} [1 - \exp(-\alpha \delta t)] \tag{5.4}$$

Where:

$$\alpha = \frac{F_{out}}{V} \tag{5.5}$$

5.2 ARCON96

ARCON96 was created with the purpose of improving dispersion models with building wake effects during calm winds. The code uses hourly meteorological data to calculate relative concentrations at control room air intakes. These concentrations are calculated for **averaging periods** ranging from one hour to 30 days in duration.

The basic diffusion model implemented in the ARCON96 code is a straight-line Gaussian model that assumes the release rate is constant for the entire period of release.

Diffusion coefficients used have three components. The first component is the diffusion coefficient used in other NRC models, such as XOQDOQ (Sagendorf, et al. 1982, ref. [13]) and PAVAN (Bander 1982, ref. [14]). The two other components are corrections to enhance the dispersion in calm winds and building wakes situations, as they are described by Ramsdell and Fosmire (1995).

5.2.1 Diffusion model

The ARCON96 code implements a straight-line Gaussian diffusion model. The basic model for a ground-level release is:

$$\frac{\chi}{Q'} = \frac{1}{\pi \sigma_y \sigma_z U} \exp\left[-0.5 \left(\frac{y}{\sigma_y}\right)^2\right] \qquad (5.6)$$

Where:

- χ/Q' = relative concentration [(Ci/m³)/(Ci/s)]
- $\sigma_y \sigma_z$ = diffusion coefficients (m)
- U = wind speed (m/s)
- Y = distance from the centre of the plume (m).

It is assumed that the release is continuous, constant, and of sufficient duration to establish a representative mean concentration. Moreover, the equation also assumes that the material being released is reflected by the ground.

This equation is completed with the **correction** of the **diffusion coefficients** σ_y and σ_z by means of **low wind** speed corrections and **building wake** corrections, section 3.2.1 to NUREG/CR 6331, ref. [10] .

The resultant model is a replacement for the dispersion model in the control room habitability assessment procedure developed by Murphy and Campe (1974), ref.[3]. Studies conducted by NRC concluded that Murphy-Campe model did not predict the variations of the concentrations in the vicinity of the buildings with precision. One of the reasons for this lack of accuracy was determined to be over predictions during low wind speed conditions.

The next graph shows a comparison for predictions made by both methods, which expressed concentrations as a function of wind speed. The executed model gathered conditions of existing diffusion experiments performed at seven reactor sites.
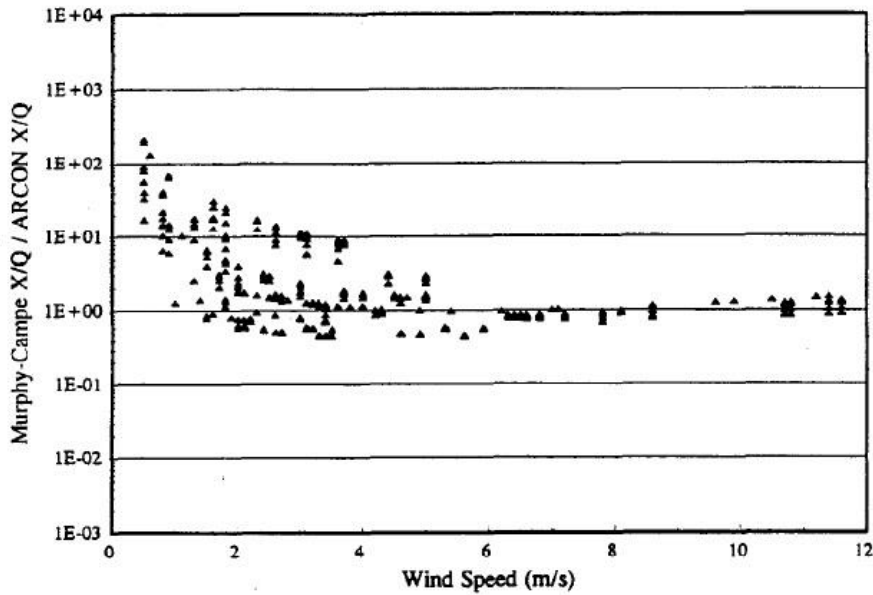
4 *Figure 5.1. Murphy-Campe / ARCON concentration ratios by observed concentration.*
Source: NUREG/CR 6331, ref. [10]

In the figure (5.1), ratios greater than one indicate that the Murphy-Campe model predicts higher concentrations than ARCON96, and vice versa for values lower than 1. As it is seen in the figure, ARCON96 estimates higher values up to a factor of 2 for wind speed values greater than 1 (m/s). However, for wind speed values lower than 1 (m/s), ARCON96 predicts concentrations that are more than a factor of 10 lower than the Murphy-Campe model predictions. Hence, it is safe to say that use of ARCON96 in place of the Murphy-Campe model would have the greatest effect at reactor sites with low average wind speeds. At those sites the effect of changing models would be a general reduction in the relative concentrations used to evaluate control room concentrations resulting from postulated accidents.

5.2.2   Sector average diffusion model

The previous equations are useful to obtain one-hour concentration periods. Nevertheless, in order to obtain larger periods values, a sector-average relative concentration model is used, in order to estimate concentrations for periods after the initial 0-8 hour period. The sector-average plume model is derived by integrating the concentration across the normal plume model to obtain a crosswind integrated concentration, CIC, which is:

$$\frac{CIC}{Q'} = \int_{-\infty}^{\infty} \frac{1}{\pi \Sigma_y \Sigma_z U} exp\left[-0.5\left(\frac{y-y_0}{\Sigma_y^2}\right)\right] dy \qquad (5.7)$$

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Where $\Sigma_y \Sigma_z$ are the corrected dispersion coefficients for low wind and building wake effects. The relative concentration is then calculated by dividing CIC/Q' by the width of the sector, W,

$$\frac{\chi_{sa}}{Q'} = \frac{2}{\sqrt{2\pi} W_S \Sigma_z U} = \frac{0.80}{W_S \Sigma_z U} \tag{5.8}$$

In most cases, the sector width is defined as the width of a 22.5° sector, which is a function of the distance downwind. This procedure works well except for small distances in unstable atmospheric conditions. In these unstable conditions the procedure gives sector average concentrations that are greater than the centerline concentration at small distances. This can be avoided by redefining the sector width.

6. ALTERNATIVE DISPERSION MODELS

Because the validated codes apply simple methodologies to estimate atmospheric dispersion, there are grounds for believing that actual realistic models could yield a finer solution to this issue. Therefore, some available codes have been assessed with the intention of providing the licensee a robust tool to face this probabilistic approach.

6.1 LAGRANGIAN PUFF MODELS

The first explored code is CALPUFF developed by Exponent Scientists®, ref. [15]. It consist of an advanced non-steady-state meteorological and air quality modeling system. The model has been adopted by the U.S. Environmental Protection Agency (USEPA) in its Guideline on Air Quality Models as the preferred model for assessing long-range transport of pollutants.

The modeling system consists of three open main components and a set of pre-processing and post processing programs. The main components of the modeling system are CALMET (a diagnostic 3-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a post processing package).

Each of these programs has a graphical user interface (GUI).

6.1.1 Advantages and drawbacks of using CALPUFF

Since it is an already **validated** code by a U.S. Public Administration, it has clearance about its use, and it would be feasible to validate in the nuclear safety field if needed.

Another advantage is that the compound of pre-processing programs, for the meteorological input data, guarantee **reliable results** for the meteorological probabilistic assessment.

On the contrary, this is a code developed for **long-range** estimations, which means that, for distances shorter than 50 km it might not be as suitable as a plume model, although the developer claim it to fit short distances estimations and complex terrains flow behaviour.

In addition to this main drawback, it is important to take into account that, the complexity of the whole package forces the user to invest an important amount of time in order to give it a proper use. Actually, it is safe to say that a complete utilization of this package could occupy a whole PhD study. There is, however, a guide user interface (GUI) that can ease the way of learning how to use it, though is not a free or an open application.

6.1.2   HYSPLIT

Another known code for atmospheric dispersion estimations is **HYSPLIT**, developed by Air Resources Laboratory, ref. [16]. The model calculation method is a hybrid between the Lagrangian approach, using a moving frame of reference for the advection and diffusion calculations, and the Eulerian methodology, which uses a fixed three-dimensional grid as a frame of reference to compute pollutant air concentrations.

This is also a model used for mesoscale estimations. Therefore, it might not be suitable for the purposes of this study.

6.2 CFD MODELS

Computational Fluid Dynamics models could fit the purpose of improving concentration predictions in the intake of the control room. This type of codes simulate realistic behaviour of atmospheric dispersion in short-range scales. Hence they may be used to get more realistic results than both EXTRAN and ARCON96.

There are some drawbacks, however, in the use of this type of code. Firstly, the computational cost has to be consider, in case it is needed to perform high number of calculations. Secondly, it requires a detailed meteorological input database, in order to build the scenarios. This might be an issue, considering that the meteorological data available is far from plentiful. Finally, there is no known open

CFD code for atmospheric dispersion estimations. Hence, in case it was suitable, it would be necessary to make an investment on it.

7. METEOROLOGICAL ANALYSIS

Given the objective of providing this study with a prospective result, it is important to analyse meteorological phenomena as well as historic data about the involved area.

On the other hand, before digging deep into meteorological data, main parameters must be selected. This refers to physical parameters that have influence on the dispersion phenomenon. In the appendix B to this document, ref. [17], can be found a brief explanation about meteorological concepts affecting atmospheric dispersion phenomena. As it is concluded, the key parameters are **wind speed**, wind **direction** and atmospheric **stability**. These parameters are likewise affected by **insolation**, which varies depending mainly on the season, the clouds and on whether is day or night. Furthermore, the degree of insolation also affects on the degree of vaporization in the case of liquid releases.

The next step consist of a selection of the methodology to establish the parameters statistics in the area of interest. With this in mind, the review of studies about wind power generation prospection might be handy for getting inspired at this stage.

One reviewed model is the MCP, ref. [18][19], which stands for "Medir Correlacionar Predecir". The meaning is measurement, correlation and prediction, and it is applied in prospection studies for wind power generation purposes.

The goal of this methodology is to perform retrospective long-term predictions in a location in which only short-term historic data is available. The procedure consist of making correlations with meteorological stations located nearby.

This method tends to be more accurate than numerical simulation models, such as WAsP (Wind Atlas Analysis and Application Program), ref. [20], especially in complex terrains with local effect on wind. The numerical models introduce uncertainties that cannot be quantified in the prediction. Therefore, the MCP method has become a standard tool in wind power prospection.

The requirements for quality assurance in data processing are established by [Brower 2016, ref. 19],

- The point of interest (the accident or site) and the reference station must be correlated in terms of meteorology,

- Both must have homogeneous series. This means that, the measurements must be taken steadily at the same place, same height and with the same instrumentation.

- The measurement period must comply with seasonal variations, in other words, it must be measured at least one year, and they must be complete.

- The station cannot be affected by buildings or vegetation.

- The height of the measurements must be the same. Differences higher than 20 meters worsen the correlation coefficient.

