## Navigating Uncertainties: Strategies for Robust Hydrogen QRA

Simon Gustafsson | Risk Management and Societal safety | LTH | Lunds universitet



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> Riskhantering och samhällssäkerhet Lunds tekniska högskola Lunds universitet Box 118 221 00 Lund

> > http://www.risk.lth.se

Telefon: 046 - 222 73 60

Division of Risk Management and Societal Safety Faculty of Engineering Lund University P.O. Box 118 SE-221 00 Lund Sweden

http://www.risk.lth.se

Telephone: +46 46 222 73 60

## Abstract

Both the EU and Sweden aim to incorporate hydrogen to decarbonize industries and reduce fossil fuel dependence. Liquid Wind, a company focused on sustainable electro-fuel production, develops facilities to convert biogenic CO2 and renewable hydrogen into green electro-fuel eMethanol. Such facilities, handling flammable substances, require quantitative risk assessments (QRA). Currently, Hydrogen QRA uses conservative estimates and worst-case scenarios. There is potential for improving uncertainty management and decision-making in QRA.

This thesis explores strategies to enhance QRA accuracy by evaluating the strength of knowledge and managing uncertainties. An iterative study, incorporating more data and Monte Carlo simulations, aims to identify the necessary detail level for QRA studies. Results indicate increased strength of knowledge, though some parameters may not need detailed distributions. Applying this approach broadly could improve QRA robustness and accuracy, especially when scaling facilities from pilot to commercial plants.

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## Nomenclature

- MCS Monte Carlo Simulation
- QRA Quantitative Risk Assessment
- CBA Cost Benefit Analysis
- LOC Loss of Containment
- **BLEVE** Boiling Liquid Expanding Vapor Explosion
- LCOH Levelized Cost Of Hydrogen
- GHG Greenhouse Gas
- RES Renewable Energy Sources Taguchi's Orthogonal Array Testing-method
- FS2 FlagshipTWO
- TOAT Taguchi's Orthogonal Array Testing-method
- ALARP As Low As Reasonably Practicable
- IPS Intresseföreningen för Processäkerhet

# Summary

Both the EU and Sweden have announced strategies for incorporating hydrogen in their solution for decarbonizing industries and reducing their dependence on fossil fuels. Liquid Wind is a company attempting to decarbonize an industry, they are a developer of sustainable electro-fuel production facilities with a vision to reduce the world's dependency on fossil fuels. They develop "replicable commercial scale" facilities to convert biogenic CO2 and renewable hydrogen and electricity into electrofuels. In general quantitative risk assessments need to be performed for facilities such as electro fuel production facilities.

The studied facility in this thesis is the second one in their pipeline of projects called "FlagshipTwo" located in Sundsvall, Sweden. It has just received its environmental permit from the Land and Environmental Court in Östersund and it is expected to be up and running in 2027, producing 130 000 tons of eMethanol annually.

Hydrogen Quantitative Risk Analysis (QRA) is today generally done in a conservative manner and when performing frequency estimation, it's done by using point estimates, conservative assumptions and worst-case probabilities. There is room for improving the management of uncertainties and increasing the strength of knowledge for decisions made in QRA's.

In this thesis, I attempt to chart different strategies to evaluate strength of knowledge and manage uncertainties which in turn will lead to a more accurate QRA. Where a lack of strength of knowledge if found will warrant further investigation and treatment of uncertainties. This will be done by performing an iterative study where the QRA will be continuously enhanced by introducing more/other data and performing a Monte Carlo simulation. It will be divided into five stages: Method research, Case Examination, Analysis, Comparison and Interpretation.

Three methods for evaluating and increasing the strength of knowledge and also reveal and decrease uncertainties were identified. Semi-quantitiative method, assumption deviation risk and Monte Carlo simulation. Were the first two would be applied to evaluate chosen assumption or parameter and the MCS used to incorporate potential changes made to the frequency analysis.

In the analysis it was limited to examining the frequency generation in four iterations. In iteration 1 the base frequency for the event trees was replaced, in iteration 2 the probabilities for ignition was altered to employ distributions which incorporate data from several sources. The same approach was used in iteration 3 were data from several sources was incorporated through distributions. Monte Carlo simulation was performed through every iteration and then used as part of the interpretation.

From the results of thesis, it is clear that the strength of knowledge has been increased but there are certain parameters that may not be necessary to employ distributions for since some of the results between iterations are negligible. But if this approach would be applied to the entire case study, on all of the substances present in the facility there is great potential for increased robustness and accuracy of the QRA, Which becomes even more necessary when facilities will be scaled up from pilot plants to commercially viable plants.

# Sammanfattning

Både EU och Sverige har tillkännagivit strategier för att införliva vätgas i sina lösningar för att minska koldioxidutsläppen i industrin och minska beroendet av fossila bränslen. Liquid Wind är ett företag som utvecklar hållbara produktionsanläggningar för elektrobränslen med en vision om att minska världens beroende av fossila bränslen. De utvecklar "kommersiellt reproducerbara anläggningar" för att omvandla biogen CO2 och förnybar vätgas till elektrobränslen. Anläggningar som dessa genererar risker, vilket är anledningen till att kvantitativa riskbedömningar måste utföras.

Anläggningen som studeras i detta examensarbete är den andra i deras pipeline av projekt som kallas "FlagshipTwo" och ligger i Sundsvall, Sverige. Den har precis fått sitt miljötillstånd från Mark- och miljödomstolen i Östersund och förväntas vara i drift 2027 och producera, up till 130.000 ton eMetanol per år.

Kvantitativ riskanalys (QRA) för vätgas görs idag i allmänhet på ett konservativt sätt. Frekvensgenereringen produceras med hjälp av punktskattningar, konservativa antaganden och sannolikheter för "värsta fall". Det finns utrymme för att förbättra hanteringen av osäkerheter och öka robustheten i de beslut som fattas i QRA.

I det här examensarbetet försöker jag kartlägga olika strategier för att utvärdera kunskapsstyrkan och hantera osäkerheter, vilket i sin tur leder till en mer exakt QRA. Om en brist i strength of knowledge upptäcks kommer det att motivera ytterligare undersökningar och hantering av osäkerheter. Detta görs genom en iterativ studie där QRA:n kontinuerligt förbättras genom att mer/annan data införs och en Monte Carlosimulering utförs. Den kommer att delas in i fem steg: Metodforskning, fallgranskning, analys, jämförelse och tolkning.

Tre metoder identifierades för att utvärdera och öka kunskapsnivån samt för att avslöja och minska osäkerheter. Semikvantitativ metod, risk för avvikelse från antagande och Monte Carlo-simulering. De två första metoderna användes för att utvärdera valda antaganden eller parametrar och MCS användes för att införliva potentiella förändringar i frekvensanalysen.

Analysen begränsas till att undersöka frekvensgenereringen i fyra iterationer. I iteration 1 ersattes basfrekvensen för händelseträden och i iteration 2 ändrades sannolikheterna för antändning genom att använda fördelningar som innehåller data från flera källor. Samma tillvägagångssätt användes i iteration 3 där data från flera källor användes genom ansättning av fördelningar. Monte Carlo-simuleringar utfördes genom varje iteration och användes sedan som en del av tolkningen.

Ur examensarbetet resultat framgår det tydligt att kunskapens styrka har ökat, men det finns vissa parametrar som det kanske inte är nödvändigt att använda fördelningar för eftersom vissa av resultaten mellan iterationerna är försumbara. Men om detta tillvägagångssätt skulle tillämpas på hela fallstudien, på alla ämnen som finns i anläggningen, finns det stor potential för ökad robusthet och noggrannhet i QRA. Detta blir ännu mer nödvändigt när anläggningar kommer att skalas upp från pilotanläggningar till kommersiellt gångbara anläggningar.

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## 1

# 1 Introduction

## 1.1 A tool for green transition

Both the EU and Sweden have announced strategies for incorporating hydrogen in their solution for decarbonizing industries and reducing their dependence on fossil fuels (European Commission, 2022). Renewable and green hydrogen can be produced via electrolysis with variable renewable electricity from cheap sources which then can be used in several ways e.g. electro fuels, energy storage, production of chemicals, and electricity grid balancing (European Commission, 2022).

In the white paper "Mainstreaming Green Hydrogen in Europe" by Material Economics (2020) it is stated that hydrogen may provide enormous economic benefits along with being essential to Europe's fight against climate changes, especially in sectors that have few other technological options. In Europe (and other regions) there already is momentum for green hydrogen with approximately 100 MW built and another 20 GW of capacity announced.

### 1.1.1 Liquid Wind

Liquid Wind is a developer of electro fuel production facilities with a vision to reduce the world's dependency on fossil fuels. The company develops "replicable commercial scale" facilities to convert biogenic CO2 and renewable hydrogen and electricity into electrofuels. Liquid Wind has the ambition of developing more than ten facilities by 2027 thanks to their standardized technology (Östersunds Tingsrätt Mark-och miljödomstolen, 2024).

The studied facility in this thesis is the second one in their pipeline of projects called "FlagshipTWO" located in Sundsvall, Sweden. It has just received its environmental permit from the Land and Environmental Court in Östersund and it is expected to be up and running in 2027, producing up to 130 000 tons of eMethanol annually.

### 1.1.2 Electro fuels

One of the main industries contributing to greenhouse gas emissions worldwide is the transportation industry. Using electro fuels as a replacement for traditional carbon fuels is one of the crucial steps that will be needed to reduce greenhouse gases. Electro fuels produced in this manner create a closed loop where carbon emissions are recycled instead of emitted into the atmosphere. Recycled CO2 gas and hydrogen from water electrolysis are combined to create electrofuels, the energy needed to create these fuels comes from renewable energy sources such as wind-, hydro- or solar power (Ababneh & Hameed, 2022).

Electrofuels have several beneficial characteristics according to Ababneh and Hameed (2022) which exacerbates their usefulness in the future energy landscape. As previously stated the production process can utilize CO2 from other production processes or gather it directly from the atmosphere as feedstock for fuel production. It will help reduce GHG (Greenhouse gas) emissions and provide a sustainable way to convert carbon into an energy carrier. Since electro fuels can be produced with RES (Renewable Energy Sources) which are intermittent the electro fuel and its production process can be used as an energy storage when there is surplus electricity available. With this possibility of storage, the resilience of renewable electricity systems is elevated (Ababneh & Hameed, 2022).

## 1.2 Hydrogen Risk Management

With the emerging green hydrogen industry in the process of scaling up from pilot facilities to more commercially viable facilities, they will manage, produce and store a greater amount of highly explosive and flammable substances. This will in turn scale up the risks that they generate, therefore there is a need to increase the accuracy and robustness of the quantitative risk assessments for this kind of facility. Especially if Sweden's and the European Union's plans are to accelerate the implementation of such industries.

Hydrogen quantitative risk assessment does not differ a lot from regular QRA (Quantitative Risk Assessment) in Sweden, IPS states this in their QRA guideline (IPS, 2022). IPS is a stakeholder association for the Swedish process safety industry. It consists of leading academics in the subject, most of the companies working in the industry and producers of these dangerous substances and they have publicised a QRA guideline in an attempt to standardize the method for professionals either producing, reading and deciding on these types of documents. IPS does recommend using HyRAM (Hydrogen Risk Assessment Models) in cases of hydrogen-specific applications, such as frequency generation and consequence modelling. It is a software with an accompanying reference manual which details a suggested approach to frequency generation and consequence modelling.

#### 1.2.1 Hydrogen Risk Assessment Models 3.1

HyRAM (Hydrogen Risk Assessment Models) is a sophisticated software toolkit designed to streamline the evaluation of hydrogen safety across its use, delivery, and storage infrastructure. It serves as a comprehensive platform that seamlessly integrates cutting-edge scientific and engineering models, alongside pertinent data, to ensure a robust assessment of hydrogen-related risks in the industry. Hydrogen Risk Assessment Models 3.1 Technical Reference Manual (Ehrhart et al., 2021) is a report detailing the algorithms, models and data used in HyRAM 3.1.

At its core, HyRAM amalgamates state-of-the-art methodologies, validated through rigorous scientific scrutiny, to deliver a thorough analysis of hydrogen safety considerations. Its risk assessment capabilities encompass a wide spectrum, incorporating generic failure probabilities for nine different component types. Furthermore, HyRAM employs probabilistic models to gauge the impact of heat flux and overpressure on both human beings and structures, enhancing its predictive accuracy (Ehrhart et al., 2021).

The program was developed by the Sandia National Laboratories for the U.S Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE) and Hydrogen Fuel Cell Technologies Office (HFTO) (Ehrhart et al., 2021).

#### 1.2.2 The New Risk Perspective

Conventional risk estimation is usually done by combining probability and consequence. This approach puts great emphasis on historical data and expert assessments to generate an accurate estimation of the risk magnitude and has successfully been applied for decades. However because of several severe accidents during the 20th century, a new approach started to be formulated. "The new risk perspective" as it is called introduces uncertainty as a core concept rather than frequency and consequence (Aven, 2013).

Risk has long been considered to represent the expected loss and as a combination of loss and probabilities but in the nuclear industry the definition of risk triplet has prevailed. The risk triplet definition consists of three questions; What can happen? How likely is that to happen? If it happens, what are the consequences? All previous definitions of risk are probability-based and there has been a significant push within the scientific community that these definitions will need to be replaced by a broader perspective which is not only linked to one parameter of uncertainty (Aven, 2013). For Hydrogen QRA's to achieve a higher degree of accuracy and robustness a new perspective on risk is needed.

The new perspective should be able to describe uncertainty in several ways, namely through probability-based thinking, knowledge dimension and black swans. The knowledge dimension could for example include the uncertainties which stem from the lack of knowledge about the assumptions upon which the probability is built. Black swans represent the "surprise" part of the risk assessment, with surprise Aven (2013) means an event or deviation which is unknown relative to the expert or consultant performing the assessment.



