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Abstract

Leaks of flammable gases from containing systems pose safety concerns in many industrial settings. In this research, state-of-the-art visual flowcharting methodology is employed to develop a probabilistic model to quantify occupational risks of fire and explosion events initiated by leaks that ignite within enclosed spaces. In this model, leak initiation time and leak type (small, medium, or large) are selected based on user-specified probability distribution function and leak probability ranges, respectively. Other inputs to the model include probability distribution of time to failure of mechanical ventilation in the enclosed space, likelihood of presence of an ignition source with energy \geq minimum ignition energy (MIE) of formed flammable gas cloud, probability of leak detection prior to ignition, and conditional probabilities of fires and explosions, given ignition. The model checks whether randomly-selected times of leak initiation and ventilation failure are within user-specified mission time. Number of personnel present near leak source is determined by a user-selected probability distribution. Uncertainties of input probabilities are propagated through the model using Monte Carlo sampling technique. Given occurrence of an undetected gaseous leak in conjunction with presence of an ignition source, ventilation failure, and presence of personnel close to the hazard source, the model calculates frequencies of risks of fire or explosion injuries, averaged over 106 Monte Carlo trials per simulation run. Functionality of proposed model is demonstrated by a hydrogen refueling station (HRS) case study in which gaseous hydrogen is postulated to leak from its compressor system. Base case and worst case scenarios as well as sensitivity cases are considered and their simulation results show that, for these postulated scenarios, compressor's small H₂ leaks (unlike medium and large leaks) pose intolerable occupational risk frequencies that exceed the acceptable risk level of 1.0E-4/year as well as NFPA's selected risk guideline of 2.0E-5/year which is driven by the comparative risk to gasoline stations. To mitigate predicted occupational risks to acceptable levels, safety control measures and best practices are recommended. The proposed model can be used as a training tool for first responders to fire and explosion events initiated by leaks of flammable gases. The model allows user-specified 'what-if' scenarios with or without risk mitigation measures. In addition to HRS, the model can be applied to a broad range of industrial applications such as natural gas refueling stations, indoor chiller systems which employ flammable refrigerants, and warehouses equipped with hydrogen-powered forklifts. Risk insights from this model's simulations can also support safety codes & standards and root cause investigations of industrial fire and explosion events.

Keywords	consequence analysis, refueling stations, first responders, flammable gases, gaseous leaks
Taxonomy	Risk Assessment, Process Safety
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August 27, 2017

Re: A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases

Dear Professor Amyotte, Editor

It is my pleasure to submit my manuscript entitled '*A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases*' for potential publication in the Journal of Loss Prevention in the Process Industries.

Best Regards,

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A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases

Highlights

- Developed a novel and robust probabilistic occupational risk quantification model using virtual-flowcharting method.
- Quantified probabilistic consequences of ignition scenarios of leaked flammable gases into confined spaces.
- Identified gaseous leak type leading to human safety consequences in excess of the acceptable occupational risk level.
- Recommended risk control measures and best practices to reduce predicted occupational risks to acceptable levels.
- Proposed a computational framework to quantify economic costs of first-party's fire and explosion injuries.

A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases

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Abstract

Leaks of flammable gases from containing systems pose safety concerns in many industrial settings. In this research, state-of-the-art visual flowcharting methodology is employed to develop a probabilistic model to quantify occupational risks of fire and explosion events initiated by leaks that ignite within enclosed spaces. In this model, leak initiation time and leak type (small, medium, or large) are selected based on user-specified probability distribution function and leak probability ranges, respectively. Other inputs to the model include probability distribution of time to failure of mechanical ventilation in the enclosed space, likelihood of presence of an ignition source with energy \geq minimum ignition energy (MIE) of formed flammable gas cloud, probability of leak detection prior to ignition, and conditional probabilities of fires and explosions, given ignition. The model checks whether randomly-selected times of leak initiation and ventilation failure are within user-specified mission time. Number of personnel present near leak source is determined by a user-selected probability distribution. Uncertainties of input probabilities are propagated through the model using Monte Carlo sampling technique. Given occurrence of an undetected gaseous leak in conjunction with presence of an ignition source, ventilation failure, and presence of personnel close to the hazard source, the model calculates frequencies of risks of fire or explosion injuries, averaged over 10^6 Monte Carlo trials per simulation run. Functionality of proposed model is demonstrated by a hydrogen refueling station (HRS) case study in which gaseous hydrogen is postulated to leak from its compressor system. Base case and worst case scenarios as well as sensitivity cases are considered and their simulation results show that, for these postulated scenarios, compressor's small H₂ leaks (unlike medium and large leaks) pose intolerable occupational risk frequencies that exceed the acceptable risk level of $1.0\text{E-}4/\text{year}$ as well as NFPA's selected risk guideline of $2.0\text{E-}5/\text{year}$ which is driven by the comparative risk to gasoline stations. To mitigate predicted occupational risks to acceptable levels, safety control measures and best practices are recommended. The proposed model can be used as a training tool for first responders to fire and explosion events initiated by leaks of flammable gases. The model allows user-specified 'what-if' scenarios with or without risk mitigation measures. In addition to HRS, the model can be applied to a broad range of industrial applications such as natural gas refueling stations, indoor chiller systems which employ flammable refrigerants, and warehouses equipped with hydrogen-powered forklifts. Risk insights from this model's simulations can also support safety codes & standards and root cause investigations of industrial fire and explosion events.

Key words: *consequence analysis, refueling stations, first responders, flammable gases, gaseous leaks*

^{*} The author of this article is the current Operating Agent (OA) of the Hydrogen Safety Task of the International Energy Agency (IEA), was the Principal Investigator of DOE Contract on hydrogen safety for on-board vehicular applications (Contract Award # DE-FG36-07GO17032), a member of NFPA-2 (Hydrogen Technologies Executive Committee, and the Engineering Manager of the Probabilistic Risk Assessment (PRA) Department at the Millstone nuclear power station in Waterford, Connecticut, USA.

1. Introduction

Concerns about global warming and climate change have spurred global impetus for use of compressed natural gas (CNG) and compressed hydrogen gas (CHG) to curb greenhouse emissions (GHG) from the petrol-based transport sector. As a result, many CNG refueling stations and CHG refueling stations (HRS) were built worldwide and many others are scheduled to be built in the near future. For example as of 12/08/2016, the U.S. has 1,729 private and public CNG stations, of which 769 are private stations (Sakamoto et al., 2016). Out of the 769 private CNG stations, there are 146 stations in California and 75 stations in New York. Out of the 960 public CNG stations, there are 176 stations in California and 101 stations in Oklahoma. Also, the U.S. has 56 public and private HRS, of which 25 stations are private. California alone has 9 HRS out of the 25 private stations and 28 stations out of the 31 public HRS. As a global-scale example, the Japan Ministry of Economy, Trade, and Industry announced its plan to construct 160 HRS by 2020 and 320 HRS by 2025 (Sakamoto et al., 2016). In a similar fashion, there is a worldwide interest among manufacturers of indoor chiller systems to replace conventional refrigerants that have high global warming potential (GWP) and ozone depletion potential (ODP) with environmentally-friendly refrigerants. Unfortunately, however, those environmentally-friendly refrigerants including propane, R1234yf and R1234ze(e) are flammable and, thus, pose safety hazards under certain conditions. The aforementioned applications are just a few examples of a broader scope of industrial settings where accidental leaks of flammable gases into enclosures present human safety risks.

Gaseous leaks have happened in the past and will continue to happen for a variety of reasons including random equipment failures, structural degradation (*e.g.*, stress corrosion cracking, gas-material incompatibility, etc.) and human-induced failures during equipment handling, installation, or maintenance activities. For example, according to the Japanese High Pressure Gas Safety Act (HPGS) database (Sakamoto et al., 2016), 21 HRS incidents were reported during the period 2005 to 2014. Of the 21 incidents, 14 were related to small H₂ leaks from flanges, valves, and seals (including deteriorated nonmetallic seals). The root causes of those leakage incidents were dominated by vibrational fatigue of piping's screw joints and the fatigue of filling hoses. Also, according to the U.S. Hydrogen Incident Reporting database (HIRD), 22 HRS incidents were reported over the period 2004 to 2012.¹ The dominant root causes of those leakage incidents in the U.S. HRS were fatigue of filling hoses and pipe welds, use of nonconforming material for components such as pressure relief valves, and poor maintenance of filling hoses, etc. The AC transit HRS in Emeryville, California was a good example of material incompatibility as the root cause of H₂ leakage incident (Harris and San Marchi, 2012).