Once the basis are established, the next step is to get meteorological data. The first data collected belongs to the plant, which has its own meteorological station. It measures wind speed, wind direction and temperature gradient. Temperature gradient is useful to estimate atmospheric stability.

Then, with the purpose of applying MCP method, historical data has been requested to Public Agency, which is regional public administration in meteorological assessment. Unfortunately, the request process takes its time. However, they finally provided the NERG with several stations data. These data contain wind velocity and direction, but not the temperature gradient for the simple reason that the station only takes one height measurements.

The same process has been followed with the SCAR agency (Servei de Coordinació d' Activitats Radilògiques), and it took time as well. The data collected happened to be richer in variety of parameters measured, although it did not comply with the seasonal requirement.

7.1 PUBLIC AGENCY DATA AND MCP EVALUATION

With the data provided by Public Agency can be studied the parameters wind speed and wind direction. A statistical study has been performed to assess these data, the correlation coefficients for wind speed values are:

```
station 1     station 1  station 2
station 2       0,814
station 3       0,817      0,763

Cell Contents: Pearson correlation
```

The stations have measured one-hour periods during more than 3 years, the sample for this study has been selected for the period starting on 01/02/2012 and ending on 01/02/2014.

As a result of correlation evaluation, it is safe to say that measurements taken by the three stations are correlated, and they provide the study with enough quality data to apply MCP method for wind speed parameter.

Secondly, the direction is studied as a function of wind speed. The reason to do that, is because there are correlations between the strength of the wind and the direction where it blows from, especially for the strongest winds.

The statistic is been calculated with more than 5e4 data points, and the distribution is been sectored as follows:

Dir\Wspeed	0-1m/s	1-3m/s	3-6m/s	6-10m/s	10-15m/s	>15m/s
N	6%	9%	9%	6%	3%	2%
NE	13%	13%	10%	2%	0%	0%
E	13%	11%	4%	1%	0%	0%
SE	5%	6%	15%	12%	2%	0%
S	7%	10%	27%	22%	5%	0%
SW	19%	12%	11%	7%	9%	3%
W	34%	33%	13%	24%	37%	33%
NW	4%	7%	13%	26%	44%	62%

Table 1. Table 7.1. Wind direction distribution as a function of wind speed

The following plot, which consist of a wind rose, helps to visualize the wind direction distribution.

Wind Direction Distribution. Station 1 (Public Agency)
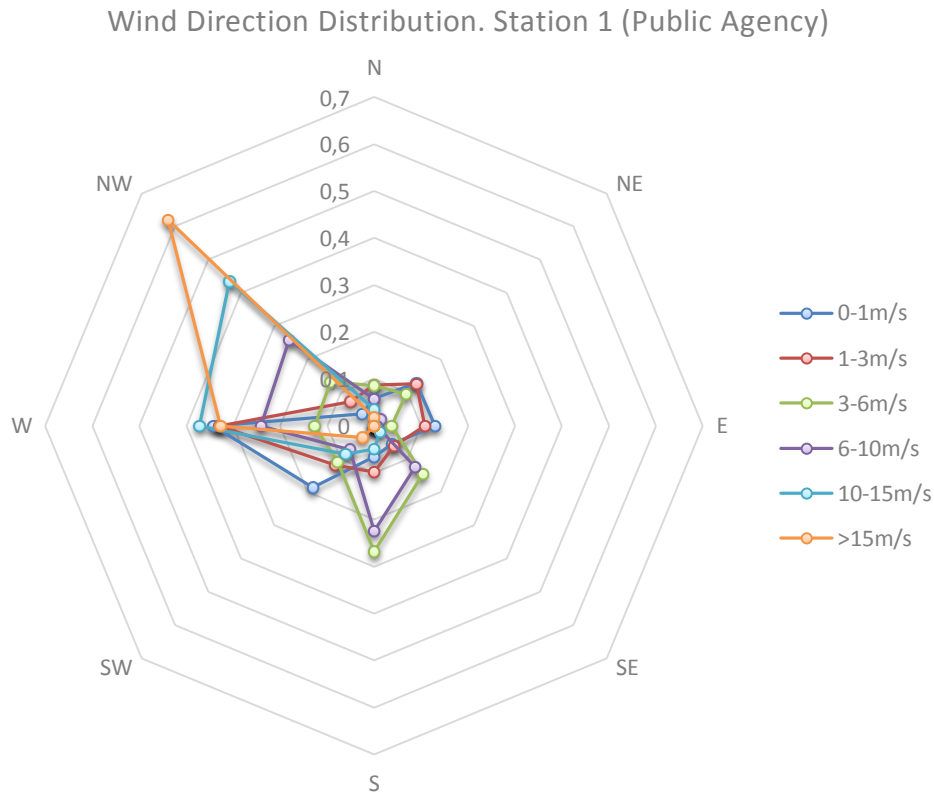
5. Figure 7.1. Wind Rose for Station 1 (Public Agency). The iso-lines stand for frequency

The measurements from Public Agency stations are reliable enough to apply the MCP method. Nevertheless, it is no possible to obtain temperature gradient parameter in these stations, since they have only one height point of measure.

7.2 SITE METEOROLOGICAL STATION

Finally, the data measured from the plant meteorological station is processed. The measured time corresponds to one complete year, and the first step is grouping velocities in bins so that their frequencies can be quantified. The bins width is 0.1 m/s and the resultant empirical probability density function is showed in the following figure:

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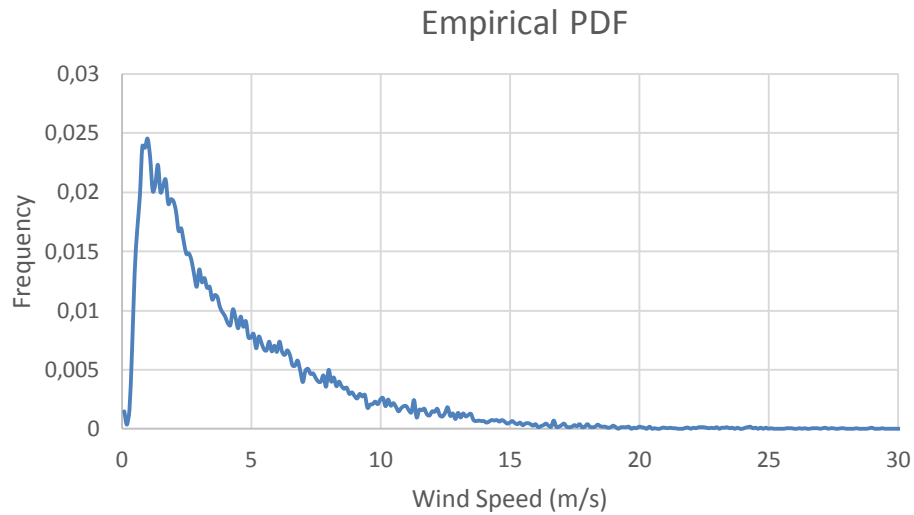
6 Figure 7.2. Empirical probability density function of wind speed measured at the plant station.

The most approximated theoretical probability function to this empirical distribution is a Weibull function. However, with a P-value < 0.01 is not fitting good enough the sample distribution. The analysis shows that the Weibull function fits the data for values greater than 1 m/s, but not for lower values.
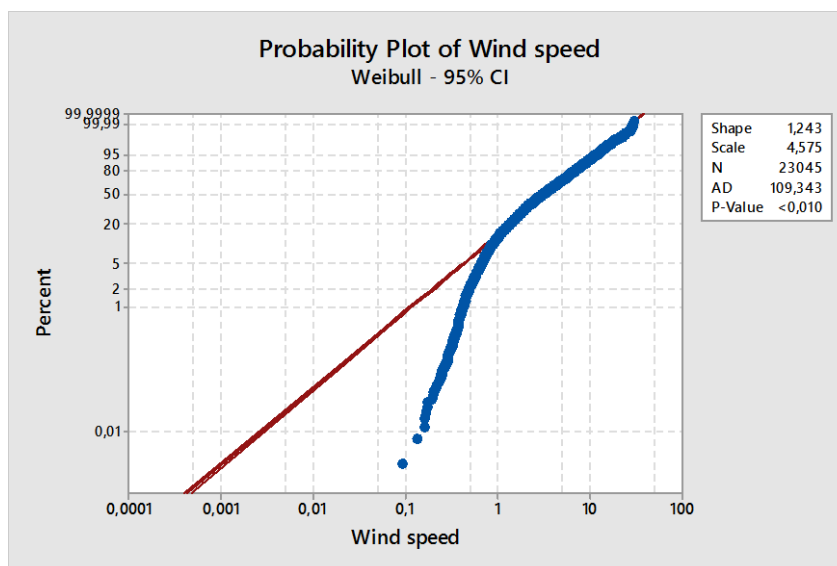
7. Figure 7.3. Probability density function analysis for wind speed measurements

Next, the cumulative distribution function is obtained from pdf, figure 7.2. The following figure 7.4 shows the result:

Empirical CDF - Plant meteo-station
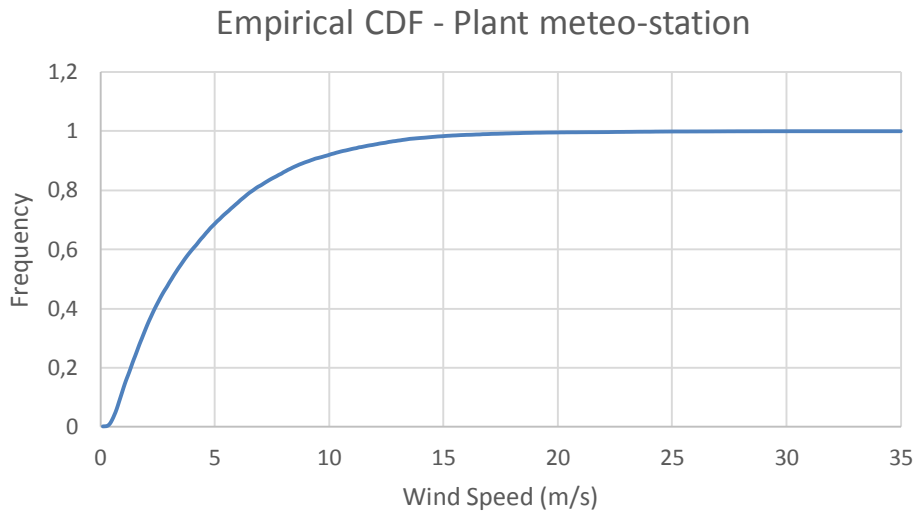
8 Figure 7.4. Empirical cumulative distribution function of wind speed measured at the plant station.