Figure 1.1: Basic features of the new risk perspectives compared to the traditional probability-based perspectives (Aven, 2013).

### 1.2.3 Strength of Knowledge

In the new risk perspective, it is highlighted that all estimations of frequencies/probabilities and consequences are founded in some sort of background knowledge. This knowledge must be incorporated as a part of the analysis where it's disclosed whether the knowledge is viewed as strong or weak. Strong and weak in this case means whether the knowledge is accompanied by more or less uncertainties (Aven, 2013). If a parameter or assumption is found to have moderate or weak strength of knowledge its uncertainties will have to be incorporated in the analysis by using and/or combining it with new data.

Within Hydrogen QRA the strength of knowledge can be considered generally as low, this is spoken about in Ehrhart et al. (2021) and it is one of the reasons why bayesian-updating had to be used to generate their input parameters.

# **2** Problem Statement and Goals

When developers such as Liquid Wind build facilities which are going to produce flammable substances with green hydrogen certain risks arise and some sort of risk assessment has to be made. Hydrogen Quantitative Risk Analysis which is represented by the QRA process according to IPS guidelines, is today generally done in a conservative manner and when performing frequency estimation, it's done by using point estimates, conservative assumptions and worst-case probabilities. Today's practice is the conservative and safe way of analysing risk and it may lead to the risk being overestimated which can be a good starting point. If the estimated risk is below set criteria no further action is needed. If it turns out to be above set criteria there is uncertainty as to whether it is because of the conservative approach or if the risk is too great.

This in turn can lead to the mandated and suggested measures being exaggerated and in turn could halt the green transition, increase costs, and prolong the legislativeand approval process for facilities in the industry. There is room for improving the management of uncertainties and increasing the strength of knowledge for decisions made in QRA's which is the purpose of this thesis and it will be done by answering these questions:

- How can the strength of knowledge of Hydrogen QRA performed according to current praxis be improved?
- What are the implications of improving the strength of knowledge of hydrogen QRAs?

In this thesis, the author attempted to chart different strategies to evaluate the strength of knowledge and manage uncertainties within the frequency generation part of a QRA. These methods were then implemented in a case study where potential differences were interpreted. A case study on an existing facility was chosen to help contextualize the differences between iterations and to be able to compare it to a "conservative QRA". This approach could then be incorporated into future assessments where there may be a need for a more accurate and robust management of uncertainties.

# 3 Methodology

For this thesis, research into methods for evaluating the SoK (strength of knowledge) and ways to manage uncertainties for the frequency generation has been done. These methods were then applied to the assumptions and input parameters which are present in the case study.

Where a lack of SoK was found, it warranted further investigation and treatment of uncertainties. This was done by performing an iterative study where the QRA was continuously enhanced by performing a Monte Carlo simulation. Each section of the frequency generation had its SoK examined in iterative steps, and if found to be unsatisfactory it was treated. Each iteration was then compared to the original case, through calculation of risk metrics, uncertainty- and sensitivity analysis. A comparison to the original QRA was done to contextualize the differences between the iterations and a "conservative QRA". The study was quantitative, and iterative and consisted of 5 stages:



Figure 3.1: Method Flowchart

## 3.1 First Stage: Method Research

The first stage consisted of research into appropriate methods for evaluating uncertainty and SoK for frequency generation. The existing standard practice in Sweden was also presented by examining IPS's suggestion for a QRA. This was done to establish a comparison and to determine which methods for uncertainty management and evaluation of SoK were appropriate.

The keywords identified from the problem statement for the thesis were Uncertainty

Management, Hydrogen, Quantitative Risk Assessment, Monte Carlo Simulation and Strength of Knowledge. These keywords were then used to search through the database LUBsearch. Several academic papers on uncertainty management and QRA's within hydrogen engineering were found but none with a direct link focusing on frequency generation.

Furthermore, a few papers were recommended to the author by its mentor Henrik Hassel, which then led to snowballing within the subject of uncertainty treatment and strengthening SoK within QRA's. The author of this thesis was already aware of different guidelines and reference manuals which are supposed to be used in process safety engineering which is used as a basis and reference manual for "standard practice".

## 3.2 Second Stage: Case Examination

The second stage consisted of examination of the case and defining the assumptions and parameters which will be assessed with the identified methods.

Other than defining the examined case, the QRA performed on the facility will be defined i.e. what method, input values and what output it generated.

## 3.3 Third Stage: Analysis

In the third stage, the frequency analysis of the case was performed according to appropriate practice guided by mentors, both from the university- and private sector. It was an iterative process where found methods were applied to found uncertainties and further explored until SoK was increased. To conduct this case study, the author needed a statistical calculation program such as Palisade's "@risk" and a program to generate event trees such as Palisade's "PrecisionTree". With these excel-plugin programs and the correct data sets a statistical model was built.

The author's mentor (Henrik Hassel) and colleagues at Sweco Sverige also served as relevant sources of information from the industry. In cases where there wasn't sufficient data, estimation was made qualitatively through discussion with these individuals and the application of found methods.

## 3.4 Fourth stage: Comparison

The fourth stage consisted of the comparison between each iteration and the original assessment. The comparison was done through the calculation of risk metrics through simulation software where the risk metrics Individual risk and Societal risk were compared. From these, the improvements through the iterations could be shown as contours and graphs with all end events combined into two metrics instead of a table. Riskcurves produced by Gexcon (Gexcon AS, 2024) is the software which was used to calculate the risk metrics. It is a sophisticated software which is broadly used among process safety experts and all manner of scenarios can be simulated such as population density, wind direction distribution, terrain, topography, different substances and release scenarios (Gexcon AS, 2024).

In the original QRA, a set of quantitative simulations was performed, these were later reused for every iteration with the original settings and environment. All substances present in the original QRA except hydrogen were removed from the simulations. Since hydrogen was the only substance present in the simulation and only two scenarios (Instantaneous and continuous) being simulated the real risk of the facility is not calculated. The calculations made were focused on supplying data to compare the different iterations and as a proof of concept for the approach used in the thesis.

## 3.5 Fifth stage: Interpretation

In the fifth stage, the discussion highlighted potential faults, uncertainties, improvements and what areas could benefit from further research. There will be an interpretation of the analysis and a conclusion will be formed on the suggested approaches for navigating uncertainties answering the problem statement and goals.

# 4 Background Theory

In this chapter potential methods for uncertainty analysis, evaluating and strengthening SoK are researched and explained. It is followed by a representation of what the author considers "the Swedish standard practice" which is IPS's (Intresseföreningen för Processäkerhet) suggestion for a QRA guideline.

## 4.1 Researched Methods

In this section researched methods for performing uncertainty analysis and evaluating SoK are presented.

### 4.1.1 Monte Carlo Simulation

In the paper by Andrade et al. (2024) attempts to compare the LCOH (Levelized Cost of Hydrogen) for two locations (Germany and Brazil) with a deterministic- and stochastic(probabilistic) approach. The authors use a deterministic approach with assumptions, point estimations and MCS as the stochastic approach for estimating LCOH with uncertainty and risk as the main perspective. Their focus is mainly financial risk and uncertainty which the stochastic process would reflect through the natural variation which is inherent to the financial industry.

Each possible investment in green hydrogen represents one outcome of the simulation which makes MCS an appropriate tool in many areas since the method is applicable, it all depends on the inputs used and the output generated. With the MCS it is possible to quantify the uncertainty and determine which factors contribute most to the uncertainty through sensitivity analysis. This will in turn depend on the accuracy of the data sets used or if the density function was established using qualitative means (Andrade et al., 2024). According to the authors, MCS will generate a distribution which represents all the possible trajectories for green hydrogen investments. According to NASA, MCS outperformed several other methods when estimating risk, cost and schedule (Andrade et al., 2024).

In the end, they compare what the deterministic- and the stochastic analysis finds for the two locations examined in the paper. They both end up with the same result but the stochastic analysis predicts a higher LCOH but it is also shown that the more expensive case (in Brazil) has a higher standard deviation and a higher variance which shines a light on potential hidden risks within that project. Sensitivity analysis further highlights uncertainties and factors which would influence the projects.

He and Weng (2020) performed an investigation into how to use a dynamic and simulation-based method for domino accidents in the chemical industry where they

propose a new six-step method. This paper focuses on simulating the frequency in event chains for domino accidents which they state is one of the more important aspects when performing this sort of study (He & Weng, 2020). They found that MCS is an appropriate method because of its quantitative, flexible and intuitive advantages. There is also no need to simplify the formulas or algorithms used since MCS can avoid complex probability calculations (He & Weng, 2020).

In the paper "Comparative analysis of deterministic and probabilistic methods for the integration of distributed generation in power systems" written by Beltrán et al., 2020 they compare three different statistical approaches. They are MCS, Two-point method and Taguchi's Orthogonal Array Testing Method (TOAT) where they find that MCS uses a greater level of precision since it runs more iterations, but the Twopoint combines the benefits of probabilistic and deterministic methods. The two-point method incorporates the characteristics of the probability density functions which the other methods do not (Beltrán et al., 2020).

Monte Carlo Simulation (MCS) can be described as any method that employs randomly generated numbers for problem-solving. According to this definition, MCS can be utilized to characterize probability distributions and estimate expectations using primary inferential techniques. In the field of computational algorithms, MCS relies on the generation of repeated random samples to derive numerical results, effectively leveraging randomness to address problems that may otherwise be deterministic (Stevens, 2022).

Aven (2016) highlights the usefulness of assigning distributions of input parameters, and performing sensitivity analysis. Further more Aven also states that an uncertainty interval is a more informative way of presenting risk rather than a point estimation. All of which can be done through Monte Carlo Simulation.

From a statistical perspective, MCS serves as an experiment employing simulated random numbers to estimate functions within a probability distribution. In this context, the method resolves the given problem by estimating the expected value through the use of a simulated sample from the distribution of the random variable. The generation of a MCS will yield several parameters from which evaluation can be done such as; uncertainty interval, sensitivity analysis and correlation diagrams (Colantoni et al., 2021).

#### 4.1.2 Hydrogen Quantitative Risk Assessment

In the paper Le et al. (2023) examines how different parameters affect the threats to the surroundings. This is done by using the standard practice described later in chapter 4.6. The frequency generation is done by using the values produced in HyRAM by Ehrhart et al. (2021) instead of using the purple book suggested value. This is also what IPS suggest when dealing with specific hydrogen applications. Le et al. chose to look at three release sizes; 1%, 10% and 100% where the frequencies for all components in the system for each release size were summarized into one "random leak frequency". The paper continues with event tree analysis where the event tree suggested by HyRAM is also used instead of the one suggested by the purple book and RIVM (Le et al., 2023).

Le et al. puts more focus on the consequence analysis than the frequency- and scenario analysis which is the opposite of this thesis and there is no direct management of uncertainties done (Le et al., 2023)

#### 4.1.3 On the use of conservatism in risk assessments

One way of dealing with uncertainties, which is also used in standard practice in the process safety industry, is to use conservative estimates and assumptions in QRAs. It is a natural tool to use in the early stages of a project since input data usually is lacking and therefore the true risks will not be underestimated. Aven (2016) where he finds that a conservative approach has several shortcomings. He finds that it "blocks" the use of the risk analysis as a comparison tool and as a means to study risk-reducing measures. He highlights that the SoK is important for the robustness of the assessment (Aven, 2016).

There is an alternative approach to the conservative one which is to assign the bestestimated value, distribution or assumption and in some way represent the uncertainties and strength of knowledge supporting the estimate. Two of the most common ways of doing this if data is not available are:

- Assign a subjective probability distribution of frequency or probability
- Specify an uncertainty interval [a, b] such that value r is  $P(a \le r \le b)$

Aven (2016) highlights the importance of using sensitivity analysis to examine what effect propagates in the output when varying the assigned values and assumptions.

### 4.1.4 Uncertainty intervals for consequences

When estimating a consequence of a given event, it is usually done with a point value e.g. 2.3 expected fatalities for a violent storm. But if it can be given as an uncertainty interval for example [0,100] with a 90% likelihood, this is more informant than a simple point value since it informs of the potential fatalities at a specific certainty. The uncertainty interval represents the first extension of the new risk perspective. If enough and relevant data is available, a probability distribution could be produced which would reflect the probability and uncertainty in a good way. If data isn't available or the situation isn't complete, the distribution would end up being "rather arbitrary" and unnecessary to produce (Aven, 2013).

## 4.1.5 Strengthening QRA's

Berner and Flage (2016) wrote an academic article where they examine how to strengthen QRA's by a systematic treatment of uncertainties. It showed that the results of QRA's

depend on the knowledge available e.g. understanding of the phenomenon, assumptions made, data and expert statements. They highlight that over usage of assumptions may lead to restrictions being put on the analysis. In the ideal scenario, every uncertain condition should be accounted for in the risk assessment, represented by some sort of uncertainty. According to the authors, this is generally dealt with by making conservative assumptions. Values are chosen unfavourably instead of choosing the most likely value, this will lead to an overestimation of the risk rather than its actual value. An overestimation of the risk will in turn lead to more risk-reducing measures and more resources being spent on it (Berner & Flage, 2016).