1.1 Research objectives, impact, and novelty

1.1.1 Objectives

This research has the following objectives:

- i) Employ probabilistic methods together with state-of-the-art visual flowcharting methodology to develop a simulation model for quantifying frequencies of risks associated with postulated accident scenarios where leaked flammable gases within enclosures could ignite under specific conditions.
- ii) Demonstrate functionality of the proposed model by a case study involving a postulated hydrogen leak scenario inside the compressor's room in a HRS. Using the HRS case study: a) quantify occupational risks to station's personnel (*i.e.*, first-party risks) in close proximity to the hazard

¹ Source: www.h2incidents.org

source and b) draw useful safety insights by comparing calculated occupational risks to first-party's risk acceptance criterion currently set at $1.0\text{E-}4/\text{year}$ (*i.e.*, one chance per 10,000 years).

- iii) Using the HRS case study, perform scenario analysis and sensitivity cases. Accident scenarios' simulations should employ Monte Carlo (MC) sampling technique for uncertainty propagation through the proposed model.
- iv) Establish a computational framework for calculating economic costs associated with the calculated occupational risks.

Risks that are not currently accounted for in the present model are: a) Property damage caused by resulting fire or explosion and b) Human toxicity caused by emission of toxic gases during combustion of leaked flammable gases of certain types (Kataoka, 2013; JSRAE, 2015).

1.1.2 Impact and novelty

As discussed in Subsections 1.2 and 1.3, the open literature contains copious deterministic predictions and experimental studies that examine phenomenological aspects of fire propagation and explosion (deflagration, detonation, and deflagration-to-detonation transition) of flammable gases within enclosures. Much less work has been done on the probabilistic consequences of those events, and in particular post-ignition human-safety consequences. This observation can be substantiated by the argument made in ASHRAE² risk studies of flammable refrigerants that current risk-related studies have only quantified frequencies of leak scenarios leading to ignition and that post-ignition probabilistic consequence assessment is currently lacking. Accordingly, this research presents a novel quantitative framework to fill the aforementioned gap in current state of knowledge by offering a user-friendly, probabilistically-driven tool for quantifying post-ignition consequences related to human injuries or fatalities. Another source of novelty in this research is related to use of visual flowcharting methodology (discussed in Subsection 2.4) to construct the simulation model without having to write complex computer algorithms. To our best knowledge, this is the first study that applies visual flowcharting methodology to quantify post-ignition human safety consequences. In this regard, Khalil (2016) was also the first to apply visual flowcharting methodology to construct a probabilistically-timed simulation model to quantify likelihood of mission success of adversary attacks that focus on exploiting specific vulnerabilities in safety systems contained within critical infrastructures.

1.2 Use of flammable gases in refueling stations

The discourse presented here focuses primarily on CHG in HRS as an example of industrial settings that use flammable gases. The deliberate choice of this infrastructure sets the stage for the postulated HRS case study (described in Subsection 2.4). However, the proposed model can be applied to quantify human safety consequences of fire and explosion events in a broader range of industrial settings including CNG refueling stations.

As noted in Subsection 1.1.2, the published literature on H₂-related risks shows more research activities on deterministic calculations of consequences of fires (flash and jet fires) and vapor cloud explosions (VCE) compared to probabilistic quantification of pre- and post-ignition events. Moreover, published studies on the deterministic consequence are based on predictions made by

² American Society of Heating, Refrigerating, and Air-Conditioning Engineers.

computational fluid dynamics (CFD) and other models such as the Process Hazard Analysis Software Tool (PHA³ST)³ and Flame Acceleration Simulator (FLACS).⁴ To name but a few examples of recently published deterministic studies, Cleaver and Cumber (2001) outlined an approach for assessing explosion hazards associated with small NG leaks into enclosures and calculated the resulting overpressurization. Houf and Schefer (2007) used CFD to calculate key parameters like the radiative heat flux (kW/m^2) and pressure rise for flammable gas fire and explosion events, given selected leak types (small, medium, or large), systems' pressures, and confinement free volume. Soman and Sundararaj (2012) performed deterministic calculations of consequences of VCE caused by catastrophically-failed H_2 storage tank in a hydrochloric acid (HCl) manufacturing plant. They used the equivalent TNT mass model, TNO multi energy model⁵, and the Baker-Strehlow model to estimate explosion's overpressurization and employed probit equations to estimate associated fatalities. Most recently, Mousavi and Parvini (2016) modeled H_2 dispersion and consequences of jet-fire and flash-fire events and validated their model using the data from a H_2 pipeline rupture study performed by Ganci et al. (2011).

With respect to quantitative and qualitative risk (QRA and QLRA) studies, Marangon and Carcassi (2006) performed a QRA case study on a 35 MPa gaseous HRS in Italy and Kikukawa et al. (2008; 2009) carried out QRA studies on 70 MPa gaseous HRS and liquid hydrogen HRS in Japan. In their later study, they used the conventional risk matrix approach to qualitatively assess the risks using a 2-factor risk matrix (probability of occurrence and severity of consequences). LaChance (2008; 2009) provided data on fire and explosion injuries as follows: Fire injuries may include, depending on the heat flux level (kW/m^2) and exposure time (i.e., harm criteria), second-degree burns resulting from exposure to $\approx 9.5 \text{ kW/m}^2$ heat radiation for 20 seconds and third-degree burns resulting from exposure to $\approx 25 \text{ kW/m}^2$ heat radiation for 10 seconds. Human fatality could result from exposure to 25 kW/m^2 heat radiation for 1 minute, exposure to 35 to 37.5 kW/m^2 heat radiation for 10 seconds, etc. Explosion injuries include eardrum rupture caused by ≈ 5 psig peak overpressure, head injury resulting from ≈ 10 psig peak overpressure, lung damage resulting from ≈ 10 psig peak overpressure, etc. The human fatality category typically results from explosion events with peak pressures of ≥ 12 psig. Zhiyong, et al. (2010) described compressor's leak as the main contributor to H_2 leak events in HRS. They employed the 350-bar Shanghai Anting HRS as a case study, assumed 365 days/year operation for this station, and used hazard and operability (HAZOP) analysis to define the accident scenarios. Mirza et al. (2011) performed qualitative risk study for information reported in the Hydrogen Incident Reporting Database (HIRD) on 32 industrial H_2 processing incidents and highlighted causes and lessons learned from those incidents. The study highlighted the types of accident initiating events that occurred such as H_2 storage vessel failure, leaks from gaskets and flanges, premature rupture of burst discs, failure of pressure relief devices (PRD), pipe failure, and H_2 compressor failure. Haugom and Friis-Hansen (2011) employed Bayesian Networks (BN) to model the risks associated with a virtual HRS with an onsite H_2 production. They applied BN to a case study that focused on leaks from H_2 gas dispenser and assumed heavy traffic at the virtual HRS. Ham et al. (2011) described a two-phase risk assessment benchmarking exercise using a virtual HRS. The exercise was conducted in collaboration with nine partners from seven countries. The authors noted that leak inside the compressor building represents a high risk scenario that would fall into the RED region of a typical risk matrix. Papanikolaou et al. (2011) used the GAJET integral code, ADREA-HF CFD code, and EFFECTS code to predict the time-dependent flammable H_2 mass and volume profiles, overpressure, heat radiation flux, and maximum horizontal and vertical distances of

³ <https://www.dnvgl.com/Search?q=PHAST>

⁴ <http://www.gexcon.com/flacs-software>

⁵ TNO = the Netherlands Organization for Applied Scientific Research.