The same way Public Agency data has been processed, so it is done for the plant meteo-station, and the direction distribution is shown in the following table:

Dir\Wspeed	0-1m/s	1-3m/s	3-6m/s	6-10m/s	10-15m/s	>15m/s
N	20%	22%	6%	3%	1%	0%
NE	12%	9%	3%	1%	0%	0%
E	7%	3%	2%	0%	0%	0%
SE	12%	12%	27%	30%	46%	24%
S	18%	22%	21%	24%	8%	5%
SW	11%	4%	1%	1%	0%	0%
W	7%	6%	14%	17%	25%	52%
NW	13%	22%	27%	25%	19%	19%

Table 2. Direction Distribution as a function of wind speed. Site station

The values are a bit different from Public Agency station measurements. It can be better appreciated in the wind rose:

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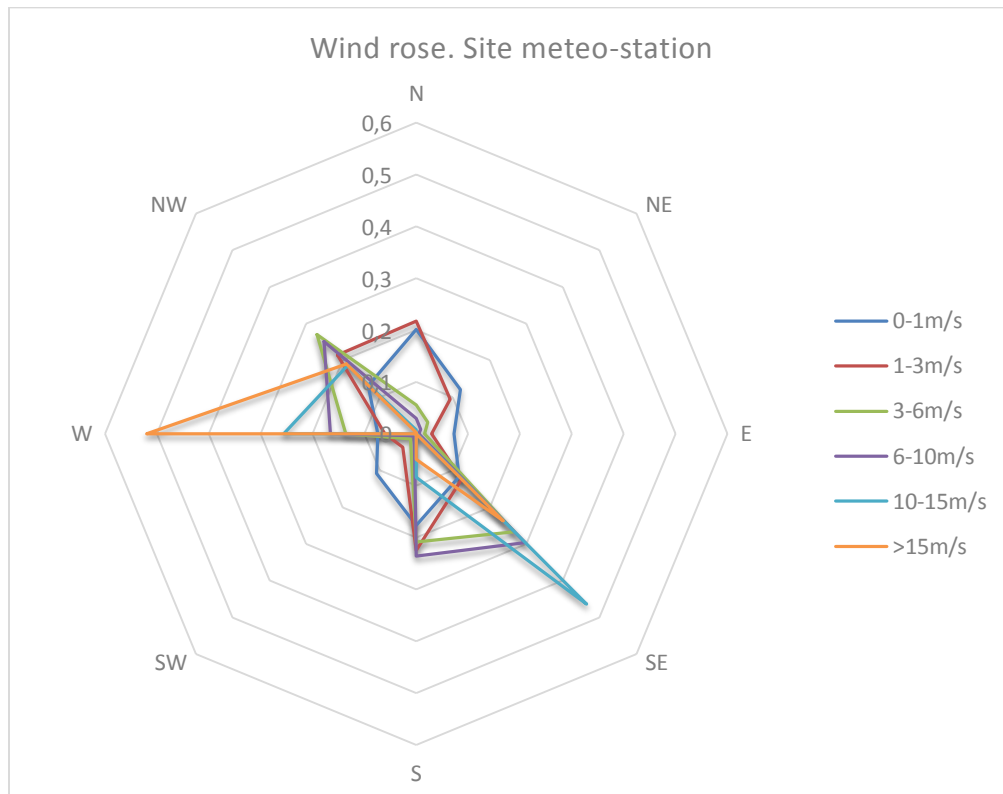
9 Figure 7.5. Wind Rose for site meteo-station.

As it is appreciated, dominant winds tend to blow from different direction in this case. However, the frequency of strong winds, in both cases, is low compared to the frequency of less than (3 m/s) winds.

Next, the temperature gradient is correlated with wind speed parameter, just the same way than direction was done. The distribution is shown at the following table:

	0-1m/s	1-3m/s	3-6m/s	6-10m/s	10-15m/s	>15m/s
stability A	1%	7%	14%	26%	24%	30%
stability B	1%	2%	4%	5%	8%	8%
stability C	1%	3%	5%	6%	9%	10%
stability D	17%	27%	38%	39%	46%	48%
stability E	43%	43%	31%	19%	12%	3%
stability F	28%	13%	3%	1%	1%	0%
stability G	6%	2%	0%	0%	0%	0%

Table 3. Stability distribution as a function of wind speed. Site meteo-station.

The following plot better illustrates stability class distribution:
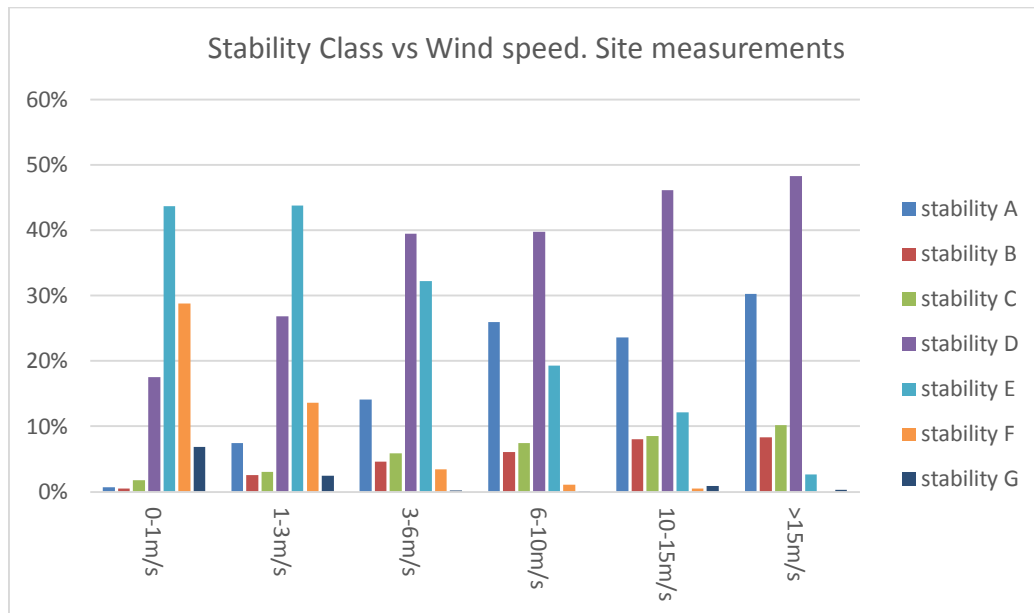
10. Figure 7.5. Stability class distribution as a function of wind speed. Site meteo-station

7.3 CONCLUSIONS ABOUT METEOROLOGICAL DATA PROCESSING

The goal of applying MCP method is to take advantage of additional stations, which have collected long-term measurements, and use it to make the forecast on the accidental release area. Since the site data only accounts for one year of collection, it would come in handy to apply this methodology.

Unfortunately, the processed data does not match the requirements described above [Brower 2016, ref. 19] to apply MCP method. The main reason is that the plant meteorological station is located higher than surrounding Public Agency stations. Thus, the wind profile is too different leaving a poor correlation between them.

Furthermore, Public Agency stations do not collect different height temperatures, so they cannot provide with temperature gradient, which is a necessary parameter to estimate atmospheric stability class.

8. SOLUTION PROPOSAL

Once the dispersion models and the meteorological data have been analysed, a solution will be selected to accomplish the objective of this study.

In accordance to RG-1.78, ref. [4], two types of accidental release must be evaluated. These consist of maximum concentration release and maximum concentration-duration release.

On the one hand, EXTRAN estimates short-term concentration dispersion by introducing worst case scenario inputs. On the other hand, ARCON96 estimates long-term concentration dispersion, and it returns cumulative distribution functions of the concentrations at the control room intake.

The way ARCON96 processes meteorological data makes it acceptable for the stochastic approach. It would be desirable, however, that this data was a forecast instead of being a collection of the past. EXTRAN, on the contrary, does not process meteorological variability.

Finally, the fact that the whole project will gather a sequence of very different nature phenomena, makes the Monte Carlo method suitable to achieve a result within a stochastic approach.

8.1 MC METHODOLOGY

Monte Carlo method is useful for simulating systems with many coupled degrees of freedom.

The scenario that is to be simulated consist of a Discrete-event System, and it is a static simulation model, by means of non-time depending simulation. The simulation of such models involve the repeated generation of the system state.

On the account that the train accident analysis will be performed separately to this study, the train accident likelihood has been postulated as a uniform distribution along the affected case area. This case area is determined, in the first place, by the RG-1.78 recommendations, and it is delimited by a 5 miles (≈8 km) radius.
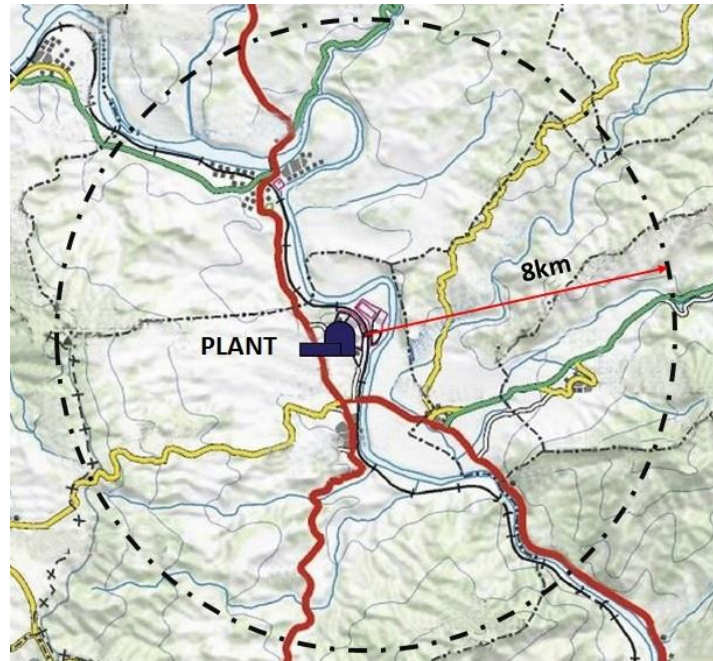
11 Figure 8.1. Case study area of interest for postulated accidents

The points of accident distributed along the rail within the area of study, have been located discreetly using UTM coordinates. Each point has associated data, such as distance to intake, direction to intake and building cross-sectional area. The building cross-sectional area is a value that will be introduced in the dispersion model in order to correct dispersion coefficients due to the building wake effects. This wake effect is produced, in this case study, by the containment building, which has a height of 45,2m over the ground level, and compared to the 22m of the control building intake, it is highly probable that this wake effect occur during toxic dispersion. No other building is affecting the dispersion.

The wind direction window is determined as follows.

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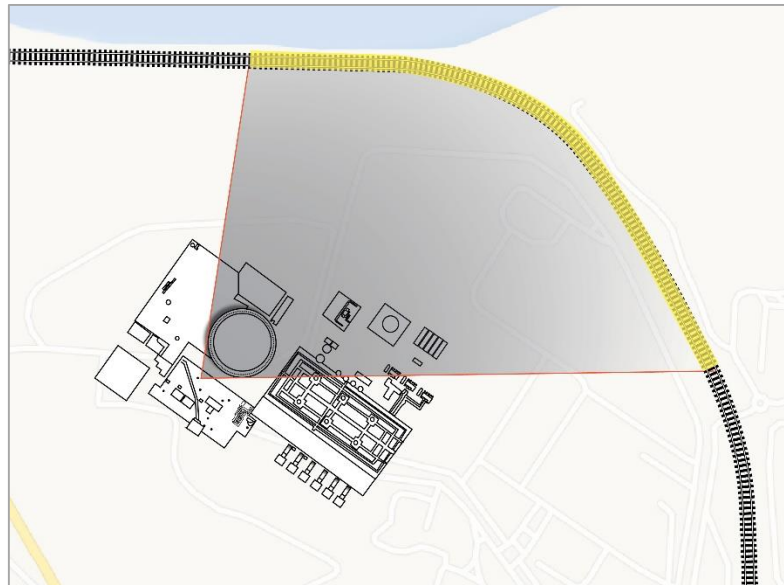
12 Figure 8.2. Rail section which includes building wake effects in its dispersion.