#### Semi-quantitative Method

When the risk or uncertainty cannot be fully encompassed by quantitative means, Berner and Flage (2016) propose a semi-quantitative method to evaluate the SoK. This method allows for hidden uncertainty factors to be revealed and assessed in a qualitative way. Using simple criteria to categorise the strength of knowledge the risk is identified and assessed, which supports the probabilistic analysis and the sensitivity of the risk magnitude. If all four criteria are fulfilled the SoK is considered high according to Berner and Flage (2016):

- a) Assumptions made are considered to be reasonable
- b) There is broad agreement and consensus among experts
- c) Large amount of reliable data is available
- d) The phenomena involved are well understood; the models used are known to give predictions with the required accuracy

The background knowledge is considered weak if one or more of these criteria are fulfilled:

- The assumptions made represent strong simplifications
- There is a lack of agreement/consensus among experts
- The phenomena involved are not well understood; models are non-existent or known/believed to give poor predictions

In situations where some but not all criteria are fulfilled the strength of the background knowledge would be considered moderate. A rudimentary analysis of the sensitivity can also be made through these classifications (Berner & Flage, 2016):

- High: Relatively small changes in base values needed to bring about altered conclusions (e.g. exceedance of risk acceptance criterion)

- Moderate: Relatively large changes in base values needed to bring about altered conclusions
- Low: Unrealistically large changes in base value needed to bring about altered conclusions

Assessing how relatively small or large a change is can be challenging since it varies greatly depending on the situation, especially if the analysis is made qualitatively. The values and aim that have been set for the risk assessment will decide if the magnitude of the deviation will alter any conclusions and the sensitivity will have to be seen relative to the risk index used (Berner & Flage, 2016).

Berner and Flage (2016) mentions Saltelli (2002)'s article where he lists four desirable characteristics of sensitivity analysis one of which is multidimensional averaging. According to him the change occurring when varying every factor or input simultaneously is important enough to not be overlooked. This is what is done when a MCS is performed. Berner and Flage (2016) further states that it is recommended to also take an extra look at assumptions where deviation is considered high and at dependent assumptions i.e. where a deviation in an assumption is also extremely unlikely without also changing the other assumption.

#### Assumption Deviation Risk

Assumption Deviation Risk is a method that Aven (2013) first presented in 2013 where one converts the assumptions to a set of uncertainty factors to the assumed values. This method will take another more thorough step compared to traditional sensitivity analysis and uncertainty analysis where the focal point is asking "What if" questions. Assumption deviation risk explicitly examines the risk of deviation on assumptions made in the QRA. In its most simple form, it can be used as a way to evaluate the strength of knowledge but it can also be used as a more robust evaluation method for evaluating the consequences of deviations, the uncertainties inherent to the assumptions (Khorsandi & Aven, 2017). These criteria should be considered:

- Magnitude of the deviation
- Probability of this magnitude to occur
- The effect of the change on the consequences

Using the four (a-d) criteria listed on the page above, a rough estimate of the deviation can be made, if the SoK is considered high a low deviation score would be given and vice versa if SoK is considered low a high deviation score would be given. As an example given by Aven (2013) the deviation magnitudes of 2, 10 and 100 would then be given a deviation score based on the three earlier criteria. Since a deviation magnitude 2 had a probability of 50% it was given the score "high" but considerably lower for the other magnitudes (1% and negligible respectively)(Aven, 2013).

## 4.2 IPS suggested QRA Best Practice

Intresseföreningen för Processsäkerhet also called IPS and Stakeholder Association for Process Safety is a Swedish association whose objective is to maintain a high level of security in the process industry, convey knowledge to individuals in the industry and support the industry with seminars, training and courses. They publicised a guide for how QRA should be performed for a process plant, what steps need to be taken and how they are done to produce a robust risk assessment. An important part of the guide is making sure that the appropriate "inputs" are used, this will lead to the use of "best practice" according to IPS (IPS, 2022).

In subchapter 1.2.3 it is discussed that the use of the most likely value for inputs should be used for the QRA to generate the actual expected value of the risk but it is important to not disregard variation in the inputs. If one parameter is chosen to be estimated more conservatively than others to manage uncertainty, the overview of how different scenarios contribute to total risk could be distorted. The distortion can lead to confusion over which measures are most effective and the accuracy of the analysis is lessened. A sensitivity analysis can be used to give the analysis a more nuanced conclusion (IPS, 2022).

### 4.2.1 IPS's guide to QRA

Step 1 which is not labelled in figure 4.1 is handled in IPS QRA guide part 1, this step contextualizes the assessment, and defines the analysis purpose.

Step 2 is the (Val av scenarier) process where the appropriate scenarios are chosen to represent the analysis. There are different methods and approaches for this process depending on the situation where QRA is performed.

Step 3 is the process of frequency analysis (Frekvensanalys), this is where you determine the failure rate of components and functions which can lead to the predefined scenarios from step 2. This data can usually be found in databases where reliability, failure rates and safety measures efficiency are available.

Step 4 is also part of frequency analysis (Frekvensanalys) and this is where source strength for the predetermined scenarios is calculated and/or decided upon.

Steps 5 and 6 are made up of consequence analysis (Konsekvensanalys) where potential emissions are modelled (step 5) and calculation of consequences and effects potential emissions will have (step 6).

Step 7 is the process where frequency- and consequence analysis are combined to calculate the chosen risk metric (Beräkning av risk).

In step 8 the calculated risk metric is evaluated and compared (Värdering av risk) to criteria that are either mandated or decided upon to determine if the risk is acceptable or if risk-reducing measures need to be implemented.

Uncertainties that are associated with the analysis are managed and treated in step 9 (Hantering av osäkerheter). In step 10 the quality of the assessment is confirmed (Kvalitetssäkring).



Figure 4.1: IPS's definition of QRA

In this thesis only relevant steps from IPS suggestion will be discussed.

## 4.2.2 Step 2: Selection of scenarios

The core of a QRA is the identification, selection and description of possible scenarios. IPS highlights the importance of rigorously describing the chain of events from the emission of a dangerous element via safety barriers to the final event. The number of identified base events must be enough to represent an accurate picture of the potential risks, for smaller facilities just a few but for larger facilities several times more may be necessary. Base events or Loss of Containment (LOC) events are the starting point of any chain of events which is used in a QRA, an accurate estimation of potential base events will in turn have the most significance for estimating the base frequencies. According to the "Purple Book" by Uijt de Haag et al. (2001) LOC is divided into four categories 1) generic base events; 2) mechanical damage; 3) during loading and unloading; 4) specific to certain processes. IPS makes a more general division of base events:

- Generic base events with starting point at relevant elements in one or more chosen parts of the facility.
- Specific base events with relevance to one or more chosen parts of the facility.

Generic base events are events where some sort of release occurs, the reason why is less important. These events are experience-based and are a collective term for events caused by corrosion, design flaws or malpractice. In IPS's definition of generic base events mechanical damage and loading/unloading is also included.

Specific base events are releases of an element at a specific part or process which is unique to the facility and cannot be described by generic terms. Specific base events are directly linked to the design, processes and operational parameters of the facility. This means that base events will be produced specifically for this part of the facility.

#### **Base Frequencies**

When coming up with a base frequency there are usually two ways, either generic data sources or self-assessment (alternatively calculation). According to standard practice, information on typical failure rates can be found in these sources:

- BEVI Risk Manual (RIVM,2009)
- HSE Failure Rate and Event Data (HSE, 2017)
- IOGP Process Release Frequencies (IOGP, 2010)
- IPS vägledning om val av numeriska data i samband med skyddbarriärsanalys (IPS,2016)
- Sandia HyRAM (Hydrthe ogen Risk Assessment Model) (Hecht & Erhart, 2021)

When performing a QRA per the IPS guide it is suggested to use the BEVI Risk Manual for appropriate approach and input data but there are certain exceptions. For loading and unloading of cryogenic substances, DSB's recommendations are more suitable. For hydrogen-specific applications, Sandia's HyRAM is more suitable but failure rates for filters are probably wrongly estimated according to DSB. Generic data for Boiling Liquid Expanding Vapor Explosion (BLEVE) should not be used, instead specific event trees should be produced to generate failure rate.

Generic base frequencies are a suitable option if the frequency is difficult to estimate, they are based on historical data and should therefore be rough estimates of the true frequency. Another benefit of using generic base frequencies is that comparison between facilities become easier to perform.

Specific or self-assessed base frequencies can be used in some situations when producing a QRA, there may be a database on similar events and similar facilities available. In this case, it can be more appropriate to generate self-assessed base frequencies. For instance, if there is a produced LOPA (Layers of Protection Analysis) it can be used directly as input for the base frequency. If there is relevant facility-specific data for base event frequency it is recommended by IPS that it be used instead of generic base frequency, especially if said facility has specific or unique components in the process. When performing self-assessments it is important to guarantee that the data sets are big enough to accurately be able to draw general conclusions.

### 4.2.3 Step 3: Frequency Analysis

After establishing the scenarios representing the analysis (base events and end events) then subevents are used to generate the analysis using event trees. The first step is to establish the base frequency but that was done in step 2, in certain cases a fault tree should be used to calculate the base frequency. This may be appropriate if there are specific scenarios which cannot be found in generic databases or if there are certain underlying causes for the scenario. Usually when establishing the base frequency an

assessment of the reliability and functionality of mitigating barriers is done and they can also be taken into account throughout the event chain.

The next step is generating event trees, which is a tool for representing the event chains of different base events which can lead to end events. Base frequencies are the main input data which is then multiplied with the probability of each subevent. This will then generate a frequency for each end event. Some of the most important subevents in process engineering are weather conditions, the probability of ignition or/and explosion and the probability of barriers performing their designed purpose. A QRA always contain event trees, one per base event. It scales quickly to a large amount of end events but if done within a QRA tool it will perform the calculations for you.

#### Ignition

Ignition subevents are usually divided into two types of events, immediate ignition and delayed ignition. IPS mentions that DSB guidelines take you through the most commonly used analysis models but highlights it has been influenced by the Norwegian offshore industry where the focus is ignition. BEVI's model is considered the most simplistic but good enough for most QRA applications with a focus on environmental impact. HyRAM should only be used for hydrogen-specific applications.

When deciding on what probabilities to use for direct ignition subevents in the event tree IPS makes the differentiation on how reactive the substance is, the amount released, source strength and whether it's a stationary or mobile container. Delayed ignition is a bit more difficult to differentiate, the value is supposed to represent the likelihood of a gas cloud of a certain size drifting in a direction and ignites. Factors that affect the likelihood are characteristics of the substance, weather conditions, source strength, duration and what type of ignition source.

#### Barriers

When performing a QRA barriers for sub-events should be included but, in most cases only technical barriers are included. It is virtually impossible to include every single barrier so the barriers with the most effect on the rest of the event chain are incorporated into the calculation. Barriers are usually divided into two groups, passive and active. Passive barriers are barriers that always are in place and need no activation such as embankments, and active barriers that need activation to perform such as safety valves. If active barriers are used there needs to be two separate scenarios generated, one where the barrier activates and one where it does not activate.

### 4.2.4 Step 6: Estimation of consequences and fatalitites

When estimating the effect an accident would have on individuals, vulnerability and fatality criteria are needed. These criteria describe what exposure levels will result
in injuries, fatalities or domino effects on equipment. For toxic substances criteria, a calculation of dosage is recommended as and for fire radiation intensity. For this thesis toxicity will not be discussed.

### 4.2.5 Calcualtion of Risk

For every scenario, a consequence and a scenario have been calculated, for this to be comparable and evaluated it needs to be turned into risk metrics. This is usually done by calculating the individual risk (IR) and societal risk.

#### Individual Risk

IR is represented as the likelihood that for one individual residing in one location continuously one full year will perish, it is location-specific. These criteria are taken into consideration:

- Location of risk source
- Wind direction
- The fictive person is residing outdoors and takes no safety measures
- Duration of damage, maximum exposure time of 30 minutes

For each end event IR is calculated with this formula:

$$IR_{x,y,i} = f_i \cdot p_{f,i} \tag{4.1}$$

 $IR_{x,y,i}$  = Individual Risk at location x, y for end event i

 $f_i$  = frequency for end event (scenario) i, per annum

 $p_{f,i}$  = probability that scenario i leads to death on location x, y

 $f_i$  value is derived from the frequency analysis and the probability  $p_{f,i}$  of death is derived from the consequence analysis and partially from the frequency analysis where the wind direction is assessed. If wind direction is not included in the event tree a generalization can be made, splitting the 360° into 12 sectors and multiplying the scenario-specific frequency with 1/12. This case is applicable to gas clouds and not explosions. Total IR is calculated by summarizing each scenario which can affect the chosen location in this formula:

$$IR_{x,y} = \sum_{i=1}^{n} IR_{x,y,i}$$
(4.2)

 $IR_{x,y}$  = Total Individual Risk at location x, y, per annum

n =total number of scenarios

IR is displayed as contours on a map since it has a clear connection to the distance of consequence, usually called risk contours or individual risk contours. If several risk sources are present it is necessary to summarize IR for each end event and each risk source at each individual location.

#### Societal Risk

Societal risk is a metric which is used to represent the possible amount of casualties in case of an accident. To evaluate the societal risk the distance of consequence will have to be translated into the expected number of fatalities and for this certain parameters have to be known:

- The spread of consequence distance
- Population data
- Time of accident

To estimate the number of fatalities for each scenario consequence distance, areas where the criteria thresholds are exceeded, population data and time of accident are needed. The consequence analysis is performed in a way to represent how large a portion of the grid is affected by the scenarios.

$$N_i = \sum_{x,y} P_{x,y} \cdot p_{f,i} \tag{4.3}$$

- $N_i$  = Number of fatalities in the scenario i
- $P_{x,y}$  = Number of indivduals at location x,y
- $p_{f,i}$  = Probability of fatalities for scenario i

$$F_N = \sum_i F_i \text{ For all scenarios } i \text{ where } N_i \ge N \tag{4.4}$$

 $F_N$  = Frequency for all scenarios that affect N or more individuals

 $F_i =$  Frequency for scenario i

With  $F_N$  and  $N_i$  a fN-curve can be generated which is a graphic representation of the frequency of scenarios which will lead to a certain number of fatalities. It shows the relationship between the frequency f for an event or accident as a function of the number of fatalities (N). They are plotted on a logarithmic scale and it is especially useful for measuring risk metrics.