the LFL from the leak source for a hypothetical gaseous HRS which they named BBC as the base Case scenario. The authors applied qualitative judgment to describe the consequence severity. The hazard scenarios were determined using the HAZard Identification (HAZID) methodology. Khalil (2011; 2015) developed and quantified a fault tree (FT) model for gaseous H₂ leakage (via permeation) through Type-III and Type-IV liners in on-board vehicular H₂ storage systems. Galassi et al. (2012) described the main features of the Hydrogen Incidents and Accidents Database (HIAD) modules, namely, the Data Entry Module (DEM), the Data Retrieval Module (DRM), and the Data Analysis Module (DAM). The HIAD structure divides the consequences of hydrogen-related incidents into five types: fatalities, injuries, environmental damage, property damage, and economical loss. According to the HIAD's reported events, 38 H₂-related events occurred in the EU between 1985 and 2006, of which 18 were explosion events and 9 were fire events. The associated onsite personnel injuries/ fatalities were 129 due to H₂ explosions and 17 caused by H₂ fires. Sun et al. (2014) used process hazard analysis (PHA) to calculate risks associated with mobile HRS and noted that compressor's leak represents the dominant risk due to its highest failure rates and the 'worst' harm from the consequence standpoint. Their study was tailored for two mobile HRS required for refueling sight-seeing cars during the World Expo in China. Accidents selected for analysis were derived from a HAZOP study and frequencies of failure are taken from the Purple Book (2005). The authors estimated the risk associated with only H₂ fires and employed three stages to calculate consequences of the postulated accident sequences. Using 1.0E-4/year as risk acceptance criterion for occupational risk, they concluded that mobile HRS are safe for both Station's personnel and fuel-cell vehicles' users during refueling time. For risk to the general public (*i.e.*, third-party), they used 1.0x10⁻⁶/year as the threshold for risk acceptance. Al-shanini et al. (2014) used a risk assessment approach driven by progressive failures of specific prevention barriers using fault tree and event tree models and used hypothetical data as space holders until actual data become available. They applied their approach, which is based on the SHIPP⁶ methodology (Rathnayaka et al., 2011a; 2011b) to a liquid HRS where H₂ is not produced onsite but transported to the station via trucks. Event consequences were classified as: safe, near-miss, mishap, incident, accident, and serious accident.

Most recently, Sakamoto et al. (2016) qualitatively analyzed HRS incidents in Japan (between 2005 and 2014) and in the U.S. (between 2004 and 2012) and expressed their concerns about potential for fire and explosion risks due to H₂ leaks in HRS. Pipe failure caused by embrittlement of incompatible structural materials as well as leaks from flanges, joints, and valves were among the root causes for those incidents. Sakamoto et al. (2016) noted that one of the key differences between the Japanese and U.S. HRS is the pipe joint approach, where most of the Japanese HRS use screw joints and use of welded joints dominates the U.S. HRS. The European Integrated Hydrogen Project (Phase 2)⁷ performed QLRA for gaseous HRS with on-site H₂ production. The project researchers employed the so-called Rapid Risk Ranking (RRR) approach (Norsk Hydro ASA and DNC, 2003) in their study and classified the risk as unacceptably high, medium or acceptably low depending on the probability vs. consequence combination. Pique et al. (2016) performed a comparative study of codes, standards, and regulations as well as best practices of HRS for light-duty vehicles in 9 countries (U.S., UK, Germany, Canada, Sweden, Norway, Denmark, and Spain). A survey questionnaire was employed to collect respondents' inputs. The authors noted that safety distances between HRS equipment and potential internal and external targets were driven by risk acceptance criteria and their definition remains as work-in-progress in both U.S. and Europe.

⁶ SHIPP = System hazard identification prevention and prediction.

⁷ Source: www.eihp.org

1.3 Use of flammable refrigerants in HVAC&R applications

Research trends in recent heating, ventilation, air conditioning and refrigeration (HVAC&R) studies show an accelerated shift from use of hydrofluorocarbons (HFCs) to low GWP and ODP refrigerants such as hydrofluoroolefins (HFOs) and blends of HFOs with HFCs. Unfortunately, environmentally-friendly refrigerants like R-290 (propane) are flammable and have been assigned an ASHRAE⁸ safety classification A3. Some of the environmentally-friendly refrigerants, however, are mildly flammable such as R1234ze(e) and R1234yf and have been assigned an ASHRAE safety classification A2L.⁹ As noted earlier, all risk assessment studies published by the Air Conditioning, Heating, and Refrigeration Institute (AHRI)¹⁰ for residential heat pumps, chillers, and commercial refrigeration units discussed in AHRI Projects 8004 (Lewandowski, 2012) and 8009 (Lewandowski, 2015) focus only on quantifying potential accident sequences leading to ignition of leaked refrigerants. None of the published AHRI reports, however, attempted to quantify post-ignition human safety consequences. In this regard, ASHRAE Standard 34 flammability subcommittee is currently seeking to evaluate the flammability of those environmentally-friendly refrigerants. Accordingly and in lights of the human safety concerns associated with use of flammable refrigerants like propane and others, our proposed probabilistic model is positioned to provide the needed methodology to address the aforementioned knowledge gap. Specifically, this simulation tool is designed to probabilistically predict post-ignition frequencies of fire-related injuries (such as burns of various degrees) and explosion-related injuries (caused by the resulting shock waves and overpressurization in confined spaces).

The rest of this manuscript is organized as follows: Section 2 discusses the proposed probabilistic visual-flowcharting-based model, assumptions made, and a postulated HRS case study to demonstrate the functionality of the proposed model. Section 3 discusses the results of applying the model to the postulated case study and Section 4 covers research conclusions, recommendations, and future work.

2. Probabilistic visual-flowcharting-based model

The structure and assumptions of the proposed model are described in Subsections 2.1 and 2.2, respectively. Subsection 2.3 introduces the visual-flowcharting methodology that has been employed to construct the proposed model. Demonstration of functionality of the proposed probabilistic model is discussed in Subsection 2.4 using a case study involving a postulated H₂ leak scenario within the compressor's room in a HRS.

2.1 Model's structure

The logical structure of the proposed model is provided in Figs. 1a through 3. The model is constructed using the visual flowcharting methodology which is part of the RENO software platform (see Subsection 2.3 for additional discussion on this methodology). The structure of this model is designed to simulate progression of postulated accident scenarios initiated by a flammable gas leak and have end states representing the calculated frequencies of fire and explosion injuries. The probability of occurrence of each event along accident progression path is conditional on the occurrence of its precursor events.

⁸ American Society of Heating, Refrigerating and Air-Conditioning Engineers.

⁹ 1806-TRP, Flammable Refrigerants Post-Ignition Simulation and Risk Assessment Update Retrieved from: <https://www.ashrae.org/File%20Library/docLib/Research/2016FallBids/1806-RFP.pdf>