In the figure 8.2 can be appreciated the rail section that has to add cross-sectional area to its dispersion estimation.

Now that the geometric parameters are determined, dispersion modeling can be developed.

8.1.1   Maximum concentration release

In the case of instantaneous release, next step is to generate meteorological conditions by MC method and launch EXTRAN as the dispersion model, subsequently running CHEM. Since EXTRAN does not take into account wind direction, that is to say, it considers that wind is blowing from the source to the intake, some filtering criteria will be applied.

Let us show an overall view of the procedure before continuing with meteorological conditions and the filtering criteria methods. Each history of the MC simulation will follow the next flow diagram:
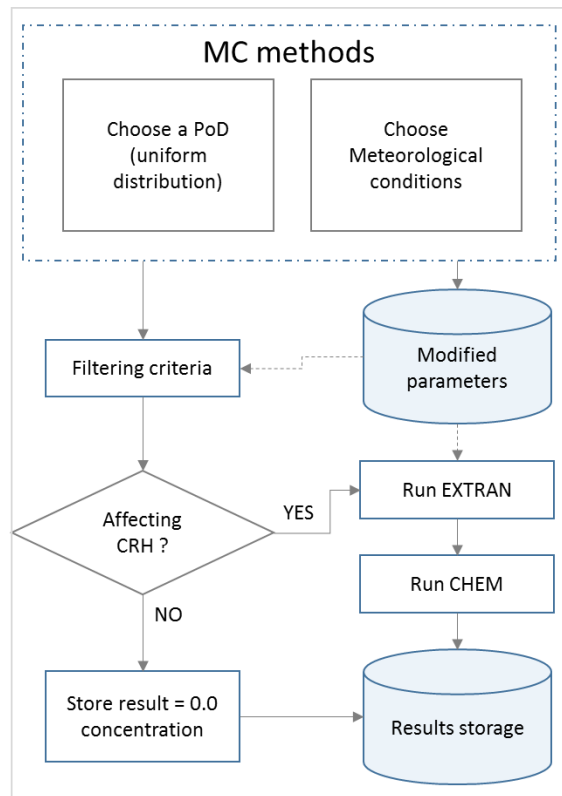
13 Figure8.3. MC Simulation methodology flow diagram for instantaneous release

By applying the filtering criteria it is saved a considerable amount of computational time, allowing to simulate greater number of histories, and therefore reducing the variance.

The procedure to obtain meteorological conditions follows a sequence of random variables generation, which starts with the generation of the first parameter, wind speed. Alter the wind speed is determined, so will be the direction and temperature gradient. Both as a function of the established wind speed. The procedure is illustrated in the following figure.
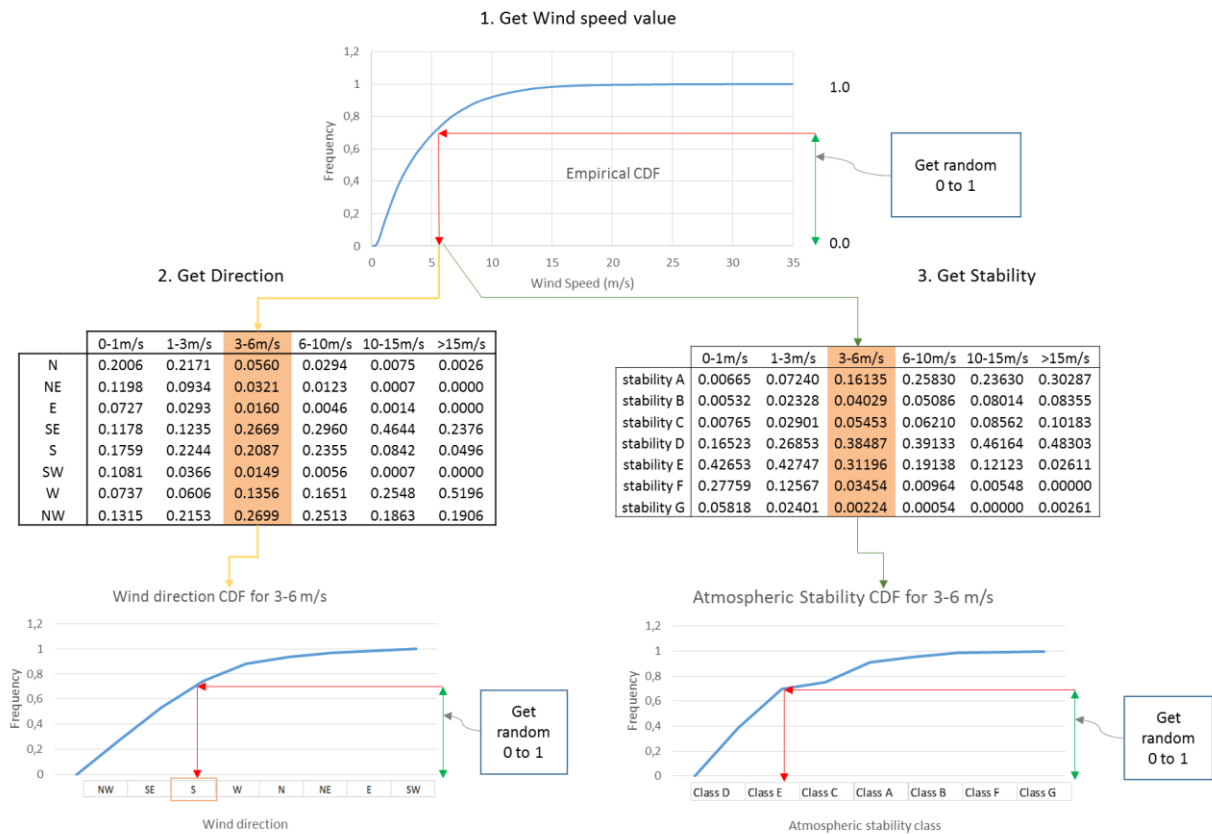
14 *Figure 8.4. How meteorological conditions are obtaining by MC method.*

The reason of obtaining atmospheric stability only from wind speed value is that wind direction can be very variable, especially during calm conditions. Hence, both direction and temperature gradient have been correlated to velocity when the conditions were generated.

With the meteorological conditions determined, the filtering process takes place. The criteria to apply could be distance as much as wind direction. Nevertheless, the distance parameter can increase uncertainties when trying to neglect the simulation. Besides, EXTRAN will neglect any condition or parameters combination that prevent the concentration to reach the intake. Therefore, the distance filtering will be done by the code.

To perform the direction selection, the plume dispersion has been taken into account. This is because EXTRAN assumes that the wind is blowing from release point to intake directly. Thus, by applying Gaussian plum dispersion, any wind direction contained within the lateral dispersion, will be considered as though it

blown straight towards the intake. Considering the wind window and the uncertainty, the filtering criterion for direction would be as it is shown next.
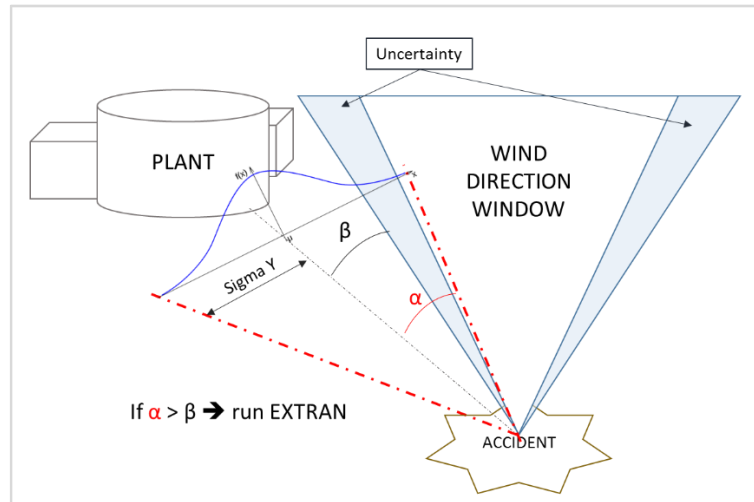
15 Figure8.5. Scheme of logical control for Direction selection

Now that the filtering is established, the dispersion codes can be run. The concentration results will be stored with the zero results from the histories that have not been selected.

8.1.2   Uncertainties

Whenever the risk is to be assessed, either by deterministic or stochastic approach, uncertainties must be quantified in order to guarantee conservative results.

On the one hand, the model contains epistemic uncertainties, which represent the lack of knowledge about the appropriate quantity to use. One example of epistemic uncertainties in this study are the dispersion mathematical model approximations, and they can be reduced by applying more realistic methods.

The technique used to model meteorological phenomena is interval analysis. In interval analysis, it is assumed that nothing is known about the uncertain input variables except that they lie within certain intervals. That is, there is no particular structure on the possible values for the epistemic uncertain variables except that they lie within bounds.

The interval analysis is the technique used to model meteorological data in this study. In the case of wind speed, the intervals have a width of 0.1 m/s, and it represents a 0,3% of the range of the measured velocities. The wind direction, however, has been classified in coarser intervals of 45º out of the total 360º. Therefore, it can be improved with finer intervals in the future.

Nevertheless, there is another type of uncertainty that might affect the result more than the epistemic uncertainties. They are aleatory uncertainties, and consist of inherent variability or randomness that cannot be reduced thought increased understanding of the phenomenon. The weather is considered aleatory uncertainty or stochastic, or type A uncertainty. Therefore, it might be useless to distribute experimental data values in fine intervals if there is too much variability. However, this stochastic uncertainty can be mixed with epistemic by studying long term retrospective meteorological data.

This retrospective analysis allows to obtain standard deviation of frequencies for the different intervals where the value is classified. As an example, let us show the next figure.
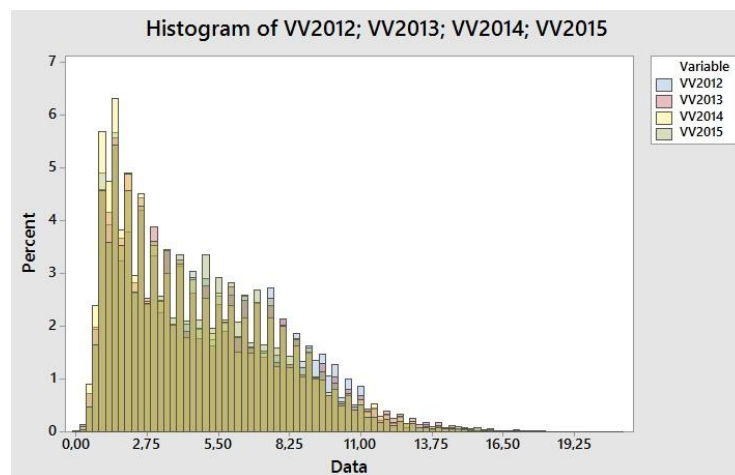
16 Figure 8.6. Wind velocities for 2012, 2013, 2014 and 2015, in Public Agency meteo-station

In order to make a qualitative assessment, the histogram is used to detect some pattern in historical data, and it has been useful to realize that slow and calm winds have more variability than strong and dominant winds. With wind direction and temperature gradient parameters the assessment of uncertainty would be done the same way.