# 4.2.6 Step 9: Management of Uncertainties

Management of uncertainties is at the core of what a QRA is, all risk analysis involve making assumptions, simplifications and establishing boundaries and all of these contribute with uncertainty. Uncertainty according to IPS in this case is represented as if appropriate scenarios have been chosen, correct input data and if the right calculation models have been used.

#### Sensitivity Analysis

Sensitivity analysis is one of the more accessible ways of manage uncertainties, it will show how robust the analysis is. It does this by showing which of the parameters affects the output data the most. If a small change on one input parameter affects the output in a significant way, that parameter would be considered sensitive. A sensitive parameter will need input data with less uncertainty, this will in turn lead to a correct and representative value calculated for the frequency, consequence and/or the risk. An effective use of resources in a QRA will leave more room for management of uncertainties for sensitive parameters or refinement of assumptions.

IPS recommends that the sensitivity analysis is performed qualitatively on the quantitatively identified parameters. It is recommended that the parameters that are expected to be most sensitive are varied with a factor of 2 i.e. half and double of the expected value. Alternatively a minimum and maximum value is used to represent a non-conservative and a conservative estimation. This will highlight what parameters are most sensitive. When this is done a qualitative discussion on how these values will affect the result and interpretation of the risks. If the sensitivity analysis shows that it varies above the ALARP (As Low As Reasonably Practicable) limit certain considerations must be shown.

Basic assumptions such as the selection of scenarios and usage of calculation models shall be included in the sensitivity analysis. They do not need to be varied but a discussion of its effects on the result is necessary.

### **Uncertainty Analysis**

According to IPS, uncertainty analysis is a more sophisticated way of managing uncertainties by varying input data on several parameters. The chosen risk metric will then be represented as a interval or statistical distribution. MCS is a more advanced approach which can be used for more complex situations where every input parameter is a distribution, these distributions are often generated from histrocial data. An even more sophisticated approach is Bayesian analysis or updating where generic failure rates are combined with a specific failure for a certain valve on a specific facility. These results from Bayesian analysis will be presented with statistical distribution.

# 5 Case examination

In this chapter, the system that was analysed in the case study was defined along with the produced original QRA.It was based on Liquid Wind's FlagshipTWO facility, located in Sundsvall, Sweden and is located adjacent to a nearby CO2-source. The location is important for the Liquid Wind facility that needs biogenic CO2 and hydrogen to produce eMethanol.

# 5.1 Chosen methods

From Chapter 4.1 and IPS's suggestion two methods were chosen primarily for the case examination. Monte Carlo simulation was used as a tool to perform uncertainty analysis throughout the iterations because of its ability to vary all of the input variables and generate an uncertainty interval. The semi-quantitative method was chosen to evaluate the strength of knowledge throughout the iterations because of its allowed the SoK to be evaluated and motivate new relevant data to be incorporated into the analysis.

# 5.2 System Description

The case study examined the hydrogen part of their production process (Red area in Figure 5.1). The hydrogen will be produced through electrolysis where water will be split into hydrogen gas and oxygen gas. The process will be operating under pressure, 7 bar but after combining with the CO2 it will be pressurized up to 90 bar (Green area in Figure 5.1). From these situational inputs, two LOC scenarios were generated with accompanying event trees. The event tree composition where found in the reference manual BEVI RIVM, 2009 which is recommended by IPS to use.



Figure 5.1: Principle process sketch. Blue area: CO2 line / Red area: Hydrogen line / Green area: Methanol Reactor (fictional hydrogen storage cylinder) (Östersunds Tingsrätt Mark-och miljödomstolen, 2024)

# 5.3 QRA

# 5.3.1 Original Event Tree

The event trees used in the original QRA are based on the suggested event trees for flammable pressurised gas in the instantaneous and continuous case. They were produced for the purple book and reused in the BEVI risk manual (RIVM, 2009).

In the original QRA, two release scenarios are assessed in which one fictional storage cylinder containing all of the hydrogen within the facility has a complete rupture (Instantanenous) or a 10-minute continuous release. In this case, with the assumption of one fictional storage container, detection is less relevant since there is no realistic way of isolating the leak. This scenario becomes more relevant as soon as a more realistic "system" is examined where potential leaks within all the components have to be considered.

The original QRA was produced with IPS (2022) as a guideline. The purple book by Uijt de Haag et al. (2001) and BEVI Risk Manual by RIVM (2009) were used for the selection of scenarios, this is most likely because hydrogen was not the only substance managed and produced within the facility. The QRA was produced in an early stage of the project which meant the level of detail and depth at which it was produced were not as high as it would be in later stages.







Figure 5.3: Suggested Event Tree for Continuous Release for Pressurised Gas(RIVM, 2009)

#### 5.3.2 HyRAM Event Tree

The guideline HyRAM would allow for a more detailed frequency analysis to be performed since it contains failure frequencies and distributions for components. The event tree suggested by HyRAM also incorporates another end event which is detection which would be possible if component-specific frequencies were to be calculated. The end events fire ball and flashfire are not included in their event tree.



Figure 5.4: Suggested Event Tree for Hydrogen Release (Ehrhart et al., 2021)

### 5.3.3 Ignition probabilities

The ignition probabilities used in the original QRA come from the purple book where it is assumed that it is 100% that it will ignite. This is because hydrogen is considered a high reactivity category 0 substance. HyRAM on the other hand which is specifically produced for hydrogen engineering deems the ignition probabilities to be less likely.

**Table 5.1:** Instantaneous Ignition probabilities (Uijt de Haag et al., 2001) & (Ehrhart<br/>et al., 2021)

Source	Mass (Flow)	P(Direct)	P(Delayed)	P(No ignition)
BEVI Risk manual HyRam	1-10  ton > 6.5  kg/s	$\begin{array}{c} 0.5 \\ 0.23 \end{array}$	$\begin{array}{c} 0.5 \\ 0.12 \end{array}$	$\begin{array}{c} 0 \\ 0.65 \end{array}$

**Table 5.2:** Continuous Ignition probabilities (Uijt de Haag et al., 2001) & (Ehrhart et al.,<br/>2021)

Source	Mass Flow	P(Direct)	P(Delayed)	P(No Ignition)
BEVI Risk manual HyRam	$<\!10 \text{ kg/s}$ $>\!6.5 \text{ kg/s}$	$\begin{array}{c} 0.2 \\ 0.23 \end{array}$	$\begin{array}{c} 0.8\\ 0.12\end{array}$	$\begin{array}{c} 0 \\ 0.65 \end{array}$

### 5.3.4 Event Probabilities

The purple book supplies probabilities for the end events that are used in their suggested event tree. For pressurised gas, they are fireball (BLEVE), jet fire, explosion and flash fire as shown in figure 5.2 and 5.3.

Event	Scenario	Purple Book (probability)	HyRAM (probability)
Fire Ball	INST	0.7	N/A
Explosion	INST/CONT	0.4	0.108
Flash Fire	INST/CONT	0.6	N/A
Jet Fire	CONT	0.2	0.207

**Table 5.3:** Event Probabilities Suggested by (Uijt de Haag et al., 2001) & (Ehrhart et al.,<br/>2021).

Since HyRAM's event tree is quite different, it does not deal with complete ruptures for storage cylinders and some event probabilities are missing compared to the purple book. It incorporates the probability of detection and isolation of the leak in the event tree which the purple book's tree has not.

As figure 5.5 shows below only the probability of the leak being isolated, direct ignition and delayed ignition are needed to calculate the end event frequencies per the event tree suggested by HyRAM.

$f_{\text{Isolated}} = f_{\text{H2 Release}} \times P(\text{Isolated})$	(5)
$f_{\text{Unignited}} = f_{\text{H2 Release}} \times P(\overline{\text{Isolated}}) \times (1 - P(\text{Immed. Ignite}) - P(\text{Delayed Ignite}))$	(6)
$f_{\text{Jetfire}} = f_{\text{H2 Release}} \times P(\overline{\text{Isolated}}) \times P(\text{Immed. Ignite})$	(7)
$f_{\text{Explosion}} = f_{\text{H2 Release}} \times P(\overline{\text{Isolated}}) \times P(\text{Delayed Ignite})$	(8)

Figure 5.5: Equations to calculate frequencies for end events according to HyRAM's suggested event tree (Ehrhart et al., 2021)

# 6 Frequency Generation

In this chapter, an iterative study of the strength of knowledge for the defining assumptions and parameters was performed and then said assumptions and parameters underwent uncertainty treatment. The employed distributions and decisions made during the analysis were done in conjunction with Alexander Lauge Pedersen, a risk consultant at Sweco Sverige AB (2024). Four iterations were made and for they implemented an improvement to the uncertainty management and strength of knowledge in the QRA:

• Iteration 1: Base frequency

Replaced base frequency for starting event with generic failure distributions using the purple book event tree.

• Iteration 2: Ignition probabilities

Employed distributions for ignition probabilities instead of point estimations using the purple book event tree.

• Iteration 3: Outcome probabilities

Employed distributions for outcome probabilities instead of point estimations using the purple book event tree.

• Iteration 4: Cumulative frequency

Component specific cumulative base frequency replacing iteration 1 base frequency with HyRAM event tree

The sensitivity analysis in this thesis was used to help identify to what level of detail it was worth performing and which parts of the analysis are necessary to enhance further.

# 6.1 Iteration 1: Base Frequency

The base frequencies used for the QRA on FS2 are found in the purple book written by Uijt de Haag et al. (2001). In this given scenario a conservative assumption has been made that all of the hydrogen in the process will be pressurized up to 90 bar. The pressure vessel will be combined into one fictional vessel which upon the scenario selection and calculations will be made. This choice was made because of a lack of facility data and that this scenario would generate conservative risks. Conservative risks would then be overestimated allowing for the approval process to move along. Here the semi-quantitative method was implemented to evaluate the SoK which then gave a basis for varying the base frequency, using the four criteria previously mentioned in Chapter 4.

# 6.1.1 Base Frequency: Evaluation of SoK

#### Assumption

The assumptions concerning that all of the hydrogen would be stored in a fictional storage cylinder are considered to be reasonable albeit conservative. Using the fictional hydrogen vessel would elevate the consequences since all of the hydrogen never would be stored in a single container during operation. The hydrogen mixed with CO2 would also have a dampened effect on the consequences and this is not included in the calculations instead consequence modelling is done with pure hydrogen.

#### Consensus

Since the original QRA was performed in the early stages of the project (FlagshipTWO) there was no exact information available except the amount of substance utilized onsite. Therefore there is a broad consensus among experts that an assumption of this kind (One single storage container) is reasonable when in the early stages and examining a facility with several different substances. But since it's hydrogen gas which is being evaluated in this thesis and IPS (2022)states in assessments where hydrogen is assessed, HyRAM by Ehrhart et al. (2021) is the appropriate guide to use. In the original QRA's case, it is not as straightforward since it examined and simulated several different substances and the hydrogen part of the risk did not exceed set criteria. If the risk would have exceeded mandated criteria a more detailed approach would have been appropriate.

#### Data

Since this facility has as of March 2024 just been constructed or is in its final steps there were not large amounts of data available. This is why in many steps conservative "standard practice" values have been used. Ehrhart et al. (2021) guideline will help bridge the gap of knowledge with generic values on probabilities and distributions specific to components used in hydrogen facilities.

#### Phenomena

The phenomena involved in the analysis are well understood, models used and simulations performed output the required accuracy.

### SoK Grade

From the evaluation of these four criteria, it is determined that the strength of knowledge is moderate to weak, this warrants further investigation and application of Monte Carlo simulation to include these uncertainties within the parameters.

# 6.1.2 Generic Component Failure Frequencies

Generic component failure frequencies in this case is a component-specific failure frequency for a component being used in a hydrogen facility. It is the input value used in the frequency generation as base frequency. The purple book supplied the failure frequencies as point estimations in the original QRA but in iterations 1 through 4 it is replaced by HyRAM's proposed generic component failure distributions.

The generic component failure frequencies presented in HyRAM were produced by Lachance et al. (2009). In this paper, they discuss the general lack of data within hydrogen safety engineering which meant certain concessions had to be made. This meant stepping away from traditional statistics and using Bayesian statistics. There are benefits and drawbacks to both approaches.

With traditional statistics, the data available poses certain restrictions if highly specific data is unavailable which leads to agglomeration of data which in itself invites uncertainties in assessment.

On the other hand with Bayesian statistics this problem is somewhat mitigated since with Bayes' rule data from several sources can be combined where the existing data may serve as "first guess" values which will then define the distributions of the leak frequency. These distributions would then be called "prior" distributions and they could then be updated with hydrogen-specific values. These updated distributions would then be called "posterior" distributions. If a hierarchical approach is used which the authors Lachance et al. (2009) used, "layers" of significance can be factored into each data set depending on the confidence in its accuracy and SoK. One drawback of bayesian statistics is the chosen "prior" as it is chosen subjectively, if it is poorly chosen or biased it may skew the output of the analysis.