¹⁰ AHRI = Air Conditioning, Heating, and Refrigeration Institute

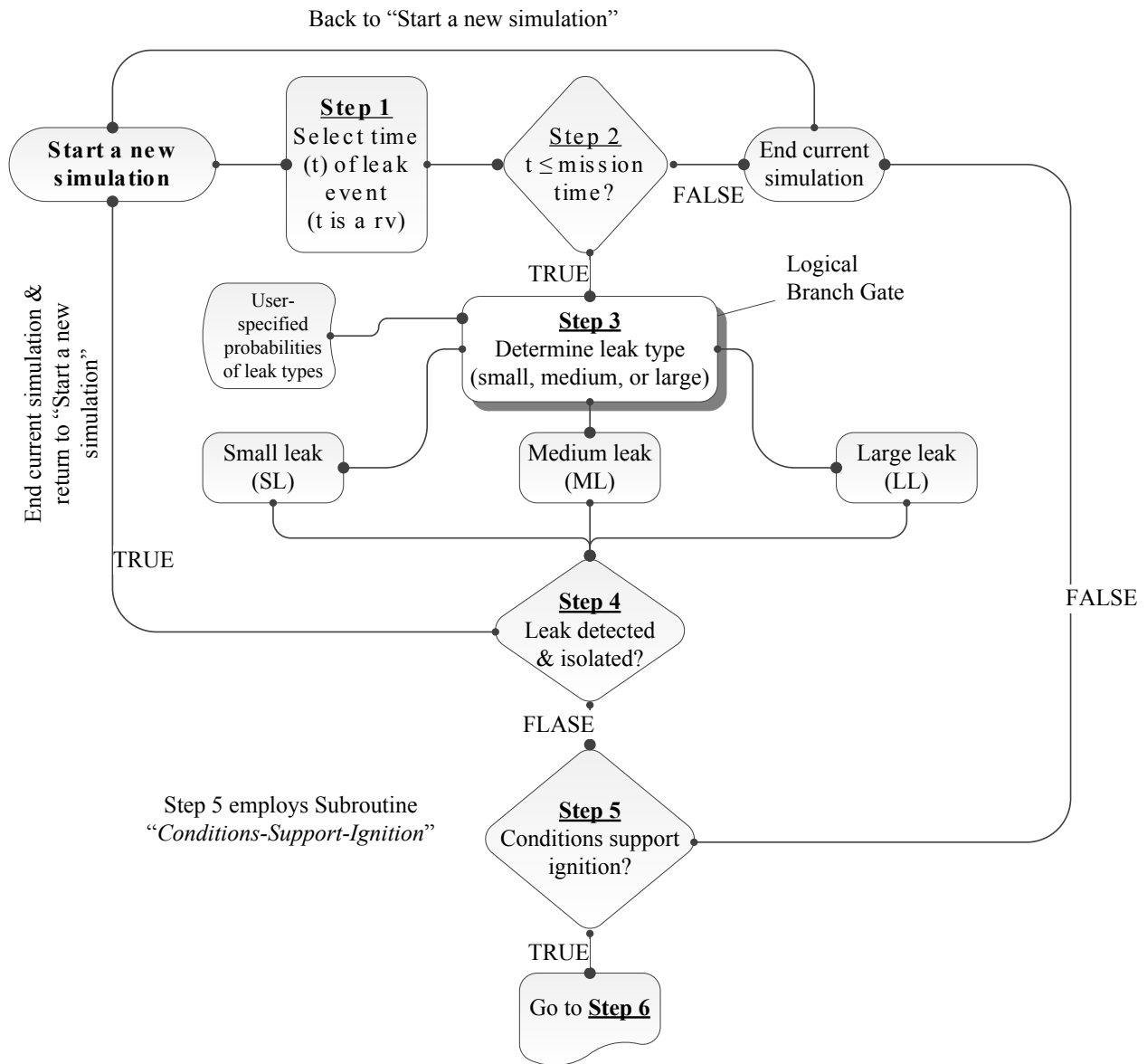


Fig. 1a. A probabilistic visual-flowcharting-based model for safety consequence assessment of fire and explosion events involving leaks of flammable gases within enclosures: *MainChart*.

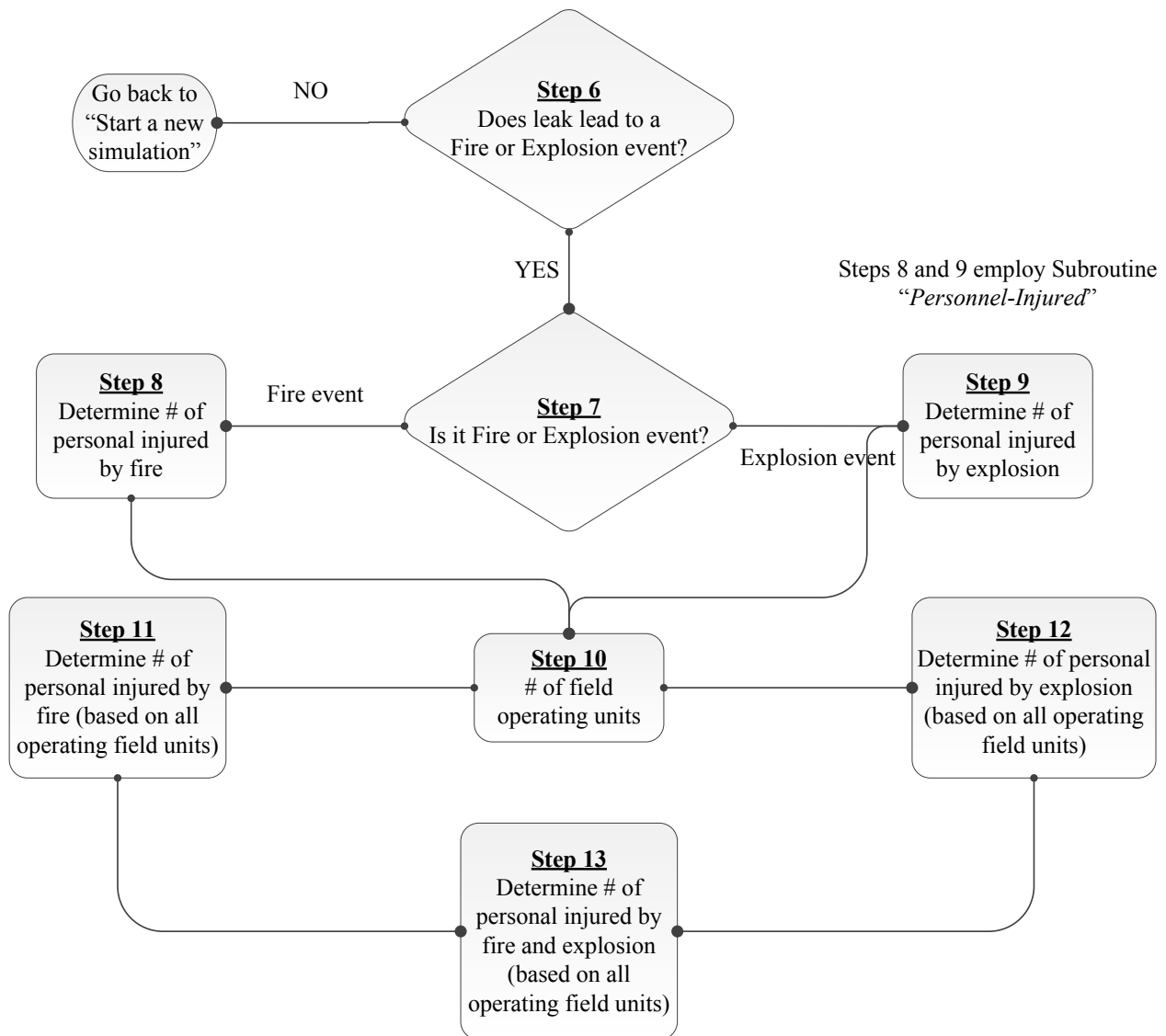


Fig. 1b. A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases within enclosures: *MainChart* (cont'd).