In addition to the methodology commented, sensitivity analysis are performed to evaluate which values affect the output significantly.

8.1.3   Maximum concentration-duration release accident.

For this type of accident, the chosen code is ARCON96. Since it processes meteorological values and returns cumulative distribution functions of relative concentrations, no Monte Carlo simulation is needed to obtain meteorological conditions. Furthermore, ARCON96 provides with relative concentrations for periods

of 0-8 hours (or 0-2 hours and 2-8 hours), 8-24 hours, 24-96 hours, 96-720 hours. These periods are recommended by regulatory guide RG-1.194, ref. [11] to be analysed for accidental release of radionuclides. The RG-1.78, on the contrary, leaves the long-term release assessment to the table C-2 of the RG-1.78 itself. Given that this type of release will be calculated by ARCON96, the relative concentrations will be estimated for the periods previously commented.

The methodology starts by running ARCON96 for each point of release established within the affected area, so that the MC simulation uses stored data instead of running ARCON96 for each history. It can be appreciated in the following figure.
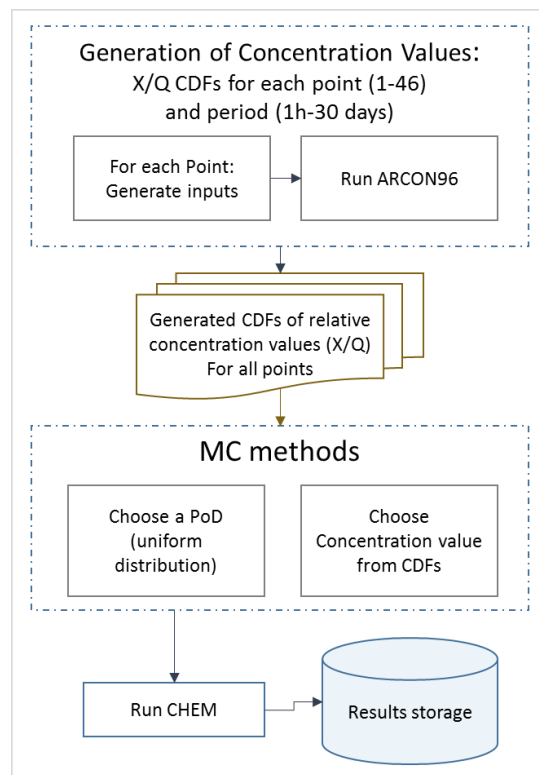
17 Figure 8.7. Overall MC methodology for Maximum concentration-duration release accident.

Then, before starting simulations, it is necessary to determine the release rate. The reason is that ARCON96 returns concentrations relative to release rate, so it is not taking into account the amount of material released.

The release rate would be calculated as the amount of hazardous material released, distributed along the period, for each period, from one hour to thirty days.

To determine release rate, in the case of liquids, the user will have to estimate how much material becomes airborne either by evaporation or flashing phenomena. The

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governing equations will be the same EXTRAN uses, see chapter 6.2.1.B.a. (Mass Balance for Liquefied Gasses and Volatile Liquids) of NUREG/CR-6210, ref. [9].

With the release rate for each period, the concentration can be estimated at the intake of the control room. Finally, by running CHEM with the concentration values obtained, the concentration levels in the control room will be estimated in order to evaluate the habitability (CRH).

8.2 COMPUTATIONAL PROCEDURES TO RUN THE MC SIMULATION

To apply a stochastic approach is necessary to yield a considerable number of samples. The better way to do that is by automating processes.

Both dispersion codes HABIT and ARCON96 are written in Fotran77, they are distributed along with Batch scripts, which, in both cases, are used to manage the introduction of the input and the execution of the fortran.exe files.

The initial idea was to call Fortran executable files directly from another programming language. This language would have been used to automate the MC process. Nevertheless, after trying different combinations, it was decided to maintain batch files as intermediary between Fortran codes and the MC script, which has been written in Python. Some issues and details of the programming tool selection process are explained in Appendix C, D and E to this document, ref. [22], [23], [24].

Even though the programming process is explained in detail in the Appendixes, it will be synthesized here to provide with an overall view of the design, as well as to inform of its possibilities.

The following diagram illustrates the design of the program.

MC Method
Instantaneous release

Python Loop Module

MC Loop:
- History generation
  - Call Exe batch
- Call Python files

Batch script

Execute Python Main:
Starts a new History

Python Main

Call Class
Define Object
Assign attributes

Ask Filter method. If True:
Call Batch-Fortran Exe

Python ClassMC Module

Meteo conditions:
Methods:

ChooseWind
ChooseDir
ChooseTG
ChoosePoint

Attributes:

MeteoFiles
Geofiles

Modify EXTRAN inputs
Method:

InputModif

Attributes:

inputFiles
MeteoFiles
Geofiles

Filtering Procedure
Method:

Filter

Attributes:

MeteoFiles
Geofiles
DispersionCoefficientsFile

MeteoFiles
Geofiles
Coeff_Files
Input Files

Batch script

Copy modified input to EXTRAN
original input

Call EXTRAN and Define output Files

Call CHEM
Define Input Files and Output Files

Call RecordingClass Python

Control Files
Collecting data Files

Input Files

EXTRAN

Output/Input Files

CHEM

Output Files

**Python Exe-Recording
Method**
From Python Main:
If Filter Method == False:
Call Recording Class

**Python Recording Class
Module**

Methods:

Reading
Recording
Controling

The process diagram in the figure 8.8 shows the program design for MC simulation in maximum concentration release evaluations. The fact that it is structured in classes, allows the user to modify simulation conditions by changing the attributes files. For instance, in case the section of possible accident must be modified, the only change needed is the Geo-Files content. Another example is the case in which the user wants to improve pre-processed meteorological data. Similarly, the only modification needed would be the data contained in Meteo-Files.

The reason of separating the looping Python module from the Python Main module is to avoid bottleneck[1] effect caused by parallel running tasks. This effect produces registering errors and collapses the process by preventing the dispersion codes to run properly.
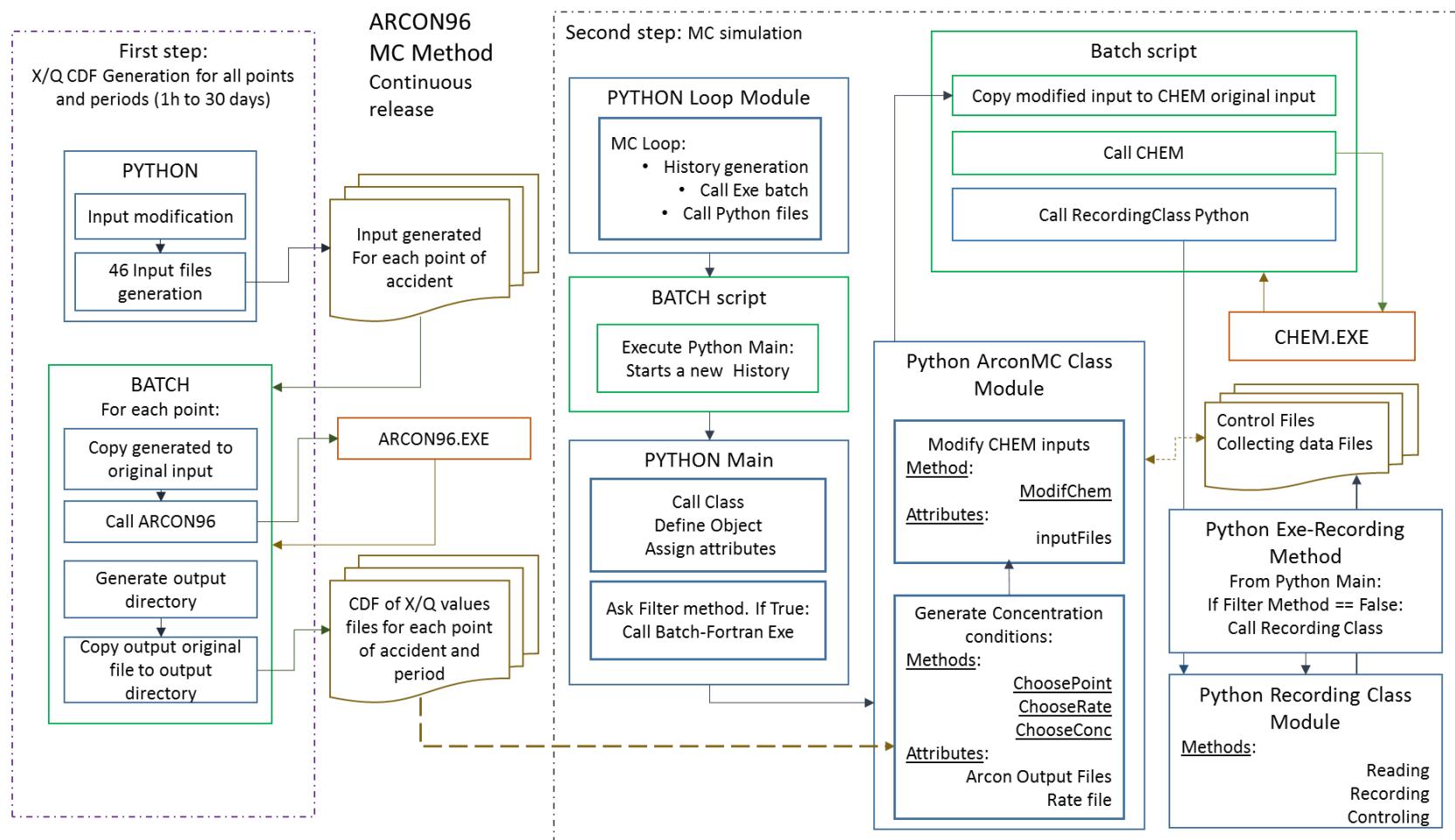
The parallel running tasks happen when Python or batch files call another program, such as fortran.exe files. Once the program is called, the script (Python or Batch) keeps doing what is programmed to, and does not wait for the other program to finish.

To prevent this situation, a control file was created so that the looping Python module can avoid starting a new loop before the simulation is finished.