# 6.1.3 Cylinder Frequency

As stated on the previous page the SoK for the base frequency was considered to be moderate and therefore an investigation into whether better data can be found was performed. Ehrhart et al. (2021) has as previously produced generic failure distributions for different components. The distribution for the component called "cylinder" was used to replace the base frequency for the pressurized storage cylinder in both the instantaneous and continuous scenarios. By using a distribution, the uncertainties were managed in a more holistic sense, and since these were specifically produced for hydrogen systems, they helped reveal the uncertainties found in the SoK investigation and, if incorporated in risk evaluation, decreased the uncertainties. The generic failure distributions found in HyRAM are divided into release sizes for each component, 0.01% through to 100%. The release sizes in this case reflect the percentage of the pipe flow area

Scenario	Component	Release Size	$\mu$	α	Distribution
Instantaneous	Cylinder	100%	-15.62	0.68	Lognormal
Continuous	Cylinder	0.01%	-13.92	0.67	Lognormal
Continuous	Cylinder	0.1%	-14.06	0.65	Lognormal
Continuous	Cylinder	1%	-14.44	0.65	Lognormal
Continuous	Cylinder	10%	-14.99	0.65	Lognormal

Table 6.1: HyRam Generic Cylinder failure distributions (Ehrhart et al., 2021)

#### Instantaneous

The distribution for the instantaneous case includes the point estimation frequency that is proposed in the purple book in the 95th percentile. This would support that the Purple Book was produced conservatively. For the instantaneous case, the base frequency of a 100% release was used which is generated from the distribution shown in 6.1.

The event tree used is the same which is a recommended event tree for pressurized gas from RIVM (2009) and the probabilities of fireball, flash fire and explosion also stayed the same since the parameter/assumption being investigated is the base frequency.

#### Continuous

For the continuous case, the rest of the release sizes ranging from 0.01% to 10% were used as a cumulative frequency as it is assumed that all of these release sizes can lead to the continuous case, see table 6.1. The cumulative frequency generated from HyRam's generic failure frequencies encompasses the base frequency suggested by the purple book.

The event tree used is the same which is a recommended event tree for pressurized gas from RIVM (2009) and the probabilities of fireball, flash fire and explosion also stayed the same since the parameter/assumption being investigated is the base frequency.

# 6.1.4 Result

In this first iteration, when only the base frequency was altered, this propagated linearly throughout the analysis. The strength of knowledge was elevated and, in this sense, made the assessment more robust. One distribution of frequency from each scenario (instantaneous and continuous) are shown since the trends they show are prevalent in all end events.

#### Instantanenous

For the instantaneous case, the base frequency was replaced, from the original mean value (5.5E10 - 7) to the new mean value (2.07E10 - 7) which gave it a decrease in all end events frequencies. Table 6.2 and 6.3 displays each end event's 5th-, 95th percentile, mean and median which was generated through MCS and compared to the point estimated original mean.

Table 6.2: Iteration 1 Instantaneous: End event frequency with replaced base frequency.

End event	5th	Mean	Median	95th	Original Mean
Fireball (direct) (I1)	1.87E - 8	7.25E - 8	5.76E - 8	1.75E - 7	1.75E - 7
Explosion (direct) $(I2)$	3.21E - 9	1.24E - 8	9.86E - 9	3.01E - 8	3.00E - 8
Flashfire (direct) (I3)	4.84E - 9	1.87E - 8	1.48E - 8	4.51E - 8	4.50E - 8
Explosion (delayed) (I4)	1.08E - 8	4.15E - 8	3.29E - 8	1.00E-7	1.00E - 7
Flashfire (delayed) (I5)	1.61E - 8	6.21E - 8	4.93E - 8	1.50E - 7	1.50E - 7
No Ignition (I6)	0	0	0	0	0
Base Frequency	5.35E - 8	2.07E - 7	1.64E - 7	5.02E - 7	5.5E - 7



Figure 6.1: Generated distribution of frequency for scenario I2 (Explosion, instantaneous case) with original mean as the top value shown as an example of how distribution will vary. (X-axis: Possible range of frequency, Y-axis: Probability density of said frequency)

Figure 6.1 displays the distribution of frequency for end event explosion I2, as can be seen it is very similiar to lognormal distrubtion, this is due to all varying inputs are lognormal distributions. he original mean frequency were used as a top value to demonstrate at which certainty it is included in the uncertainty interval.

		INST					End Event	Frequency (base freq replaced)
				70,0%	25,55%		11	7,25767E-08
			Fireball (BLEVE)	0	0			
		Direct0	Chance					
			1		Explosion 40,0%	4,38%	12	1,24417E-08
					0	• 0		
			Explosion	30,0%	Chance 0			
					Elashfire 60,0%	6,57%	13	1,86626E-08
BaseFreq Hyram					0	0		
	Hyram INST	Chance 0						
		1	Explosion	40,0%	12,4%		14	4,14724E-08
				0	- 0			
		Delayed 31,0%						
			Flashfire	60,0%	18,6%		15	6,22086E-08
				0	0		10	
		No ignition 32,5%	32,5% 0				16	0
							Tot	2,07362E-07

Figure 6.2: Event Tree for Instantaneous case with mean values generated from replaced base frequency for end event frequencies.

When calculating this in risk metrics there should be a significant difference in the result considering the frequency for the events is about 58% (for the mean value) less than the original assessment for the instantaneous case.

#### Continuous

For the continuous case, the base frequency was replaced, from the original mean value (5.5E-7) to the new mean value (3.123E-6) which gave it an increase in all end events frequencies. Table 6.2 and 6.3 displays each end event's 5th-, 95th percentile, mean and median which was generated through MCS and compared to the point estimated original mean.

End event	5th	Mean	Median	95th	Original Mean
Jetfire (direct) (C1)	3.23E - 7	6.29E - 7	5.82E - 7	1.10E - 6	1.10E - 7
Explosion (delayed) $(C2)$	5.16E - 7	1.01E - 6	9.32E - 7	1.77E - 7	1.76E - 7
Flashfire (delayed) $(C3)$	7.74E - 7	1.51E - 6	1.40E - 6	2.65E - 6	2.64E - 7
No Ignition $(C4)$	0	0	0	0	0
Base Frequency	1.58E - 6	3.13E - 6	2.94E - 6	5.28E - 6	5.5E - 7

Table 6.3: Iteration 1 Continuous: End event frequency with replaced base frequency.

The base frequency suggested and generated from Ehrhart et al. (2021) is significantly larger than the one used in the original assessment which was provided by the purple book. This is in large part due to the amount of release sizes which were included in the generated base frequency. Le et al. (2023) only uses the 1% and the 10% release sizes to represent the continuous case, no reason is given other than that they were chosen. This is most likely because the 0.01% and 0.10% release sizes were considered to be too

small and negligible. In this first iteration, a release size of 0.01% and 0.10% cannot be considered negligible since it is one fictional storage cylinder being examined. A release of that size would still pose a risk to the facility and its surroundings.

Figure 6.3 displays the distribution of frequency for end event explosion C2, as can be seen it is very similar to lognormal distrubtion, this is due to all varying inputs are lognormal distributions. The original mean frequency were used as a top value to demonstrate at which certainty it is included in the uncertainty interval.



Figure 6.3: Generated distribution of frequency for scenario C2 (Explosion, continuous case) with original mean as the top value shown as an example of how distribution will vary. (X-axis: Possible range of frequency, Y-axis: Probability density of said frequency)

	CONT			End Event	Freq
		Jetfire			
	Direct 2006	20,0%		C1	6,27584E-07
/		0			
HyRam CONT	Chance				
	0				
		Explosion 40	32,0%	C2	1,00413E-06
	/	0	0		
	Delayed 8	Chance			
	0	0			
		Elashfire 6000	48,0%	C3	1,5062E-06
		0	0		
	No Ignition	0,0%		C4	0
		0			
				Tot	3,13792E-06

Figure 6.4: Event tree for the continuous case with mean values generated from replaced base frequency for end event frequencies.

#### Sensitivity analysis

The tornado diagram for the instantaneous case was very simple with only one parameter, which was the base frequency. This was because it comprised only one distribution, and the rest of the inputs were point estimations.



Figure 6.5: Effect on output frequency for end event C2 explosion in iteration 1 for the continuous case.

For the continuous case, there were four parameters because the base frequency was a summarization of four different distributions. It showed that the smaller release sizes, 0.01% and 0.10%, contributed the most to the uncertainty of the output. The output in this sensitivity analysis was the distribution of frequency generated for the end event, C2 Explosion, which was performed to evaluate the uncertainty contribution by

each input parameter. In this case only one end event was shown due to trends shown in Figure 6.5 are prevalent for remaining end events. This was the case for iteration 2 and 3 aswell.

### 6.1.5 Summary

The SoK was determined to be moderate to weak, warranting further investigation and MCS. For the MCS, a base frequency for the instantaneous and continuous cases was employed. This base frequency was found in HyRAM, a hydrogen-specific reference manual. A decrease in the instantaneous frequency could be seen in Table 6.2 and an increase in continuous frequency could be seen, see Table 6.3.

# 6.2 Iteration 2: Ignition Probabilities

The next step in the iterative process was examining the probabilities for direct, delayed, and no ignition. (Event trees will not be shown as they are the same as in iteration 1.)

As previously stated in Chapter 5, the two guidelines being examined differ substantially in both likelihood and the dimensioning flow. HyRAM does not present any probabilities for a complete rupture in the same way the Purple Book does. Implementing the suggested semi-quantitative approach to examine the ignition probabilities provided further insight into the SoK of the used values.

# 6.2.1 Evaluation of SoK: Ignition Probabilites

There were arguments to be made for both guidelines, with their scopes being slightly different. HyRAM, as previously stated, was specifically developed for hydrogen safety engineering, making it fitting for this application, but it lacked data for large amounts and releases. The Purple Book, on the other hand, was more generic, dealing with a majority of flammable or toxic substances and having data for larger amounts.

### Assumptions

The assumptions made were considered to be reasonable, albeit conservative. Using the ignition probabilities from the Purple Book is the standard practice within process safety engineering, but as IPS suggested, when working with hydrogen, HyRAM's guidelines may be more accurate to use. The Purple Book assumes a 100

#### Consensus

There was a broad consensus among experts that an assumption of this kind was reasonable. However, since hydrogen gas was being evaluated and IPS (2022) states that in assessments where hydrogen is present, Ehrhart et al. (2021) is the appropriate guide to use. In the original QRA's case, it was not as straightforward since it examined and simulated several different substances, and the hydrogen part of the risk did not exceed the set criteria. If the risk had exceeded mandated criteria, a more detailed approach would have been appropriate.

#### Data

Since this facility has as of March 2024 just been constructed or is in its final steps there are not large amounts of data available. This is why in many steps conservative "standard practice" values have been used. Ehrhart et al. (2021) guideline will help bridge the gap of knowledge with generic values on probabilities and distributions specific to components used in hydrogen facilities.

#### Phenomena

The phenomena involved in the analysis were well understood, and the models used and simulations performed provided the required accuracy of output.

# 6.2.2 SoK Grade

From the evaluation of these four criteria, it was determined that the strength of knowledge was moderate to weak. This warranted further investigation and the application of Monte Carlo simulation to include these uncertainties within the parameters.

# 6.2.3 Employed Distributions: Ignition Probabilities

Given the differing data, the author employed uniform distributions with the probabilities using the available data from The Purple Book and HyRAM, where they represent the lowest and highest values. This was done to encompass all of the uncertainty that the difference in data from the guidelines gives way to.

Table 6.4: Suggested distributions for Ignition Probabilities for Instantaneous Scenario

Event	Distribution	Mean
Direct Ignition (DIR)	Uniform(0.23;0.5)	0.365
Delayed Ignition (DEL)	Uniform(0.12;0.5)	0.31
No Ignition (NO)	P(No) = 1 - P(DIR) - P(DEL)	0.325

Event	Distribution	Mean
Direct Ignition (DIR) Delayed Ignition (DEL)	Uniform(0.2;0.23) Uniform(0.12;0.8)	$\begin{array}{c} 0.215\\ 0.46\end{array}$
No Ignition (NO)	P(No) = 1 - P(DIR) - P(DEL)	0.325

 Table 6.5:
 Suggested distributions for Ignition Probabilities for Continuous Scenario

#### Instantaneous

Ehrhart et al. (2021) supplies probabilities for direct and delayed ignition specific to hydrogen systems, although the mass flows described are on the smaller side, especially when calculating a rupture of a storage cylinder under pressure. This gives way to some uncertainties and reason to propose distributions which include both probabilities from HyRam and the Purple Book.

#### Continuous

In the continuous case, the mass flows are more similar in their dimensioning size, this would lead to less uncertainty when employing a uniform distribution that includes values from both HyRAM and the purple book for the ignition probabilities.

# 6.2.4 Result

In this second iteration, both the base frequency and ignition probabilities were changed. The base frequency remains the same as in iteration 1, but the employed distributions for ignition probabilities were implemented in the Monte Carlo simulation. Table 6.6 and 6.7 display each end event's 5th and 95th percentile, mean, and median, which were generated through MCS and compared to the point estimated original mean. One distribution of frequency from each scenario (instantaneous and continuous) are shown since the trends they show are prevalent in all end events.

**Table 6.6:** Iteration 2 Instantaneous: End event frequency with replaced base frequency and employed distributions for ignition probabilities.

End event	5th	Mean	Median	95th	Original Mean
Fireball (direct) (I1)	1.25E - 8	5.30E - 8	4.07E - 8	1.305E - 7	1.75E - 7
Explosion (direct) $(I2)$	2.13E - 9	9.08E - 9	6.98E - 9	2.24E - 8	3.00E - 8
Flashfire (direct) (I3)	3.20E - 9	1.36E - 8	1.05E - 8	3.35E - 8	4.50E - 8
Explosion (delayed) (I4)	5.24E - 9	2.57E - 8	1.96E - 8	6.83E - 8	1.00E - 7
Flashfire (delayed) (I5)	1.61E - 8	3.86E - 8	4.93E - 8	1.50E - 7	1.50E - 7
No Ignition (I6)	1.15E - 8	6.74E - 8	5.18E - 8	1.81E - 7	0
Base Frequency	5.35E - 8	2.07E - 7	1.64E - 7	5.02E - 7	5.5E - 7

Figure 6.6 displays the distribution of frequency for end event explosion I2 from iteration 2. It was observed that the uncertainty interval at which the original frequency for this end event is included have increased. A decrease in standard deviation was also observed. The original mean frequency were used as a top value to demonstrate at which certainty it is included in the uncertainty interval.