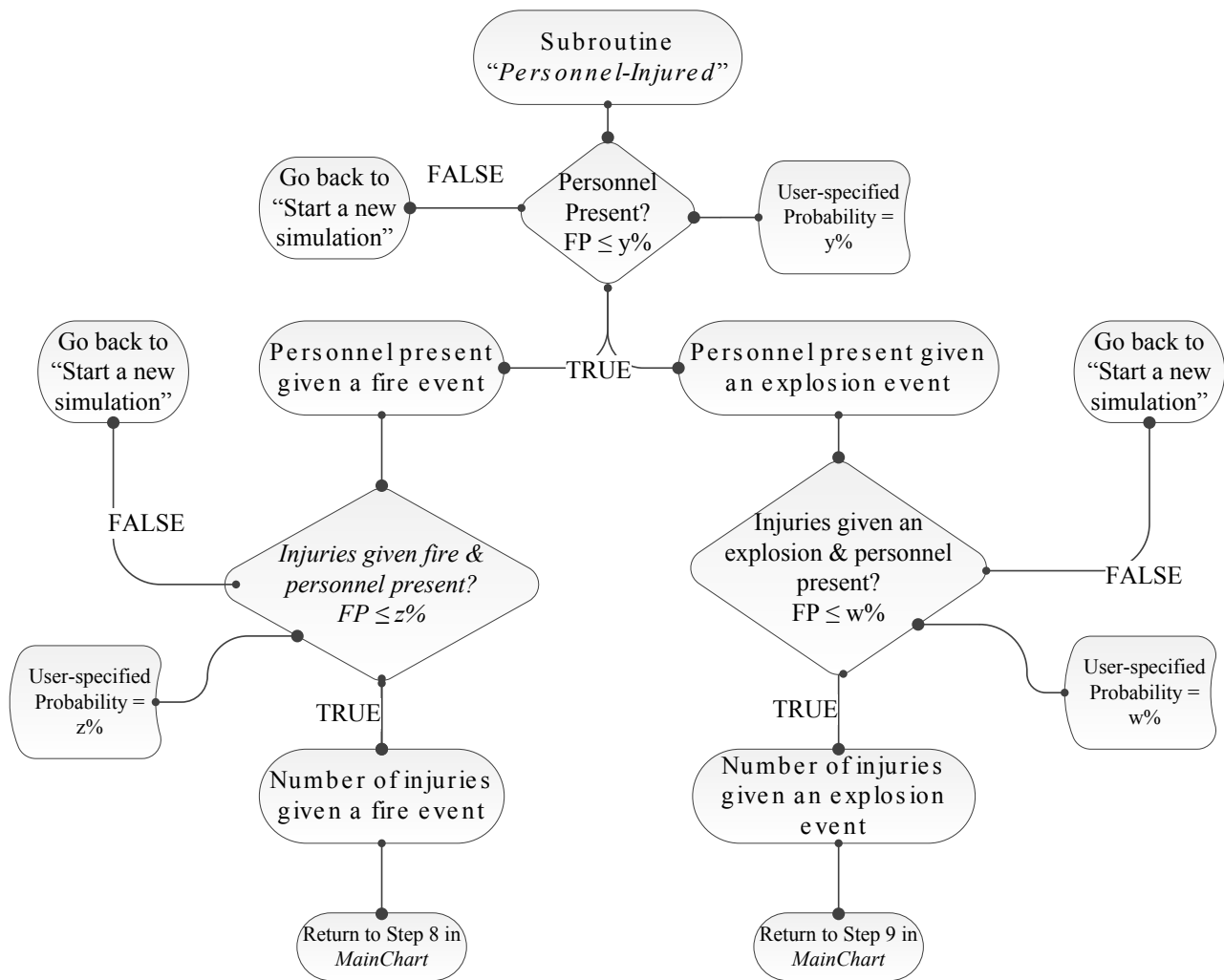


Fig. 2. A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases with enclosures: Subroutine "Personnel-Injured."

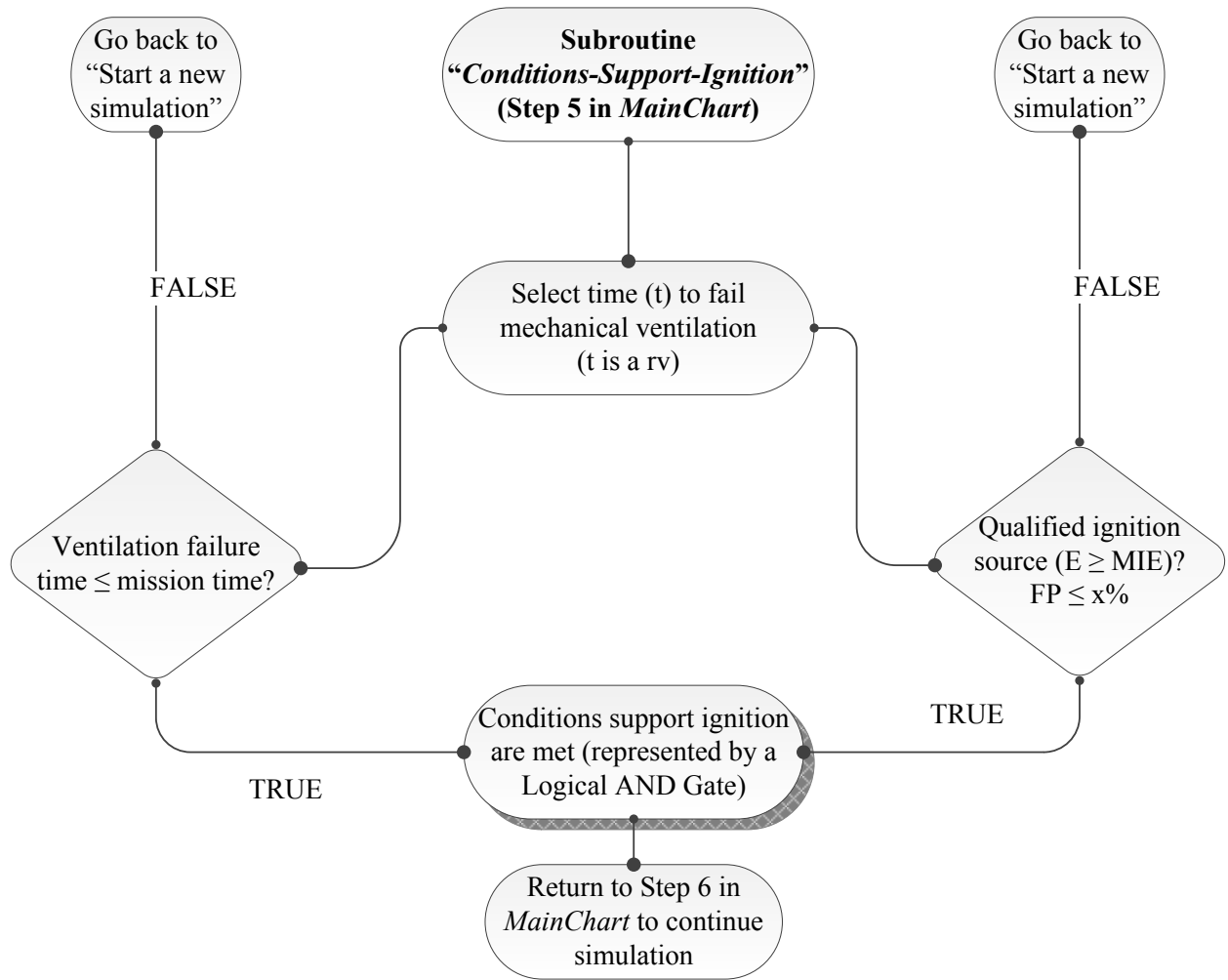


Fig. 3. A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases: Subroutine ‘Conditions-Support-Ignition.’

As shown in Figs. 1a through 3, the proposed probabilistic model contains 13 steps organized in a logical order as follows:

Steps shown in MainChart (Figs. 1a and 1b):

- Step 1: In this step, a random time (t) for occurrence of flammable gas leak is selected using an embedded user-specified probability distribution function (in our HRS case study, a 2-parameter Weibull model with $\beta = 2$, $\eta = 24,000$ hours has been assumed).
- Step 2: A conditional logic is contained in this step to check whether the flammable gas leak time occurs within a user-specified mission time (assumed to be 1 year in HRS case study). If the condition is met (*i.e.*, TRUE), the simulation progresses to Step 3. If the condition is not met (*i.e.*, FALSE), current simulation ends and a new simulation starts.

Step 3: This Step is represented by a logical Branch Gate to probabilistically determine the leak type (SL, ML, or LL), given occurrence of leak. The output of Step 3 represents one-out-of-three (1-o-3) mutually exclusive leak scenarios; namely, a small leak (SL), medium leak (ML), or large leak (LL) scenario.

Step 4: A user-specified detection probability is embedded in this step which checks whether the leak is detected and isolated. If the answer is TRUE, current simulation ends and a new simulation run starts. If the answer is FALSE, the simulation logic progresses to Step 5.

Step 5: In this Step, the *MainChart* simulation logic transfers to “*Conditions-Support-Ignition*” Subroutine (Fig. 3) which checks whether the conditions within the confined space are sufficient to support ignition. If the answer is TRUE, the simulation logic returns to Step 6. If the answer is FALSE, current simulation ends and a new simulation run starts.

Step 6: This step (shown in Fig. 1b) checks, using an embedded function $FP \leq \%$, the likelihood that the formed flammable gas cloud within the confined space could ignite leading to a fire or an explosion event. If the answer is FALSE, then ignition does not occur and current simulation ends and a new simulation start. If the answer is TRUE, then ignition leading to a fire or explosion could happen with a user-specified probability and the simulation logic progresses to Step 7. The detail on how $FP \leq \%$ function operates is provided in Table 2.

Step 7: This Step uses an embedded function $FP \leq \%$ to determine, based on a user-specified probability of fire, whether the occurring ignition event is a fire or an explosion event. If the event is determined to be a fire event, the output of this step is TRUE (*i.e.*, a fire event) and the logic progresses to Step 8. If it is an explosion event, the output of this step is FALSE (*i.e.*, an explosion event) and the logic progresses to Step 9.

Step8: This Step probabilistically determines the number of personnel injured by fire using Subroutine *PersonnelInjured* (shown in Fig. 2). Note that Subroutine *Personnel-Injured* determines the number of injured personnel, given personnel presence near the hazard source.

Step 9: This Step determines (using logic similar to Step 8) the number of personnel injured by an explosion using Subroutine *PersonnelInjured*.