8.2.1 Some features about programming design for continuous release

The procedure previously explained is for instantaneous release calculations. To perform continuous release calculations, the same approach than for instantaneous release will be used. ARCON96 is called by Batch script, which copies modified input to original input and calls fortran.exe file. The Python modification module generates a directory for each point of accident, and calls batch file to run ARCON96. Alter the files are created, it is designed a Python script that executes MC simulation by stored cumulative distribution function from ARCON96. Next, a Batch script runs CHEM using ARCON96 output values. Then, the Looping Python module can be used, as well as the method "choosePoint" from ClassMC to get point of accident, see figure 8.8 (previous diagram). More methods are needed to run MC simulation through the cumulative distribution functions of each period that ARCON96 returns.

---

[1] Bottleneck is used, as in other languages, to express a constriction in one of different possible paths in a multitask process. Thus, the Bottleneck source will set the pace of the process.

First step:
X/Q CDF Generation for all points and periods (1h to 30 days)

ARCON96
MC Method
Continuous release

Second step: MC simulation

PYTHON

Input modification

46 Input files generation

Input generated
For each point of accident

PYTHON Loop Module

MC Loop:
- History generation
  - Call Exe batch
  - Call Python files

Batch script

Copy modified input to CHEM original input

Call CHEM

Call RecordingClass Python

BATCH
For each point:

Copy generated to original input

Call ARCON96

Generate output directory

Copy output original file to output directory

ARCON96.EXE

BATCH script

Execute Python Main:
Starts a new History

PYTHON Main

Call Class
Define Object
Assign attributes

Ask Filter method. If True:
Call Batch-Fortran Exe

Python ArconMC Class Module

Modify CHEM inputs
Method:
    ModifChem
Attributes:
    inputFiles

Generate Concentration conditions:
Methods:
    ChoosePoint
    ChooseRate
    ChooseConc
Attributes:
    Arcon Output Files
    Rate file

CHEM.EXE

Control Files
Collecting data Files

Python Exe-Recording Method
From Python Main:
If Filter Method == False:
Call Recording Class

Python Recording Class Module
Methods:
    Reading
    Recording
    Controling

CDF of X/Q values files for each point of accident and period

9. CASE STUDY

In order to test the proposed solution, a case study is executed and evaluated. The case study is developed as follows:

1. Scenario description:
   - Type of release, chemical and physical properties
   - Type of control room
   - Boundary conditions
2. Calculations for both instantaneous and continuous release types
   - MC simulation for maximum concentration evaluation
   - MC simulation for maximum concentration-duration evaluation
3. Results comparison

9.1 SCENARIO DESCRIPTION

The scenario consist of a train derailment with a toxic substance release, near a nuclear power plant. The initial area of study is delimited by a 8 km radius circumference.

9.1.1 Type of release, chemical and physical properties

The postulated accident produces and accidental release of 50 tons of chlorine. The chemical and physical **properties** of chlorine are detailed in the following table:

Chemical name	Chlorine
Molecular Wt. (g/mole)	70.9
Boiling point(°C)	-34.1
Vapor pressure pure liquid (psig)	85.3
Liq. heat capacity (J/g/°C)	0.946
Density, Gas @ 0° C., 1 atm. (g/l)	3.214
Density, Liquid @ 0° C., 3.65 atm.(g/l)	1.468
Heat of Vaporization. (J/g)	288
Specific gravity	1.57
Mol. Diff. Coef. (cm^2/sec)	0.0792

Table 4. Chlorine Chemical properties

Chlorine gas can be pressurized and cooled to change it into a liquid so that it can be shipped and stored. When **liquid** chlorine is **released**, it quickly **turns** into a **gas** that stays close to the ground and spreads rapidly.

The dangerous concentration is determined by NIOSH. Originally, the chlorine IDLH was 30 ppm:

The chosen IDLH is based on the statement by ILO [1971] that exposure to 30 ppm will cause intense coughing fits, and exposure to 40 to 60 ppm for 30 to 60 minutes or more may cause serious damage. [NIOSH, ref. 23]

This threshold was revised and reduced to 10 ppm. As it is shown:

The revised IDLH for chlorine is 10 ppm based on acute inhalation toxicity data in humans [Freitag 1941; ILO 1971; NPIRI 1983]. [NIOSH, ref. 23]

9.1.2   Type of control room

The control room has a volume of 1727,3 (m^3) . The ventilation system has a flow rate from unfiltered intake source of 6,6 (m^3/s). Additionally, it has a filtered makeup air of 0,29 (m^3/s), and an emergency filtered recirculated air with an external inflow of 2,88e-2 (m^3/s). Finally, it has a bottled air system with a flow rate of 6,6 (m^3/s).

The time required to isolate the control room once a toxic gas is detected is 15,5 seconds.

These data are introduced in CHEM input file in order to calculate control room concentrations evolution.

9.1.3   Boundary and initial conditions

The toxicity limits are determined in order to assess the results of this study. Furthermore, there are environmental conditions that are introduced in the input files and are not variables in this case. They are described next.

Exposure categories and toxic limits for chlorine in control room habitability
The NUREG-0800 defines three types of categories as a function of time exposure. protective action exposure (2 minutes or less), short-term exposure (between 2 minutes and 1 hour), and long-term exposure (1 hour or greater).

Despite the limits commented in previous chapter, the acceptable concentrations in the control room are established by RG-1.78 and, specifically, by the RG-1.95, where the concentration limit for chlorine in the control room cannot exceed **15 ppm** by volume (45 mg/m^3) within **two minutes** after the operators are made aware of the presence of chlorine.

For greater periods of exposure time, the guide NUREG-0800, ref. [6], recommends to establish allowable limits on the basis that the operators should be capable of carrying out their duties with a minimum of interference caused by the gas and subsequent protective measures. The limits for the three categories are established as follows:

   a. Protective action (0-2 min): 15 ppm by volume
   b. Short-term (2-60 min): 4 ppm by volume
   c. Long-term (>60 min): 1 ppm by volume

Solar radiation and ground temperature

The insolation degree parameter is not contained in the meteorological data available, so the radiation is not be simulated as a stochastic phenomenon. Its values are the same for both instantaneous and continuous release evaluations, and they guarantee conservative results.

Hence, the conditions in the following table have fixed values for both instantaneous and continuous releases. These parameters are:

Air temperature (°C)	20
Atmos. Pressure (mm Hg)	760
Solar radiation (W/m²)	500
Cloud cover (tenths)	2
Ground temperature (°C)	25

Table 5. Initial evaporation conditions for chlorine case study

Additionally, due to the physical properties of the chlorine, the phenomenon that will take place, at the moment of release out of the shipment containment, will be flashing, and the equation to estimate the mass that become airborne by flashing is detailed at Chapter 6.2.1.b in NUREG/CR-6210, ref. [9],

$$m_f = m_r c_p (T_a - T_b)/h_v \tag{9.1}$$

Where:

   - m_f : Mass that flashes (kg)
   - m_r : Mass released (kg)
   - c_p : Heat capacity (j/g °C)
   - T_a : Air temperature (°C)
   - T_b : Boiling-point (°C)

- h_v : Heat of vaporization (j/g).

The amount of mass that flashes is then calculated for 50 tones of mass released, with the parameters detailed in tables 4 and 5, the resulting mass that flashes is 8885 tones of Cl_2.

Any substance that does not flash, forms a liquid pool, and the equations to estimate the amount of material are detailed in the following chapters or the guide NUREG/CR-6210.

9.2 MC SIMULATION FOR MAXIMUM CONCENTRATION EVALUATION

For instantaneous release, they have been simulated 5.0e4 histories, and the results are shown in the next figure.

```
                 Total
Variable         Count       N   N*    CumN      Mean  SE Mean    StDev  Minimum        Q1   Median
Total Results    50002   50002    0   50002   0,07436  0,00220  0,49196  0,00000   0,00000  0,00000


Variable            Q3  Maximum
Total Results  0,00000  9,59204
```
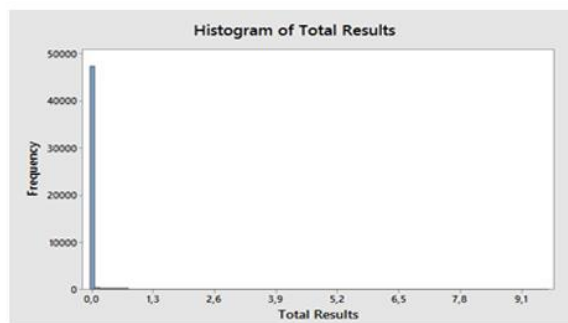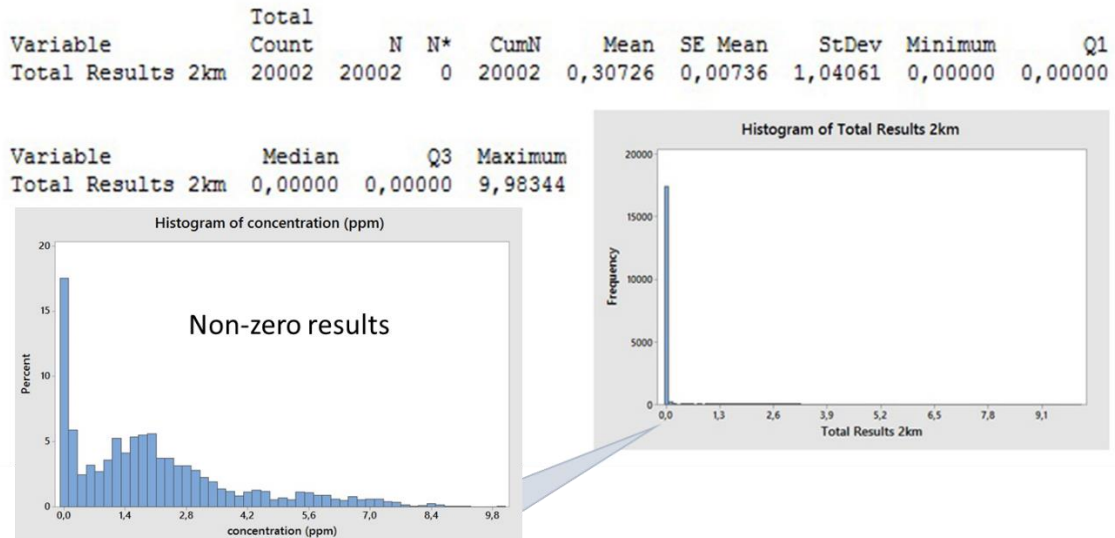
The values from figure 9.1 are shown just to illustrate that the results are not acceptable for the stochastic approach. From the 5.0e4 simulations, only 5815 times some concentration has been estimated in the control room, and 2078 times EXTRAN has neglected any concentration at the intake. As it is appreciated at the stats, the third quartile is 0.0 and the mean is much smaller than standard deviation.

All these factors might indicate that the selected area of study is too conservative in terms of sector length (8km radius). Thus, more calculations with a reduced area of study are needed. This conclusion is to be checked and confirmed with the continuous release evaluation.

Hence, another simulation is implemented, with an area of study that covers radius < 2 km and 2.0e4 simulations. The results are shown next.