Figure 6.6: Generated distribution of frequency for scenario I2 (Explosion, instantaneous case) with original mean as the top value shown as an example of how distribution will vary. (X-axis: Possible range of frequency, Y-axis: Probability density of said frequency)

 Table 6.7: Iteration 2 Continuous: End event frequency with replaced base frequency and employed distributions.

End event	5th	Mean	Median	95th	Original Mean
Jetfire (direct) (C1)	3.68E - 7	6.75E - 7	6.16E - 7	1.21E - 6	1.10E - 7
Explosion (delayed) $(C2)$	1.67E - 7	5.77E - 7	5.09E - 7	1.23E - 7	1.76E - 7
Flashfire (delayed) $(C3)$	2.50E - 7	8.66E - 7	7.64E - 7	1.84E - 6	2.64E - 7
No Ignition $(C4)$	5.71E - 8	1.02E - 6	8.74E - 7	2.58E - 6	0
Base Frequency	1.58E - 6	3.13E - 6	2.94E - 6	5.28E - 6	5.5E - 7

Figure 6.7 displays the distribution of frequency for end event explosion C2 from iter-

ation 2. It was observed that the uncertainty interval at which the original frequency for this end event is included has increased. A decrease in standard deviation was also observed. The original mean frequency was used as a top value to demonstrate at which certainty it is included in the uncertainty interval.



Figure 6.7: Generated distribution of frequency for scenario C2 (Explosion, continuous case) with original mean as the top value shown as an example of how distribution will vary. (X-axis: Possible range of frequency, Y-axis: Probability density of said frequency)

The most significant change throughout iteration 2 was that the probability of no ignition was not 0. This, in turn, led to decreases in remaining frequencies. When employing uniform distributions like these for ignition probabilities, it opened up to greater variation where the accuracy may have been affected.

#### Sensitivity Analysis

Figure 6.8 showed that for the instantaneous case, the employed distribution of direct ignition did not affect the output more than the chosen base frequency. On the other hand, for the continuous case, the parameter which affected the output the most was the employed distribution for delayed ignition. This was most likely due to the wide uniform distribution used.



Figure 6.8: Effect on end event frequency for end event explosion I2 and C2, Instantaneous (bottom) and Continuous (top) from iteration 2.

This trend was prevalent throughout most of the end events with small changes. Those changes occurred when the interval in the employed distributions for ignition probabilities was narrow.

### 6.2.5 Summary

The SoK was determined to be moderate to weak, warranting further investigation and Monte Carlo simulation. For the Monte Carlo simulation, a base frequency for the instantaneous and continuous case was employed. Uniform distributions for ignition probabilities were employed, with the bottom value supplied by HyRAM and the top value supplied by the Purple Book in most cases. This led to a decrease in all event frequencies compared to iteration 1 and the original QRA, as could be seen in Table 6.6 and 6.7. In the sensitivity analysis, it was shown that the employed distribution, delayed ignition for continuous release, contributed more to the effect on the output, which was a change from iteration 1, highlighted in the previous paragraph.

# 6.3 Iteration 3: Outcome probabilities

Examining the outcome probabilities was the third step in the iterative process. It was not as straightforward as the base frequency or the ignition probabilities since the event trees were constructed differently, and there was no need for specific probabilities for outcome's in the HyRAM event tree. (Event trees will not be shown as they are the same as iteration 1).

# 6.3.1 Outcome Probabilities: Evaluation of SoK

There were arguments to be made for both guidelines, with their scopes being slightly different. HyRAM, as previously stated, was specifically developed for hydrogen safety engineering, making it fitting for this application, but it does not provide probabilities for all the end events that the purple book makes use of.

#### Assumption

The event tree from the Purple Book was likely produced to handle both small and larger quantities of specified substances, and therefore the end events differed compared to HyRAM's event tree. For instance, Uijt de Haag et al. (2001) included the event fireball for direct ignition for the instantaneous release scenario, and for delayed ignition, it included the end event flash fire. HyRAM did not include any of these end events, and it was most likely because of the different dispositions of the two guidelines.

#### Data and Consensus

Since the end events were very different, which was probably because of their slightly differing purposes and dispositions, it led to a lack of consensus among experts. There was a considerable amount of data available for process safety engineering, but as previously mentioned, there was a lack of data generally when discussing hydrogen safety engineering.

Le et al. (2023) decide to combine the outcome probabilities in their specific event tree for hydrogen energy storage systems since neither HyRAM nor the purple book fully captures the situation or supplies enough data.

#### Phenomena

The phenomena involved in the analysis are well understood, models used and simulations performed output the required accuracy.

#### SoK Grade

From the evaluation of these four criteria, it was determined that the strength of knowledge was moderate to weak. This warranted further investigation and application of Monte Carlo simulation to include these uncertainties within the parameters.

# 6.3.2 Employed Distributions: Outcomes

Because of the uncertainties discussed in the previous section regarding the outcome probabilities distributions was employed to incorporate said uncertainties.

Event	Scenario	Purple Book	HyRAM	Distribution
Fire Ball	INST	0.7	N/A	Uniform(0.525; 0.7)
Explosion	INST/CONT	0.4	0.108	UniForm(0.108; 0.4)
Flash Fire	INST/CONT	0.6	N/A	1-P(Explosion)
Jet Fire	CONT	0.2	0.207	Uniform(0.2; 0.207)

 Table 6.8: Event Probabilities Suggested and employed distributions.

For the end event Fireball, there was no similar end event represented in HyRAM, which is why it was chosen to employ a uniform distribution with its lower value being a 25% decrease of the point estimate given from the Purple Book. The supplied point estimate was considered to be conservative, which is why only a lower value was chosen for the distribution.

Both the Purple Book and HyRAM supplied a probability for explosion, but they were significantly different. A uniform distribution with a lower value given by HyRAM

and a higher value supplied by the Purple Book was employed. This incorporated uncertainties stemming from the two guidelines.

HyRAM did not supply a probability for flash fire as it was not represented as an end event in their event tree, as seen in Figure 5.4. Since the event tree represented in RIVM (2009) and in figures 5.2 and 5.3 was the chosen selection of scenarios for this thesis, the probability of explosion and flash fire had to be summarized to 100%. In this case, it was employed as: P(FlashFire) = 1 - P(Explosion).

The probability of jet fire was given from both guidelines and was relatively similar; this, in turn, did not yield a lot of uncertainties. In this case, the Purple Book's value represented the lower end and HyRAM the higher end.

# 6.3.3 Result

In the third iteration, the outcome probabilities were given distributions instead of point estimations because of the strength of knowledge being valued at a weak to moderate strength. Given the nature of some of the employed distributions, minor changes in the end event frequencies were observed. One distribution of frequency from each scenario (instantaneous and continuous) are shown since the trends they show are prevalent in all end events.

Table 6.9 displayed each end event's 5th and 95th percentile, mean, and median, which were generated through MCS and compared to the point estimated original mean.

As could be seen in Figures 6.9 and 6.10 the interval at which the original QRA's mean value is included have yet again increased. A decrease in standard deviation could also be observed.

Table 6.9:	teration 3 Instantaneous: End event frequency with replaced base frequency
	employed distributions for ignition- and end event probabilities.

End event	5th	Mean	Median	95th	Original Mean
Fireball (direct) (I1)	1.095E - 8	4.62E - 8	3.56E - 8	1.19E - 7	1.75E - 7
Explosion (direct) $(I2)$	1.45E - 9	7.44E - 9	5.40E - 9	1.98E - 8	3.00E - 8
Flashfire (direct) $(I3)$	4.85E - 9	2.18E - 8	1.65E - 8	5.70E - 8	4.50E - 8
Explosion (delayed) (I4)	2.90E - 9	1.64E - 8	1.16E - 8	4.95E - 8	1.00E - 7
Flashfire (delayed) (I5)	9.36E - 9	4.78E - 8	3.54E - 8	1.29E - 7	1.50E - 7
No Ignition (I6)	9.74E - 9	6.75E - 8	4.89E - 8	1.81E - 7	0
Base Frequency	5.35E - 8	2.07E - 7	1.64E - 7	5.02E - 7	5.5E - 7



Figure 6.9: Generated distribution of frequency for scenario I2 (Explosion, instantaneous case) with original mean as the top value shown as an example of how distribution will vary. (X-axis: Possible range of frequency, Y-axis: Probability density of said frequency)

 Table 6.10: Iteration 3 Continuous: End event frequency with replaced base frequency and employed distributions for continuous case

End event	5th	Mean	Median	95th	Original Mean
Jetfire (direct) (C1)	3.56E - 7	6.74E - 7	6.24E - 7	1.16E - 6	1.10E - 7
Explosion (delayed) $(C2)$	7.78E - 8	3.69E - 7	3.01E - 7	872E - 7	1.76E - 7
Flashfire (delayed) $(C3)$	2.88E - 7	1.08E - 6	9.32E - 7	2.31E - 6	2.64E - 7
No Ignition $(C4)$	4.43E - 8	1.02E - 6	9.03E - 7	2.34E - 6	0
Base Frequency	1.62E - 6	3.14E - 6	2.90E - 6	5.38E - 6	5.5E - 7



Figure 6.10: Generated distribution of frequency for scenario C2 (Explosion, continuous case) with original mean as the top value shown as an example of how distribution will vary. (X-axis: Possible range of frequency, Y-axis: Probability density of said frequency)

#### Sensitivity Analysis

For the instantaneous case, it was the base frequency affecting the output the most, especially high inputs. But for the continuous case, it was the delayed ignition and explosion probability which affected the output the most. This was due to the employed distribution used for delayed ignition being a uniform distribution ranging from 12% to 80%, and the explosion distribution being a uniform range from 10.8% to 40%.



Figure 6.11: Effect on end event frequency for end event explosion I2 and C2, Instantaneous (bottom) and Continuous (top) from iteration 3.

# 6.3.4 Summary

The SoK was determined to be moderate to weak, warranting further investigation and Monte Carlo simulation. For the Monte Carlo simulation, a base frequency for the instantaneous and continuous case was employed. Uniform distributions for outcome probabilities were employed where a value from HyRAM and the Purple Book exists, but for the end event Fire Ball, a variation of 25% was applied, see table 6.8. This led to minor changes in all event frequencies as can be seen in table 6.9 and 6.10.

# 6.4 Iteration 4: Component Specific Base Frequency

For iteration 4, there were plans to generate a facility-specific failure frequency, but due to only public information being used, it was not possible. Therefore, a qualitative description of how it would have been done and a calculation example will be presented instead.

# 6.4.1 Scenario Identification

In this iteration, the plan was to step away from the original assumption that all of the hydrogen present would be stored in a storage cylinder and instead spread out throughout the system. This would have allowed the analysis to use the HyRAM event tree (Figure 5.4 This, in turn, would have increased the strength of knowledge overall by using an event tree specifically produced for hydrogen applications.

# 6.4.2 Frequency Generation

If a component list had been available, a cumulative frequency for the entire hydrogen line could have been generated. This would have later been used to calculate detailed end event frequencies. The cumulative frequency would have been substantially greater. However, in this case, the assessment that Le et al. (2023) made should be applicable to this case. Le et al. (2023) decided to only use 1%, 10% and 100% release sizes for their QRA which in this case would most likely be appropriate as well.

When the number of components which are present in the system has been established the equation shown in figure 6.12 then is the input for each component in the event tree shown below.

$$f_{\text{Random Releases},k} = \sum_{i} N_{\text{Component}_i} \times f_{\text{Leak}_{i,k}}$$

Figure 6.12: Equation for calculation of summarized component and release size specific failure frequency (Ehrhart et al., 2021)

A fault tree such as this would be used to establish a cumulative frequency for each release size depending on the number of components in the system:



Figure 6.13: Example of fault tree which can be used to calculate failure frequency for a release size (Ehrhart et al., 2021)

In this case, Monte Carlo Simulation would have also been applied to generate uncertainty intervals as input for the consequence modelling but this was not within the scope of this thesis. The authors of HyRAM Ehrhart et al. (2021) had also developed software which was free to use. Since it had somewhat more sophisticated consequence models and was suited for the HyRAM event tree and its end events, the HyRAM software would have been used instead.

For this iteration, the employed distributions generated in iterations 2 and 3 would have been reused. This decision was made to keep the strength of knowledge as high as possible. Since no component list was available, a calculation example was set up based on information from earlier QRA and in conjunction with Sweco. In this component-specific frequency, the electrolyzer failure frequency was not included since no information on its exact size, make, and model was available.

 Table 6.11:
 Iteration 4 example case component list

Component	Number of
Compressor	1
Cylinder	1
Flanges	4
Pipes	30
Valves	4
Instruments	3

This component list was then used to calculate the release size-specific frequency with the equation in figure 5.5 and component-specific distribution list (see appendix 10.1) followed by using those frequencies in the fault tree in figure 6.13. When the release size-specific base frequencies had been calculated the equations (see figure 5.5) for end event frequencies were applied but with employed distributions from iterations 2 and 3.



Figure 6.14: Release size specific end event frequency generated from example system with of fault tree which can be used to calculate failure frequency for a release size (Ehrhart et al., 2021)

Figure 6.14 shows an example of how the end event frequency would be calculated for the release size specific end event distributions. These would then be used as input in the software HyRAM produced by Sandia National Laboratories. (Ehrhart et al., 2021)

# 6.5 Distribution Comparison

Figure 6.15 shows how the distribution of frequency for the chosen example end events changes throughout the iterations.