Steps 10 through 13: In Step 10, the number of personnel injured by fire and number of personnel injured by explosion are multiplied by a user-defined number of field operating units to calculate the corresponding total number of personnel injured by fire (Step 11) and injured by explosion (Step 12) in the specified population of operating units. Step 13 sums up the outputs from Steps 11 and 12. Simulation results in Steps 11, 12, and 13 are normalized over 10^6 MC trials.

Subroutine ‘Conditions-Support-Ignition’ (Fig. 3)

This Subroutine checks for simultaneous presence of the following conditions:

- a) A qualified ignition source is present in the confined space where the leaked flammable gas cloud is formed. The qualified ignition source means that the source has energy \geq minimum ignition energy (MIE) of the flammable gas cloud. A function $FP \leq \%$ is embedded in this step to check whether a user-specified probability of presence of a qualified ignition source is met. The output of this step is TRUE if the condition is met; otherwise it is FALSE and the simulation is terminated and a new simulation starts.

- b) Failure of mechanical ventilation is the confined space. A user-specified probability distribution function (rvm(FailureToVentilate)) is used to randomly select failure time of ventilation and then compares this time to the user-defined mission time. If the failure time is within the mission time, a TRUE output is generated which signifies condition is met, otherwise a FALSE output is generated and current simulation stops and a new simulation starts.
- c) This step is represented by a logical AND Gate. The Gate opens only when presence of a qualified ignition source is TRUE and ventilation failure (within the mission time) is also TRUE. In such case, this Subroutine returns to Step 6 in the MainChart (Fig. 1b) to continue the simulation.

Subroutine '*Personnel-Injured*' (Fig. 2)

As indicated before for each of the 10^6 MC trials where the leaked flammable gas ignites, the *Main Chart* (Figs. 1a and 1b) passes a binary value (Step 7 in Fig. 1b), either '0' to signify an explosion event or '1' to signify a fire event, to the *PersonnelInjured* Subroutine (Fig. 2) which determines the number of personnel injured (Step 8 for fire-related injuries and Step 9 for explosion-related injuries). This Subroutine contains a conditional step with an embedded function $FP \leq \%$ that checks, using a user-specified probability, whether personnel are present near the hazard source. If the condition is met, the output of this step is TRUE otherwise the output is FALSE. In the latter case, current simulation ends and a new simulation starts. In this regard, the function $FP \leq \%$ draws a random number as a percent from a uniform distribution from 0 to 100% and checks if this number \leq a user-defined probability of personnel presence near the hazard source. If the condition is met (i.e., TRUE), the binary value generated (0 or 1) by block (Step 7 in Fig. 1b) is passed on to the next conditional steps that determine using embedded $FP \leq \%$ functions which of the following two mutually-exclusive conditions is met: a user-specified conditional probability of injuries by fire, given a fire event or a user-specified conditional probability of injuries by explosion, given an explosion event. If none of the two conditions is met, then no personnel injuries would be expected and current simulation ends and a new simulation starts. If one of these mutually exclusive conditions is met, the corresponding probability is multiplied by number of personnel present near the hazard source. A user-defined probability distribution function, rvm(NumberOfPersonnel), is used to randomly select the number of personnel present near the hard source (see Table 2 for more discussion on this function). There are two outputs from Subroutine *Personnel-Injured* (Fig. 2): Number of personnel injured by fire injuries (Step 8) and number of personnel injured by explosion (Step 9) as shown in Fig. 1b.

In summary, the model simulates three mutually-exclusive scenarios namely: SL scenario, ML scenario, and LL scenario. Each scenario has two end states, one of which represents the total number of personnel injured by fire and the second represents the total number of personnel injured by explosion. Therefore the model has a total of six end states (two for each of the aforementioned leak scenarios). Accordingly in HRS case study, 10^6 MC trials have been selected per simulation and the probabilistic results of each MC trial are passed on to one of the following six end states (bins):

- 1) Number of fire-injured personnel caused by SL scenario.
- 2) Number of explosion-injured personnel caused by SL scenario.
- 3) Number of fire-injured personnel caused by ML scenario.
- 4) Number of explosion-injured personnel caused by ML scenario.
- 5) Number of fire-injured personnel caused by LL scenario.
- 6) Number of explosion-injured personnel caused by LL scenario.

Each of the above-mentioned six end states (bins) has a built-in logic that normalizes the sum of results. Also, it should be noted that one or more of the 10^6 Monte Carlo trials per simulation could be terminated before reaching its end state if ignition did not occur or no personnel were present near the hazard zone where the fire or explosion occurred.

2.2 Model's assumptions

Tables 1 and 2 provide the user-specified probabilities and probability distribution functions, respectively, that are used in the base case simulation of HRS case study. The model probabilistically determines whether ignition of formed flammable gas cloud within the confined space could lead to fire or explosion injuries based on user-specified probabilities (Table 1). However, the model does not differentiate between jet fire and flash fire.

Table. 1. User-specified probability data (base case) as used in the HRS case study.

Model's Inputs	User-Specified Probabilities	Sources of probability data
Leak type: Large leak (LL) Medium leak (ML) Small leak (SL) <ul style="list-style-type: none"> The LL type represents catastrophic, instantaneous rupture of pressure boundaries of systems containing the flammable gas. Examples LL include compressed gas storage tanks and full-bore (i.e., double-ended guillotine) rupture in compressors' connecting pipes, etc. The ML and SL leak types represent gradual gaseous discharge over time from pipe connections, flanges, seals, valves, etc. 	0.6% 4.8% 94.6%	<ul style="list-style-type: none"> IAEA (1988). Cox et al. (1990). E&P Forum (1992). Spencer and Rew (1996). Purple Book (1999). Lees (1006). Spencer and Rew (1997).
Fire or explosion event given ignition of formed gas cloud.	40%	<ul style="list-style-type: none"> Daycock and Rew (2004). Energy Institute (2006). LaChance (2008; 2009). Zhiyong et al. (2010). HSE (2012). Sun et al. (2014). Sakamoto et al. (2016).
Fire event given ignition of undetected SL.	80%	
Presence of a qualified ignition source (IS) in the confined space. A qualified ignition source means: $E_{IS} \geq (MIE)_{\text{Flammable gas-air-mixture}}$	20%	
Fire event given ignition of LL	99%	
Explosion event given ignition of LL	1%	
LL detection in the confined space	90%	
Fire event given ignition of undetectable ML	80%	
Explosion event given ignition of undetectable ML	20%	
Personnel presence near the hazard source	30%	
Personnel injury given a fire event	50%	
Personnel injury given an explosion event	99%	

Table 2. User-specified (assumed) probability distribution functions.

Model Parameter	Assumed Probability Distribution Function
In <i>MainChart</i> (Fig. 1a): Flammable gas leak initiation time within the confined space.	Weibull probability distribution function with $\beta = 2$ and $\eta = 24,000$ hours A function <code>rvm(WB(2, 2400))</code> returns a random time which is then checked against the user-specified mission time. If selected time is within the mission time, a value of 1 (signifying TRUE condition) is then passed on to the next step in the model to determine the leak type (SL, ML, or LL).
In <i>MainChart</i> (Fig. 1a): Leak type (SL, ML, or LL)	Leak type (SL, ML, or LL) is determined using a random variable (rv) selected from a uniform probability distribution (<code>rv_uniform(rand, 0, 1)</code>) in conjunction with the user-specified probability range for each leak type. In the uniform distribution, the argument ' <i>rand</i> ' is a random number generator.
In <i>Personnel-Injured</i> Subroutine (Fig. 2): Number of personnel injured by fire (explosion) within the confined space.	Normal distribution function with mean (μ) = 5 persons and standard deviation (σ) = 1 person The embedded function <code>rvm(NOR(5, 1))</code> returns a random value of the number of injured personnel, given a fire (or an explosion).
In <i>Conditions-Support-Ignition</i> Subroutine (Fig. 3): Confined space mechanical ventilation failure time.	Exponential distribution function with mean time between failure (MTBF) = 24,000 hours A random time to failure of the installed ventilation system in confined space is generated from the user-specified exponential probability distribution using the following embedded function: <code>rvm(EX2(1000, 0))</code> If the determined time is within the specified mission time, a 1 (signifying TRUE) is passed to the next step in the model.
<p>Conditional function <code>PF <= %</code></p> <p>This conditional function, which is one of RENO's internal functions, has been used in several steps defined in the proposed probabilistic model. The function draws a random number that is uniformly distributed (between 0 and 100) and then evaluates whether the value of the input variable to this function is \leq the user-specified value for this variable. If the condition (TRUE), the function's output is 1 and if the condition is not met (FALSE), the output of this function is 0.</p> <p>For example, <code>PF <= %</code> is used to check whether the specified probability of personnel presence near the hazard source is met. The function generates a random value and compares it against the specified probability value. If the condition is met, then 1 (signifying TRUE) is passed on the next step.</p>	

Additional notes and assumptions:

- For leak type determination, a uniform probability density function (pdf) has been assumed with minimum value '*a*' equal to zero, a maximum value '*b*' equal to 1, and a uniform distribution height equals $1/(b-a)$. A random value '*x*'; where $a \leq x \leq b$ is generated by a '*rand*' function

embedded in the model and the inverse of the calculated uniform cumulative probability ' $F(x) = (x - a)/(b - a)$ ' is mapped to the user's specified probability ranges to probabilistically determine the leak type.