Variable	Total Count	N	N*	CumN	Mean	SE Mean	StDev	Minimum	Q1
Total Results 2km	20002	20002	0	20002	0,30726	0,00736	1,04061	0,00000	0,00000

Variable	Median	Q3	Maximum
Total Results 2km	0,00000	0,00000	9,98344

19 Figure 9.2 Statistical analysis second simulation with 2.0e4 histories and 2 km of radius.

Despite the results look the same as previous execution, it can be appreciated that the difference between the mean and the standard deviation has decrease. With a total of 2.0e4 histories, the number of times it is been estimated some concentration in the control room is 2991, and the number of times EXTRAN has neglected any chance of having concentration at the intake is 326. That is, the percentage of filtered histories by the angle criteria is ≈16% for both simulations, but the percentage of times EXTRAN rejects the process has decreased from 4.1% to 1.6% when reducing the accident sector. Indeed, the portion of times that concentration has been estimated has increased from 11,6% to 15,0%. It can be better appreciated in the following figure.
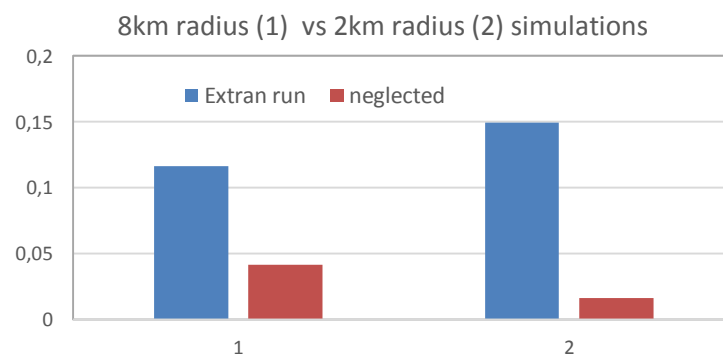

20 Figure 9.3. Comparison for 8 km radius sector versus 2 km radius sector simulations.

As a conclusion, the initial area of study was too conservative returning an excess of null results. Hence, the area in which a train accident with toxic release is relevant for the probabilistic assessment can be reduced below 2 km radius.

Additionally, one thing that can be appreciated is that the number of histories has been reduced from 50e4 to 20e4. One reason to do that is the fact that the decreased area is yielding higher ratio of run EXTRAN cases. On the second hand, the computational price would increase in excess.

Nevertheless, in order to optimize the computing time without increasing variance, a statistical control of the simulation evolution is performed, so that the sensitivity analysis do not run more histories than needed.

A stats control is added to Loop module and the result is shown as follows,
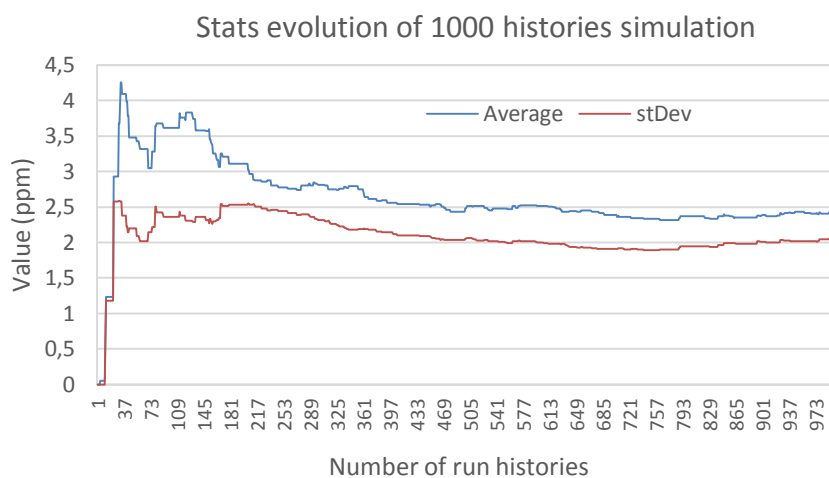
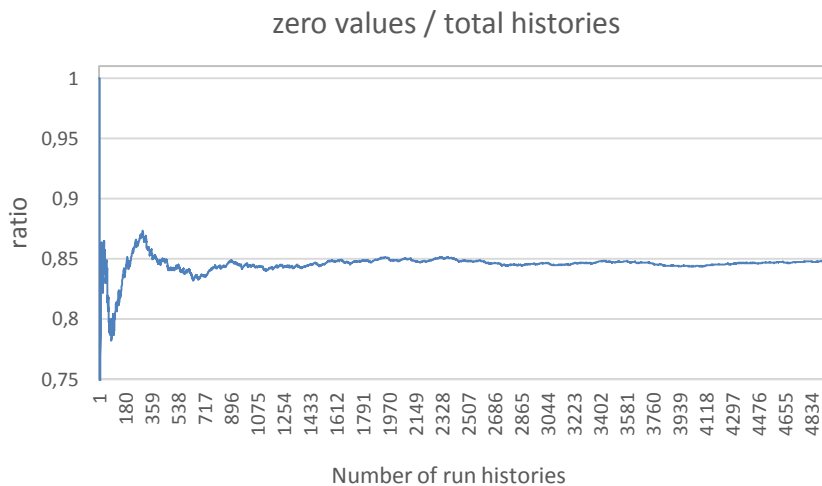*21 Figure 9.4. Stats evolution during 1000 histories simulation. Average and stDev.*
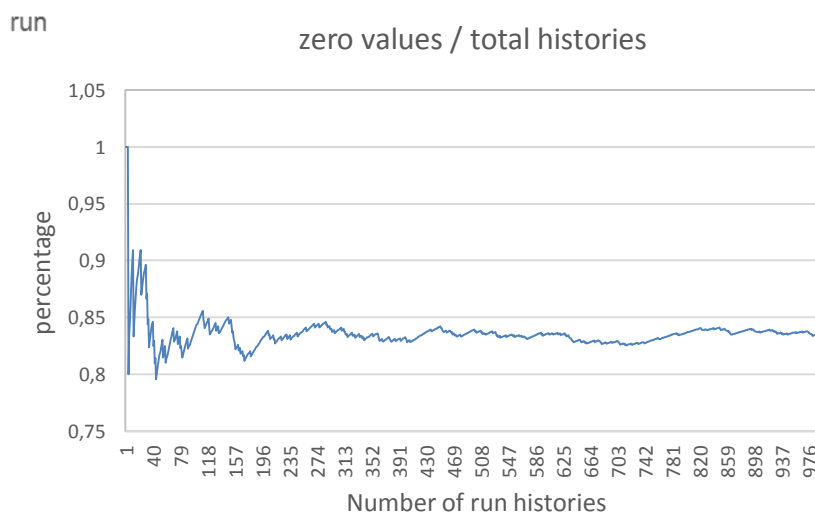
22 Figure 9.5. Stats evolution during 1000 histories simulation. Zero values percentage over the total

It can be appreciated that the values have not stabilized with 1000 simulated histories. The next test is done for 5000 histories, and the results are shown next.

Stats evolution of 5000 histories simulation
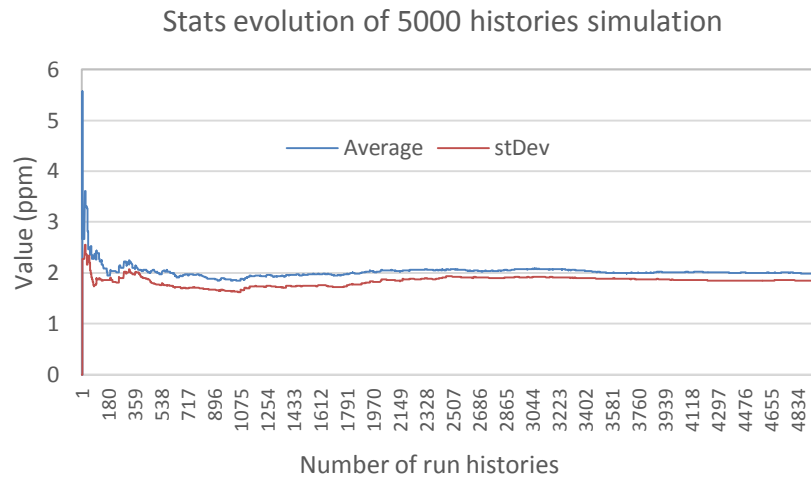
23 Figure 9.6. Stats evolution during 5000 histories simulation. Average and stDev. For instantaneous release

zero values / total histories

24 Figure 9.7. Stats evolution during 5000 histories simulation. Zero values percentage over the total

As the values are stabilizing with this last simulation, the sensitivity analysis is to be done with 5000 histories simulations. By performing the sensitivity analysis, it can be evaluated the uncertainty within a qualitative approach.

9.2.1   Wind direction sensitivity analysis for instantaneous release

As an example of how a sensitivity analysis is used to assess uncertainty, it is performed one for wind direction parameter. The same way is to be done for the rest of parameters when the whole project is carried on.

The goal of this sensitivity analysis is to assess the influence of wind direction variability on concentration results. It starts testing different combinations of 10% modifications in the wind direction frequencies established for the wind speed intervals, see table 2. Then more simulations are run with different combinations of

20% modifications in the wind direction frequencies. The result is shown in the next figure.

Sensitivity analysis - wind direction parameter
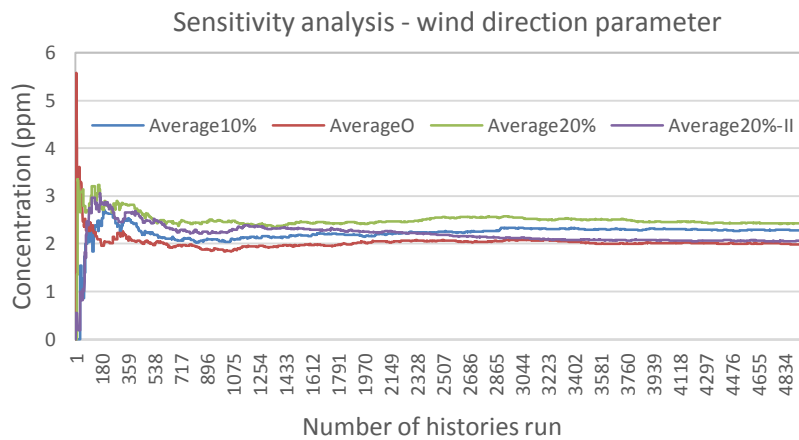
25 Figure 9.8. Sensitivity analysis for wind direction parameter, from original to 10% and 20%

The sensitivity analysis for 10% variances in wind direction returns an increase of 14% in the mean concentration value. The 20% variances return mean values in a range of 2,3% to 20,9% higher than the original one.

These increases in concentration values indicate that wind direction not only affect to filtering criteria to launch EXTRAN, but to concentration values in the CHEM output. Hence, uncertainties of this parameter must be evaluated. Furthermore, it is recommended to convert aleatory uncertainties to epistemic as much as possible by getting better historical data of the meteorological stations.

9.3 MC SIMULATION FOR MAXIMUM CONCENTRATION-DURATION EVALUATION

The first part of this evaluation consist of pre-processing the meteorological data. The procedure has some difficulties that are detailed in Appendix D to this document, ref. [24]. The following task consist of creating input files with modified values of distance, angle and cross-sectional area if needed, for each point of the sector. Once the input files are created, they are executed in ARCON96. This is done by a Batch file that copies modified inputs on original one and calls ARCON96. This script also creates output directories and files in which the relative concentration values are stored.