For the instantaneous case, it can be seen that the distribution less and less becomes a lognormal distribution. The original value for explosion (I2) needs a wider uncertainty interval for it to be included.

For the continuous case there is a similar trend between iterations 1 and 2 but for iteration 3 it shows greater variation. This is most likely due to the characteristics of the employed distributions.



Figure 6.15: Figure showing how the distribution for the end event explosion varies from iteration 1 to 3 for instantaneous (Right column) and continuous case (Left Column)

# 7 Risk Metric Comparison

In this chapter a comparison between the iterations was performed. It was done by calculating risk metrics individual risk and societal risk through the software Riskcurves 12 by Gexcon AS (2024) with the situational input data shown in appendix 10.2 and 10.3.

# 7.1 Iteration 1: Replacing base frequency

# 7.1.1 Individual Risk

Some changes in the Individual Risk (IR) were found, as shown in the risk contours generated by the software "Riskcurves". For iteration 1, there was a significant change in the frequency for both the instantaneous and continuous cases. The instantaneous mean frequency was decreased by 58%, while the continuous case was increased by 569%. This led to very similar risk curves and virtually no difference in individual risk for the mean value. In iteration 1, a low-value simulation was not produced because HyRAM recommended only using mean values for leak frequencies, as it was yet to be produced as a guideline which takes full advantage of the distributions.

For iteration 1, the two most significant end events which affected the risk metrics were stated to be fireball for the instantaneous case and jet fire for the continuous case.



Figure 7.1: Risk contours generated from iteration 1 (left and the original assessment (right). Yellow: 1E-7 /year, Green: 1E-8 /year, Blue: 1E-9 /year.
#### 7.1.2 FN-curve

Since there were few LOC scenarios and only hydrogen present, the fN-curve was not as informative as it would have been given more scenarios, but there were significant changes in the frequencies.



**Figure 7.2:** FN-curves produced from iteration 1 (left) and original assessment (right) with software Riskcurves.

From these graphs, a decrease in the expected value E(n) can be seen, namely a decrease of 62%. This was most likely because of a significant decrease in the base frequency for the instantaneous case, since it was the most lethal one with the most severe consequences.

The fN-curves generated with Riskcurves looked this way because of the way the simulation was run. Since only two scenarios (instantaneous and continuous) with hydrogen release were included and the consequences simulated were relatively small, the societal risk was too low for the software to register. But what was important to take from these graphs (see figure 7.2 and table 7.1) was that the frequency at which 1 fatality is expected is decreasing.

Assessment	Expected Value	No. Fatalities
Original	7.39E - 8	1
Iteration 1 (mean)	2.78E - 8	1

Table 7.1: Values from fN-curves generated from simulation with Riskcurves for iteration1 and original case.

#### 7.2 Iteration 2: Employing distributions for direct-, delayed- and no ignition Probabilities

For iteration 2, the replaced base frequency was still used, and the ignition probabilities were also varied. When using the software Riskcurves for calculating the risk metrics, the output generated by the Monte Carlo simulation, which is a probability density function, cannot be used. In this case, the lower amount for direct and delayed ignition was used for the instantaneous and continuous case to generate a "best case" scenario. The "worst case" scenario for iteration 2 is the same as iteration 1 because the top values of the employed distribution are the values used in the calculation of the risk metrics in iteration 1.

For iteration 2 the two most significant end events which affect the risk metrics was stated to be fireball for the instantaneous case and jet fire for the continuous case.

#### 7.2.1 Individual risk

Iteration 1 and Iteration 2 (low) represented the uncertainty interval generated from the Monte Carlo simulation, with Iteration 2 (mean) representing the most likely value from said interval. The individual risk was considerably lessened between iteration 1 and 2, especially between iteration 1 (mean) and iteration 2 (low). The green and blue risk contours stayed the same, but the yellow contour was significantly smaller in both of iteration 2's cases. This was because of the wind direction distribution and the decreased probabilities of certain end events, such as fireball and jet fire.



Figure 7.3: Risk contours generated from iteration 2 with mean- (left) and low input values (right). Yellow: 1E-7 /year, Green: 1E-8 /year, Blue: 1E-9 /year.

#### 7.2.2 FN-curve

Since there were few scenarios, the fN-curve was not as informative as it would have been given more scenarios, but there were significant changes in the numbers. For iteration 2, there were further decreases at what frequency there was expected to have occurred 1 fatality. This was also because certain end events decreased in probability, such as fireball and jet fire.

As previously stated The fN-curves generated with Riskcurves looked this way because of the way the simulation was run. But what was important to take from these graphs (see figure 7.4 and table 7.2) was that the frequency at which 1 fatality is expected is decreasing. For further explanation, see page iteration 1.



Figure 7.4: FN-curves produced from iteration 2 with mean- (left) and low input values (right) with software Riskcurves.

**Table 7.2:** Values from fN-curves generated from simulation with Riskcurves for iterations1, 2 and the original case.

Assessment	Expected Value	No. Fatalities
Original	7.39E - 8	1
Iteration 1	2.78E - 8	1
Iteration $2 \pmod{2}$	2.03E - 8	1
Iteration $2 \ (low)$	1.28E - 8	1

### 7.3 Iteration 3: Employing distributions for end event probabilities

In iteration 3, changes from iterations 1 and 2 were kept, and the third change was implemented. Namely, the base frequency (iteration 1), ignition probabilities (iteration 2), and end event probabilities (iteration 3) were all considered.

For iteration 3, the two most significant end events which affected the risk metrics were stated to be fireball for the instantaneous case and jet fire for the continuous case.

#### 7.3.1 Individual Risk

As can be seen in Figure 9.5 and Figure 9.3, the changes between iterations 2 and 3 were negligible concerning individual risk. This was due to minor changes in the end event frequencies after the changes from iteration 3 were implemented.



Figure 7.5: Risk contours generated from iteration 3 with mean- (left) and low input values (right). Yellow: 1E-7 /year, Green: 1E-8 /year, Blue: 1E-9 /year.

#### 7.3.2 FN-curve (expected number of fatalities)

The difference for the frequency at which one fatality was expected to happen did decrease, but not to the extent it did for iterations 1 and 2. This was also due to the minor changes in the end event frequencies after the implementation of iteration 3.

As previously stated the fN-curves generated with Riskcurves looked this way because of the way the simulation was run. But what was important to take from these graphs (see figure 7.6 and table 7.3) was that the frequency at which 1 fatality is expected is decreasing. For further explanation, see page iteration 1.



Figure 7.6: FN-curves produced from iteration 3 with mean- (left) and low input values (right) with software Riskcurves.

Table 7.3:	Values from	fN-curves	generated	from	simulation	with	Riskcurves	for	iterations
	1, 2, 3 and $c$	original cas	se.						

Assessment	Expected Value	No. Fatalities
Original	7.39E - 8	1
Iteration 1	2.78E - 8	1
Iteration $2 \pmod{2}$	1.95E - 8	1
Iteration $2 \ (low)$	1.25E - 8	1
Iteration 3 (mean)	1.63E - 8	1
Iteration $3 \ (low)$	9.34E - 9	1

## 8 Discussion

Consultants specialised in Risk Management were hired to perform the original QRA were all of the calculated risk were found to be below the set criteria.

In the discussion potential uncertainties, enhancements, results and faults were discussed. First all four iterations were examined followed by the two guidelines mainly used for input data, potential use of this approach and finally the next steps according to the author.

#### 8.1 Iteration 1

In iteration 1, the original base frequency was replaced by the generic component failure distributions from HyRAM. Using these distributions of frequencies certainly increased the strength of knowledge around the selection of the base frequency for the event trees. This was due to the new ones in iteration 1 being specifically developed for hydrogen applications and because they were distributions instead of point estimations, produced through Bayesian statistics (Lachance et al., 2009).

In the paper by Le et al. (2023), the component "cylinder" was translated into the storage cylinders which were used in the calculation. This was the same reasoning which I used when I replaced the original base frequencies.

For the instantaneous case, there was only one varying parameter which was the "Cylinder 100% release size," but in the Continuous case, there were several. This was because the base frequency for the continuous case was a sum of four distributions. It could be seen that the two smaller distributions contributed more to the uncertainties in the output, and there could be made an argument that 0.01% and 0.10% release sizes were negligible and would not lead to a continuous 10-minute release scenario. As previously mentioned in Chapter 6.1.4, the paper Le et al. (2023) only used 1%, 10%, and 100% release sizes for their calculations.

As discussed in Chapter 7.1, there was negligible change in the individual risk contours due to a decrease in the instantaneous and an increase in continuous case, although the frequency in fN-curve decreased substantially.

#### 8.2 Iteration 2

In iteration 2, the replaced base frequency of iteration 1 was kept, but the ignition probabilities were changed. Given that there were conflicting probabilities used by the

purple book and HyRAM, distributions were employed to incorporate them. There was a significant change in the individual risk and the frequency of the fN-curve. This was because for some of the uniforms used, there was significant variation, especially for the delayed ignition in the continuous case (see Table 6.5).

It was the author's belief that because of the two dispositions of the guidelines, the ignition probabilities differed greatly for most of the scenarios. This led to a great variation within the employed uniform distributions, which in itself led to greater uncertainty, but the potential variations were made explicit, and the strength of knowledge was increased.

As previously mentioned, some of the distributions employed in iteration 2 had significant variation, as seen in Figure 6.8, especially in the continuous case. This result warranted further research to improve the distribution in accuracy or decrease the interval at which the probability is based upon.

In iteration 2, some changes in the calculated risk metrics could be seen, which, as previously stated, were a result of the decreased frequency for the end events and that the probability of no ignition was not 0% as it was in iteration 1. Between iteration 1 and iteration 2 (low), there was a significant difference for the yellow risk contours (1E - 7/year), but since the sensitivity analysis showed a great effect on the output from the employed distributions, it had diminished value for the analysis as a whole.

#### 8.3 Iteration 3

In iteration 3, the changes made in iterations 1 and 2 were kept, but the end event probabilities were changed. Given that there were conflicting probabilities used by the purple book and HyRAM, distributions were employed to incorporate them, and when no corresponding value existed, a 25% variation was employed (Fireball, see Table 6.8).

The two guidelines' differing dispositions became even more apparent when examining the end event probabilities since they differed significantly, and because of the different event trees, they had different end events. This led to greater uncertainty when attempting to employ distributions since corresponding values did not exist, see Table 6.8. However, there was a precedent for this; in the paper by Le et al. (2023) a combination of values from the two guidelines has been made.

There were minor changes to both the individual risk and fN-curve, which directly corresponds to the minor changes in end event frequencies. However, since the strength of knowledge has been elevated by the implementation of distributions based on the two guidelines, this benefits the analysis's robustness.

From the frequency generation of iteration 3, it could be deduced that for the instantaneous case, the employed distributions for end events did affect the output but not to a significant degree. The same is true for the continuous case except for the explosion distribution, as can be seen in Figure 6.11. This was due to the relatively wide interval of the distribution compared to other employed distributions for end events and the way it was set up. The probability of flashfire is:

P(Flashfire) = 1 - P(Explosion)

#### 8.4 Iteration 4

When performing a QRA on a component-specific level, the event tree made by HyRAM becomes even more applicable since it includes detection/isolation, which is significantly more plausible when the system examined includes pipes, shut-off valves, detection instruments, etc. Given that detection/isolation has a probability of 90%, it would decrease the "negative" end events greatly.

Since the entire system would be examined and the hydrogen present at the facility would not be located in one storage cylinder during normal operation, potential releases would be significantly smaller. As previously stated, Le et al. (2023) set a precedent when they only used 1%, 10%, and 100% release sizes, which I determined to be a reasonable assumption.

The output from HyRAM's frequency generation differs greatly from the one generated when following the purple book's process. This would alter the consequence modeling because a different software is supposed to be used, and the end events are not the same.

#### 8.5 QRA standard practice

The standard practice suggested by IPS was generally thorough with great emphasis on the steps leading up to the risk evaluation, which was all positive. However, it did not focus on uncertainty management. This might have been due to the increased complexity it usually brings, the receiving party may not have had the expertise to make use of that knowledge, or the approach and input values used from Uijt de Haag et al. (2001) and RIVM (2009) may have been inherently conservative. Inherently conservative input generated conservative output, which led to the risk being overestimated. If the risk were calculated to be below set criteria, there was no need to treat uncertainties. If the risk were calculated above the set criteria, it would mean more expensive risk-mitigating measures, a delayed project and approval process, and potentially halting/slowing the green transition.

#### 8.6 Usage of this approach

Each step of the iterations kept lowering the risks except for iteration 3, but the strength of knowledge throughout the iterations was elevated. This meant that the robustness of the assessment was increased as well. A thorough assessment such as this one may not have been necessary in all cases; for instance, in the early stages and

approval process, it was usually not necessary. However, when a more detailed risk assessment was needed or using the standard approach may have yielded too high risks, this iterative approach could have been the solution. For this thesis, adding iteration 3 did not require much more work compared to iteration 2, and since the strength of knowledge was increased, it was only beneficial. However, the same case may not have been true for another QRA on another facility with different circumstances. It was something which most likely would have been revealed only after it had been produced, and if the need had arisen.

#### 8.7 Risk Insights

Throughout the simulations, fireball and jet fire were stated to be the most significant events in regards to the risk metrics, even though the probabilities of those two events had been altered. This was due to the relatively high distance of consequence for these two end events.

#### 8.8 IPS vs. HyRAM

Both guidelines served as manuals to perform QRA, although IPS did not perform its own calculations. They referred to the purple book and BEVI risk manual for input values, calculation methods, and scenario suggestions, where many of these were old, not based on anything substantial, generic, and adapted for a variety of substances. HyRAM, on the other hand, was recently produced, hydrogen-specific, with a major part of the input values being produced by the same institute that produced HyRAM. This gave weight to why it was appropriate to use when producing a hydrogen QRA.