- Subroutine '*Conditions-Support-Ignition*' (shown in Fig. 3) checks whether a qualified ignition source is present in the confined space where the gaseous leak occurs. To determine whether a qualified ignition source is present, the model draws a random number that is uniformly distributed between 0% and 100% and checks if this number \leq the user-specified probability. Also, this Subroutine contains a logical AND Gate, the output of which can be TRUE only if the following two conditions occur simultaneously within the user-specified time: a) A qualified ignition source is present and b) Mechanical ventilation in confined space failed. If one of these two conditions is not TRUE there is no risk of ignition and current simulation ends and a new simulation starts using the MainChart (Fig. 1a).
- In HRS case study, the mission time in the simulation is assumed to be one year. Hence, the calculated frequency of personnel injuries, given a fire or an explosion would be per year.
- The model allows calculation of conditional frequency of injuries, given fire or explosion, per user-specified field operating units. The word 'unit' signifies the industrial system experiencing leak failure, at some point in time during its expected service life. In HRS case study for example, the unit signifies the H₂ gas compressor which is assumed to experience the leak failure.

2.3 Visual-flowcharting methodology

RENO simulation platform from ReliaSoft¹¹ has been employed to construct the proposed probabilistic model using a visual flowcharting methodology which replaces need for writing complex computer algorithms to build the simulation model. RENO's simulation platform contains a set of blocks and internal functions that can be used to construct a variety of accident scenarios. In addition to the built-in mathematical functions, the flowcharting methodology allows inclusion of user-defined variables and functions using an equation's editor. Use of conditional if-statement blocks, go-to-flag blocks, stop flags, reset blocks, logic gates, branch gates, look-up tables, result storage blocks, flag markers, binary nodes, summation nodes, and do-loop counter blocks are among the options available in the flowcharting methodology. The RENO platform also contains an integrated utility to debug the constructed flowchart-based model for errors checking by allowing the model builder to cycle through all steps represented in the flowchart and observe interim calculated values as each block or resource in the model is executed. Results of execution of the visual flowcharting-based model can be displayed during the simulation in the form of graphs, spreadsheets, or as numerical displays next to each block in the constructed visual flowchart. Moreover, sensitivity analysis can be performed by allowing one or more of the model variables to vary across the simulation based on user-assigned starting, increment, and ending values. In its optimization mode, RENO platform allows multiple runs to be performed automatically to determine the value that minimizes or maximizes a specific result of interest to the end user.

2.4 HRS case study

This case study serves as an example for demonstrating functionality of the proposed probabilistic model. Additionally, applying the case study to HRS is motivated by the need for better understanding of potential occupational risks and mitigation measures related to these infrastructures

¹¹ Source: www.raliasoft.com

as their global presence continues to grow. The postulated accident scenario involves H₂ gas leak from the compressor's discharge line into the station's compressor room. The choice of the H₂ compressor as the leak source is driven by the conclusions reported by Zhiyong et al. (2010), Ham et al. (2011), Sun et al. (2014), and Sakamoto et al. (2016) that H₂ compressor's SL leak is the main contributor to first party risk in HRS.

The base case scenario assumes that the compressor's room is equipped with H₂ detection and mechanical ventilation as risk mitigation measures. However, these hardware systems could randomly fail in conjunction with occurrence of the compressor's gaseous leak. Under such conditions and in presence of an ignition source, the leaked H₂ gas cloud could ignite causing a fire or an explosion or both. The ignition source could be an electrical spark, smoking, mechanical friction, hot work during maintenance or repair activities, static electricity, hot surfaces, etc. Given coincidental presence of station's personnel in the compressor's room at time of accident initiation, the simulation model calculates potential risks of fire and explosion injuries associated with the postulated scenario.

Probability values used in the base case simulation are taken from the Purple Book (2005), published articles like LaChance (2008; 2009), Zhiyong et al. (2010), Ham et al. (2011), and Sun et al. (2014) as well as the author's experience as a subject matter (SME) expert on risk assessment and hydrogen safety.¹² For example, compressor's leak probabilities by type are taken from Zhiyong et al. (2010) as well as LaChance (2008) who defined H₂ leak sizes as a percent of the flow area and calculated the safe separation distance for HRS based on postulated H₂ SL (representing 3% of system flow area) scenarios. In the present work, the proposed cumulative probabilities for LL, ML, and SL are 0.6%, 4.8%, and 94.6%, respectively (Table 1).

Throughout the remaining sections of this manuscript, reference to the HRS's base case scenario signifies that the H₂ compressor's room is equipped with H₂ detection and mechanical ventilation. However, these safety controls could randomly fail with some finite probabilities during progression of the postulated gaseous leak scenario. If these safety controls were operating properly as designed during time of leak occurrence, no H₂ ignition would be expected. Additionally, reference to HRS's worst case scenario (in Subsection 3.2.1) signifies that the H₂ compressor's room is not equipped with the aforementioned safety controls. Also, because hydrogen minimum ignition energy (MIE) is very small ≈ 0.02 mJ (Khalil, 2011), ignition of the leaked H₂ from the compressor would be a likely event.

3. Results and discussion

The results and discussion provided in this section are relevant to HRS case study described in Subsection 2.4. The proposed probabilistic model has been employed to quantify the annual occupational risks of fire and explosion injuries associated with the postulated scenarios in this case study. Whether the implied consequence is fire-related injuries or explosion-related injuries, the frequency of occupational risk can be calculated as described by Eq. (1).

¹² Dr. Y.F. Khalil was the Engineering Manager of the Probabilistic Risk Assessment (PRA) Department at the Millstone Nuclear Power Station in Waterford, Connecticut, USA and the Principal Investigator for hydrogen storage materials reactivity and safety contract sponsored by the U.S. Department of Energy. He is also the current Operating Agent of the Hydrogen Safety Task of the International Energy Agency (IEA) and a member of NFPA 2 Hydrogen Technologies Committee.

$$\text{Risk Frequency} = (\text{Probability of Leak Occurrence}) \times (\text{Consequence Frequency}) \quad \dots \dots (1)$$

In HRS case study, the calculated risks using Eq. (1) are compared against occupational risk acceptance threshold of $1.0\text{E-}4/\text{year}$ to identify the conditions under which the calculated occupations risks are deemed unacceptable and, hence, additional risk mitigation would be required.

3.1 Base case scenario's risks and uncertainty quantification

Before executing the base case scenario simulation, a test scenario is executed to confirm soundness of the logical structure of the proposed model. In the test scenario, the probability of H₂ leak detection and isolation before ignition is set to 1.0 in the simulation model. Obviously, the expected outcome of this case should be no adverse safety consequences since H₂ ignition did not occur. Having confirmed this expected outcome from the test scenario, the base case simulation has been executed.

Fig. 4 shows the calculated annual risks of fire and explosion injuries for the base case scenario where the H₂ compressor's room in HRS is assumed to be equipped with contain H₂ leak detection and mechanical ventilation. A total of 30 million Monte Carlo trials (30 simulation runs and each simulation consists of 1 million Monte Carlo trials) were conducted to generate the base case results shown in Fig. 4. Base case probability data are shown in Table 1. As depicted in Fig. 4, the calculated occupational risks are provided as best estimate (BE), lower bound (LB), and upper bound (UB) values. The LB represents the 5th percentile and UB represents the 95th percentile. The occupational risk acceptance criterion of $1.0\text{E-}4/\text{year}$ is also shown (horizontal dashed line) in the same graph.