Nevertheless, the relative concentration values are not enough to assess the control room habitability, in fact, the concentration must be estimated in (g/m^3) or in (ppm). This is accomplished by introducing the release rate, which is calculated considering

initial amount of material, the release rate from the shipping containment and the mass becoming airborne by flashing.

As is has been calculated by equation (9.1), the mass that flashes is 8885 kg out of the 50 tones released. This mass is distributed in each time period from 1h to 720h,

Period	1h	2h	4h	8h	12h	24h	96h	168h	360h	720h
Rate (g/s)	2468.10	1234.05	617.03	308.51	205.68	102.84	25.71	14.69	6.86	3.43

Then the resultant values are converted to ppm units, which are the units CHEM expect. The next step is to run MC simulation.

To decide the number of simulations, a statistic control is done with the concentration values, the same way it was done for instantaneous release. A first simulation of 1000 histories shows that more histories need to be simulated.
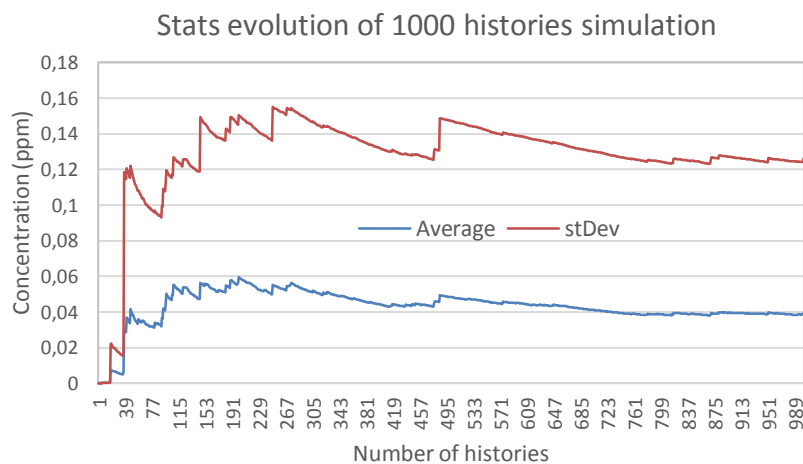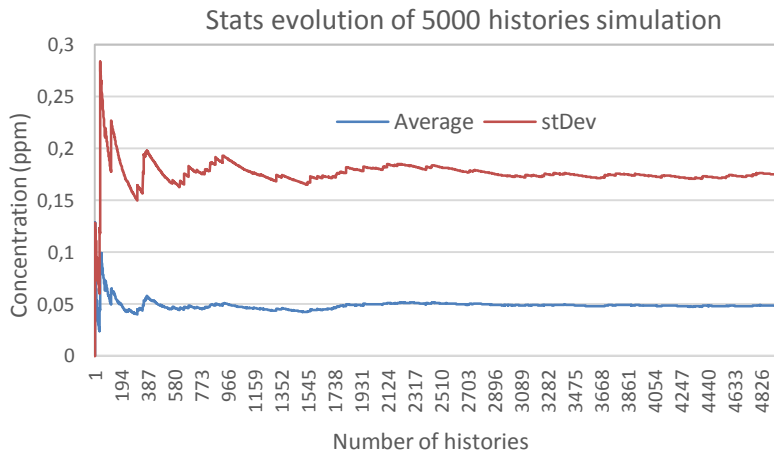

26 *Figure 9.9. Stats evolution during 1000 histories simulation. Average and stDev. Continuous release*
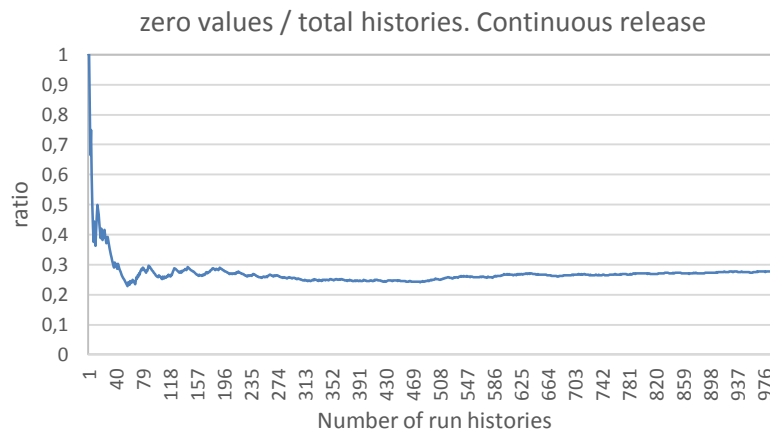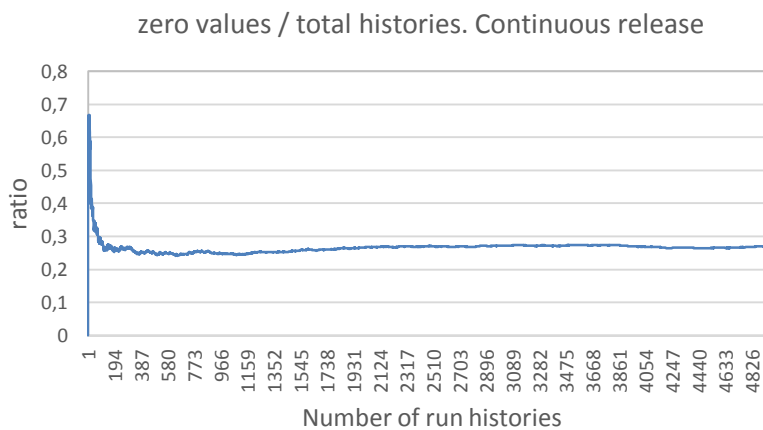

27 *Figure 9.10. Stats evolution during 5000 histories simulation. Zero values percentage over the total*

The results do not indicate stability achievement, so a simulation with 5000 histories is performed next. Let us, however, comment the results before starting new simulation. Firstly, as it is appreciated in figure 10.8, the average concentration values tend a very small number, especially if they are compared to instantaneous release concentration values. Additionally, the standard deviation is considerably greater than mean. Both facts have to do with the big amount of small concentration values that are returned with the use of ARCON96 and, of course, with the fact that continuous release involve small release rate. These appreciations are analysed deeper after all the calculations are done.

The following figures show 5000 histories simulation results.

28 Figure 9.11. Stats evolution during 5000 histories simulation. Average and stDev. Continuous release

29 Figure 9.12. Stats evolution during 5000 histories simulation. Zero values percentage over the total

The results for 5000 histories show that average value seems to reach stability, although standard deviation is still instable.

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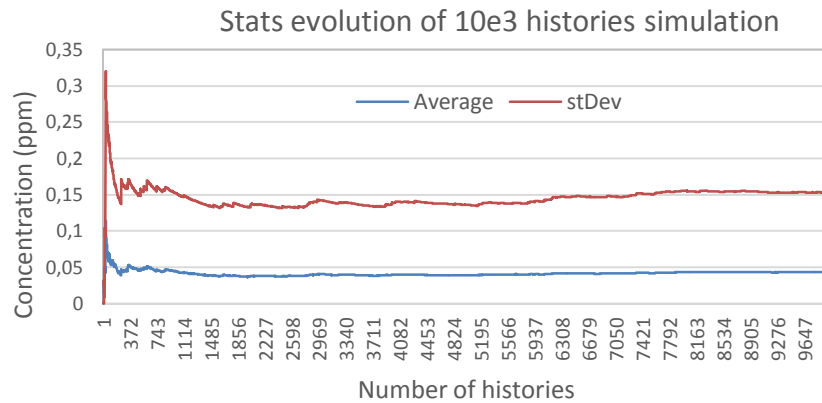
30 Figure 9.13. Stats evolution during 10e3 histories simulation. Average and stDev. Continuous release

Finally standard deviation seems to stabilize when approaching to 10e3 simulated histories.

9.4 RESULTS

The results for instantaneous results indicate that maximum values tend to 2 ± 0.25 ppm in volume of chlorine in the control room. The maximum value obtained is 9,98 ppm and the third quartile is 2,9 ppm. The limiting values, as commented before, are establish for 15 ppm for the first 2 minutes and 4 ppm for the rest first hour.

The results of the continuous release evaluation indicate that even making the selection for the closest points to the plant, the concentration values are very small. The maximum value returned is 1,42 ppm and the third quartile is 4,69e-3 ppm. The limiting value for more than one hour of exposure is 1 ppm.

The factors that may have influence in this low results for ARCON96-CHEM are,

On the one hand, the fact that the larger periods have low release rate but high frequency of returning concentration, causes a big amount of close to zero values. The shorter periods, however, have higher release rate, but they only occur 30% (1h period) of the time, returning zero value the rest of the times.

On the other hand, the coupling between ARCON96 output and CHEM input has been done by modifying an EXTRAN output with the concentration calculated by ARCON96 results. Nevertheless, EXTRAN returns short period evolution in time values, and exposure evolution. This might be creating errors in the final result that lead to wrong values.

10. CONCLUSIONS

This thesis establishes a partial methodology to implement a **probabilistic approach** on external event risk assessment. This external event consist of a train accident shipping hazardous toxic material, which produces a toxic atmospheric dispersion that reaches control room ventilation systems of a nuclear power plant, thus affecting its safety.

The methodology is partial because only atmospheric dispersion is treated. Two types of release are postulated, which are instantaneous release and continuous release.

The methodology used to achieve probabilistic approach is the **random variable** generation in a static model of a discrete-event system. However, the way it is applied differs from both types of release.

Instantaneous release is simulated by generating meteorological conditions, and continuous release is simulated by the distribution functions that the validated code ARCON96 returns after processing meteorological.

The tools used for these purposes, allow the user to change boundary and initial conditions without needing any code modification. This is useful to adjust area of interest or to change the hazardous material properties, for instance.

In the presented methodology it has been established how to treat uncertainties. However, in the case study they have not been quantified, but just evaluated by qualitative assessment of one parameter, as an example.

The results of **uncertainties** qualitative assessment indicate that variability must be analysed in future applications of the method. This fact also involves the necessity of improving the quantity and quality of historical meteorological data measured, so that randomness in meteorological parameters can be reduced. This may be achieved by applying MCP correlation method for surrounding stations.

The results of the case study are useful as a guidance and they do not represent real nor ultimate risk values. Furthermore, the comparison between both types of release codes has been performed with CHEM output, and the coupling between ARCON96 and CHEM is not accurate enough to validate its final result.

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Hence, if both types are to be compare, it is recommended to just compare EXTRAN output with ARCON96 output converted to concentration in volume. On the other hand, when continuous release is to be evaluated, the calculations of control room diffusion after ARCON96 output, must be adapted or improved in order to validate this method.

The methodology presented for **instantaneous** release, however, returns reliable values that can be **validated**, as long as meteorological data is completed.

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