Although both were reference manuals, there appeared to be slightly different dispositions and could be used for hydrogen QRA. It appeared that the purple book and BEVI risk manual should have been used for facilities with larger amounts and HyRAM for facilities with smaller amounts of substance. It was the suggested event tree from HyRAM and the tabulated mass flow rates which led to this belief. Or it could have been that HyRAM should have been used at a more detailed level on a component-specific level.

#### 8.9 Next steps

The obvious next step is performing the QRA on a more detailed level using HyRAM because of its ability to perform QRA on that level. This would most certainly increase the strength of knowledge and decrease the completeness uncertainty because of the level of detail. As previously mentioned some of the employed distributions have quite a wide interval and efforts into making these more accurate and not as wide would be beneficial, especially when facilities like these are being scaled up and in turn the risk of being scaled up.

## 9 Conclusion

From the results of thesis, it is clear that the strength of knowledge has been increased but there are certain parameters that may not be necessary to employ distributions for since some of the results between iterations are negligible.

But if this approach would be applied to the entire case study, on all of the substances present in the facility there is great potential for increased robustness and accuracy of the QRA. This becomes even more necessary when facilities will be scaled up from pilot plants to commercially viable plants. This could then lead to less expensive risk mitigating measures implemented, faster approval processes, and overall a smoother and faster green transition.

With that said the original QRA and the simulations that the author has done in this thesis show that this particular facility with its circumstances did not benefit from this analysis since the individual risk and societal risk already were assessed to be below the set criteria.

The standard practice for process safety engineering is well underway to be established and uncertainty management is included within it although not as thorough as sometimes may be needed. As SoK is a relatively new perspective IPS have not included it as a "proper" step in the QRA process but they implore the reader of their guideline to keep it in mind and strive to keep the SoK as high as possible. MCS is included in the uncertainty management chapter but it is labeled as a more complex way of performing uncertainty analysis and according to IPS it is usually not necessary. With the methods found it could be seen that the strength of knowledge could be increased and the risks made explicit.

# 10 Appendix

## 10.1 Appendix A

Table 2-2 Parameters for frequency of random leaks for individual components							
Component	Release Size	μ	σ	Mean	5 <sup>th</sup>	Median	95 <sup>th</sup>
	0.01%	-1.73	0.22	$1.8 \times 10^{-1}$	$1.2 \times 10^{-1}$	$1.8 \times 10^{-1}$	$2.6 \times 10^{-1}$
	0.10%	-3.95	0.50	$2.2 \times 10^{-2}$	$8.5 \times 10^{-3}$	$1.9 \times 10^{-2}$	$4.4 \times 10^{-2}$
Compressors	1%	-5.16	0.80	$7.9 \times 10^{-3}$	$1.5 \times 10^{-3}$	$5.8 \times 10^{-3}$	$2.2 \times 10^{-2}$
	10%	-8.84	0.84	$2.1 \times 10^{-4}$	$3.6 \times 10^{-5}$	$1.4 \times 10^{-4}$	$5.7 \times 10^{-4}$
	100%	-11.34	1.37	$3.0 \times 10^{-5}$	$1.3 \times 10^{-6}$	$1.2 \times 10^{-5}$	$1.1 \times 10^{-4}$
	0.01%	-13.92	0.67	$1.1 \times 10^{-6}$	$3.0 \times 10^{-7}$	$9.0 \times 10^{-7}$	$2.7 \times 10^{-6}$
	0.10%	-14.06	0.65	$9.6 \times 10^{-7}$	$2.7 \times 10^{-7}$	$7.8 \times 10^{-7}$	$2.3 \times 10^{-6}$
Cylinders	1%	-14.44	0.65	$6.6 \times 10^{-7}$	$1.8 \times 10^{-7}$	$5.4 \times 10^{-7}$	$1.6 \times 10^{-6}$
	10%	-14.99	0.65	$3.8 \times 10^{-7}$	$1.1 \times 10^{-7}$	$3.1 \times 10^{-7}$	$9.0 \times 10^{-7}$
	100%	-15.62	0.68	$2.1 \times 10^{-7}$	$5.3 \times 10^{-8}$	$1.6 \times 10^{-7}$	$5.0 \times 10^{-7}$
	0.01%	-5.25	1.99	$3.8 \times 10^{-2}$	$2.0 \times 10^{-4}$	$5.3 \times 10^{-3}$	$1.4 \times 10^{-1}$
	0.10%	-5.29	1.52	$1.6 \times 10^{-2}$	$4.2 \times 10^{-4}$	$5.0 \times 10^{-3}$	$6.1 \times 10^{-2}$
Filters	1%	-5.34	1.48	$1.4 \times 10^{-2}$	$4.2 \times 10^{-4}$	$4.8 \times 10^{-3}$	$5.5 \times 10^{-2}$
	10%	-5.38	0.89	$6.9 \times 10^{-3}$	$1.1 \times 10^{-3}$	$4.6 \times 10^{-3}$	$2.0 \times 10^{-2}$
	100%	-5.43	0.95	$6.9 \times 10^{-3}$	$9.1 \times 10^{-4}$	$4.4 \times 10^{-3}$	$2.1 \times 10^{-2}$
	0.01%	-3.92	1.66	$7.9 \times 10^{-2}$	$1.3 \times 10^{-3}$	$2.0 \times 10^{-2}$	$3.0 \times 10^{-1}$
_	0.10%	-6.12	1.25	$4.8 \times 10^{-3}$	$2.8 \times 10^{-4}$	$2.2 \times 10^{-3}$	$1.7 \times 10^{-2}$
Flanges	1%	-8.33	2.20	$2.7 \times 10^{-3}$	$6.4 \times 10^{-6}$	$2.4 \times 10^{-4}$	$9.0 \times 10^{-3}$
	10%	-10.54	0.83	$3.7 \times 10^{-3}$	$6.7 \times 10^{-6}$	$2.6 \times 10^{-3}$	$1.0 \times 10^{-4}$
	100%	-12.75	1.83	$1.5 \times 10^{-3}$	$1.4 \times 10^{-7}$	$2.9 \times 10^{-6}$	$5.9 \times 10^{-3}$
	0.01%	-6.83	0.28	$1.1 \times 10^{-3}$	$6.8 \times 10^{-4}$	$1.1 \times 10^{-3}$	$1.7 \times 10^{-3}$
	0.10%	-8.73	0.61	$1.9 \times 10^{-4}$	$5.9 \times 10^{-3}$	$1.6 \times 10^{-4}$	$4.4 \times 10^{-4}$
Hoses	1%	-8.85	0.59	$1.7 \times 10^{-4}$	$5.4 \times 10^{-3}$	$1.4 \times 10^{-4}$	$3.8 \times 10^{-4}$
	10%	-8.96	0.59	$1.5 \times 10^{-4}$	$4.9 \times 10^{-5}$	$1.3 \times 10^{-4}$	$3.4 \times 10^{-4}$
	100%	-9.91	0.88	$7.3 \times 10^{-3}$	$1.2 \times 10^{-3}$	$5.0 \times 10^{-3}$	$2.1 \times 10^{-4}$
	0.01%	-9.58	0.17	$7.0 \times 10^{-3}$	$5.2 \times 10^{-3}$	$6.9 \times 10^{-3}$	$9.1 \times 10^{-3}$
	0.10%	-12.92	0.81	$3.4 \times 10^{-6}$	6.4 × 10 <sup>-7</sup>	$2.4 \times 10^{-6}$	9.3×10 <sup>-6</sup>
Joints	1%	-11.93	0.51	7.5×10-6	$2.8 \times 10^{-6}$	$6.6 \times 10^{-6}$	$1.5 \times 10^{-3}$
	10%	-12.09	0.58	$6.7 \times 10^{-6}$	$2.2 \times 10^{-6}$	$5.6 \times 10^{-6}$	$1.5 \times 10^{-3}$
	100%	-12.22	0.61	$6.0 \times 10^{-6}$	1.8×10 <sup>-6</sup>	$4.9 \times 10^{-6}$	$1.3 \times 10^{-5}$
	0.01%	-11.91	0.69	8.5 × 10 <sup>-6</sup>	$2.1 \times 10^{-6}$	$6.7 \times 10^{-6}$	$2.1 \times 10^{-3}$
	0.10%	-12.57	0.71	$4.5 \times 10^{-6}$	$1.1 \times 10^{-3}$	$3.5 \times 10^{-5}$	$1.1 \times 10^{-5}$
Pipes	1%	-13.88	1.14	$1.8 \times 10^{-5}$	$1.4 \times 10^{-7}$	9.3×10 <sup>-7</sup>	6.1 × 10 <sup>-6</sup>
	10%	-14.59	1.10	$9.1 \times 10^{-7}$	$0.8 \times 10^{-8}$	4.6 × 10 <sup>-7</sup>	$3.1 \times 10^{-6}$
	100%	-15.75	1.72	6.4 × 10 <sup>-7</sup>	8.8 × 10 <sup>-2</sup>	1.5×10 <sup>-7</sup>	$2.5 \times 10^{-5}$
	0.01%	-5.19	0.18	5.7×10 -4	4.2 × 10 -4	5.6 × 10 -4	7.5 × 10 <sup>-2</sup>
Values	0.10%	-7.51	0.42	7.3 × 10 <sup>-4</sup>	5.4 × 10 <sup>-4</sup>	6.0 × 10-5	$1.3 \times 10^{-3}$
valves	170	-9.71	0.98	9.8 × 10 <sup>-5</sup>	1.2 × 10 <sup>-5</sup>	$0.0 \times 10^{-5}$	5.0 × 10 <sup>-4</sup>
	10%	-10.34	0.69	4.1 × 10 <sup>-5</sup>	$1.0 \times 10^{-7}$	5.2×10 -6	1.0 × 10 <sup>-5</sup>
	100%	-12.00	0.71	1.5 × 10 <sup>-4</sup>	6.9 × 10 <sup>-4</sup>	6.1 × 10 °	5.5 × 10 <sup>-2</sup>
Instruments	0.01%	-1.38	0.71	0.0 × 10 <sup>-4</sup>	1.9 × 10 <sup>-4</sup>	0.2 × 10 <sup>-4</sup>	2.0 × 10 <sup>-3</sup>
	0.10%	-6.34	0.82	$2.7 \times 10^{-4}$	$3.1 \times 10^{-5}$	$2.0 \times 10^{-4}$	7.5 × 10 <sup>-1</sup>
	170	-9.10	1.00	$1.7 \times 10^{-4}$	$2.4 \times 10^{-5}$	$1.1 \times 10^{-4}$	$5.1 \times 10^{-4}$
	100%	-9.21	1.40	$1.8 \times 10^{-4}$	$1.7 \times 10^{-6}$	$3.7 \times 10^{-5}$	$4.3 \times 10^{-4}$
	100%	-10.21	1.49	1.1 × 10	3.2 × 10 °	5.7 × 10 °	4.5 × 10

Figure 10.1: (Ehrhart et al., 2021)

## 10.2 Appendix B

Table 10	.1: Mon	te Carlo	Simulatio	on settings
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Setting	
Number of simulations	1
Iterations	1000
Sampling type	Monte Carlo

### 10.3 Appendix C

Process Conditions	
Chemical name	HYDROGEN ~
Initial temperature in vessel	80 °C
Initial (absolute) pressure in vessel	90 bar
Calculation Method	
Outcome / phenomena	Gas or BLEVE Fireball Gas or BLEVE Blast Flash fire (with VCE) Toxic cloud Combined (auto detect)
Expansion type	Adiabatic ~
Use GAME overpressure method	No ~
Fraction cloud involved in explosion	0,08 -
Curve number	10 (Detonation) $\sim$
Process Dimensions	
Vessel volume	308,18 m3
Height of the vessel (fireball offset Z)	1m
Environment	
Roughness length description	Regular large obstacle coverage (suburt $\scriptstyle \!$
Reporting/receiver distance (Xd)	n m
Ignition time flammable cloud	User defined V
Time t after start release	U s
Use 50% LFL for cloud contour	No
Use mass between LFL and UFL	No ~
Use defined dose contour	No ~

Figure 10.2: Simulation settings in Riskcurves for instantaneous case (Gexcon AS, 2024)

### 10.4 Appendix D

#### **Process Conditions**

Chemical name	HYDROGEN	v ~
Initial temperature in vessel	80	]°C
Initial (absolute) pressure in vessel	90	bar
Calculation Method		
Outcome / phenomena	<ul> <li>Jet fire</li> <li>Flash fin</li> <li>Toxic cl</li> <li>Combin</li> </ul>	re (with VCE) oud ned (auto detect)
Use which representative rate	First 20% a	verage (flammable) $\vee$
Type of vessel outflow	Vessel emp	oty in specified time 🗸 🗸
Vessel emptying duration	600	s
Expansion type	Adiabatic	~
Use GAME overpressure method	No ~	]
Fraction cloud involved in explosion	0,08	]-
Curve number	10 (Detona	tion) 🗸
Process Dimensions		
Vessel volume	308,18	] m3
Hole rounding	Rounded e	dges 🗸
Discharge coefficient	1	] -
Outflow angle in XZ plane	0	deg
(0°=nonzoniai; 90°=vertical) Height of release (7-coordinate)	1	lm
Environment	-	]
Environment		
Roughness length description	Regular lar	ge obstacle coverage (suburt 🗸
Reporting		
Reporting/receiver distance (Xd)	100	] m
Ignition time flammable cloud	User define	ed 🗸
Time t after start release	0	s
Use 50% LFL for cloud contour	No ~	]
Use mass between LFL and UFL	No ~	
Use defined dose contour	No ~	

Figure 10.3: Simulation settings in Riskcurves for continuous case (Gexcon AS, 2024)

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