For the risks associated with base case fire injuries, the following insights can be drawn:

- The LB, BE, and UB occupational risks of LL and ML scenarios are below the $1.0\text{E-}4/\text{year}$ threshold and, hence, first-party risks could be tolerated without need for additional risk mitigation.
- With exception of LB occupational risk, the calculated BE and UB occupational risks of SL scenarios have exceeded the occupational risk acceptance threshold of $1.0\text{E-}4/\text{year}$. Hence, additional risk mitigation actions would be needed. For example, use redundant H₂ detectors or use highly reliable H₂ detector and mechanical ventilation system.
- As a frame of reference, the Hydrogen Technologies Committee of the National Fire Protection Association (NFPA 2),¹³ proposed that the acceptable risk levels to HRS's workers (first party) and customers (second party) should not exceed $1.0\text{E-}4/\text{year}$ and proposed a risk value of $2.0\text{E-}5$ fatalities/year as a guideline driven by the comparative risk to gasoline stations. In this regard, NFPA data for gasoline service stations in U.S. suggests a frequency of $2.0\text{E-}5/\text{year}$ for fire fatalities and $3.0\text{E-}4/\text{year}$ for fire injuries (LaChance, 2008). According to the aforementioned risk of fire injuries data reported by LaChance (2008), namely, $3.0\text{E-}4$ injuries /year, our calculated frequency of fire injuries risk associated with base case SL scenario, namely, $6.62\text{E-}4/\text{year}$ (BE value) and $4.26\text{E-}3/\text{year}$ (UB value) represent intolerable risk levels.

¹³ Source: <http://www.nfpa.org/codes-and-standards/all-codes-and-standards>.

For the risks associated with base case explosion injuries, the following insights can be drawn:

- The calculated LB, BE, and UB risks associated with LL scenario are below the risk acceptance threshold. Hence, the occupational risks associated with LL scenario could be tolerated without need for adding additional risk mitigation measures in the compressor's room.
- With exception of the calculated UB occupational risk, ML scenario leads to LB and BE occupational risk values that are below the $1.0\text{E-}4/\text{year}$ risk acceptance threshold. Nonetheless, the fact that ML scenario could probabilistically lead to UB risk of explosion injuries that exceed the risk acceptance threshold could justify the need for additional risk mitigation measures.
- The calculated occupational risks (LB, BE, and UB) for the SL scenario exceed the acceptable risk threshold of $1.0\text{E-}4/\text{year}$. Accordingly, additional risk mitigation actions would be needed in the H2 compressor's room to bring first-party risks to acceptable levels.

Clearly, the simulation results show that SL base case scenario leads to more severe consequences compared to ML and LL cases. This simulation outcome can be attributed to the following: a) SL frequency is about two orders of magnitude higher than that of ML and LL (Zhiyong et al., 2010). b) The likelihood of detection of ML and LL are greater compared to SL case. This insight is also supported by the quantitative and qualitative findings of Zhiyong et al. (2010), Ham et al. (2011), Sun et al. (2014), and Sakamoto et al. (2016).

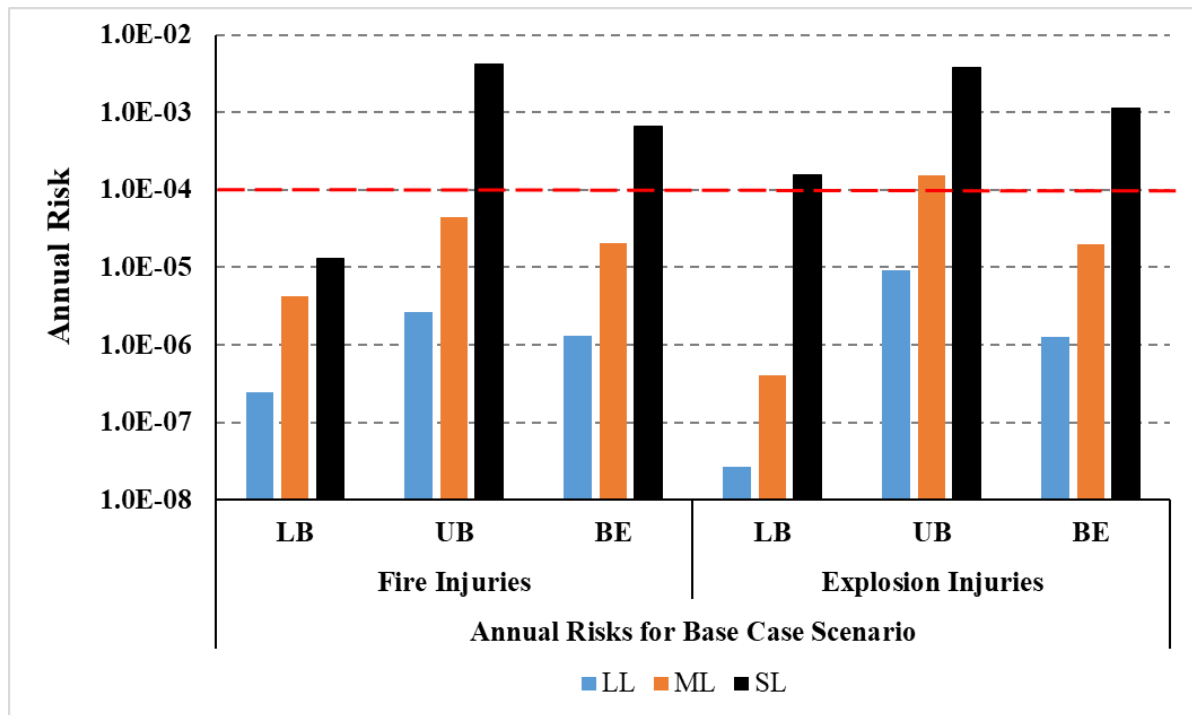


Fig. 4. Calculated annual risks of fire and explosion injuries for the base case scenario. Note: the horizontal dashed line represents the occupation risk acceptance threshold of $1.0\text{E-}4/\text{year}$.

The following are recommended risk migration actions to reduce the aforementioned occupational risks to an acceptable level:

- Employ more reliable (lower failure rates) H₂ leak detectors.
- Use redundant H₂ detectors.
- Install detectors with low detection threshold ($< 1\%$ of LFL).
- Implement capabilities to isolate leak failures (*i.e.*, fail safe design).
- Increase the ventilation rate (*i.e.*, number of air changes per hour) in the compressor's room to prevent buildup of leaked H₂ and formation of a flammable gas cloud.
- In addition to the above-mentioned hardware considerations, implement administrative controls such as daily visual inspection of the compressor's pipes and connections, restrict HRS's workers presence in the compressor's room to only during equipment shutdown periods, perform period maintenance on the compressor to minimize the mechanical vibrations which can accelerate the potential for H₂ leaks from pipe connections such as those on the compressor' discharge line, and eliminate sources of ignition in the compressor's room.

As it is always the case, predictions made by data-driven simulations require performance of uncertainty analysis. The types of uncertainty could be aleatory, epistemic, or related to the degree of completeness of the simulation model. As discussed by Khalil and Mosher (2008), aleatory type of uncertainty results from components' random failures and epistemic uncertainty is related to physical phenomena such as combustion of flammable gases within enclosures and the resulting fires (jet or flash) or explosions (deflagration, detonation, and deflagration-to-detonation transition). Because of its stochastic nature, aleatory uncertainty cannot be reduced by improving our state of knowledge about the mechanisms of hardware failures. To the contrary, however, epistemic uncertainty is reducible by improving our understanding of the phenomenology being investigated. Uncertainty related to model completeness (*i.e.*, how realistic the simulation model is relative to a real-world situation) is rather subjective and depends on several factors including the needed levels of details in the model structure, tradeoff between accuracy of results and model's complexity.

In HRS case study, MC sampling technique has been employed to propagate uncertainties through the proposed model. As shown in Table 2, several probability distribution functions are used instead of best estimate probabilities. The results of each simulation are averaged over one million Monte Carlo trials. A total of 30 million MC trials (corresponding to 30 simulation runs with each simulation consisting of 1 million MC trials) are performed to generate the LB, BE, and UB risk values shown in Fig. 4. In cases where best estimate probabilities are used in the model (see Table 1), either these probabilities are taken from peer-reviewed publications (Table 1) or based on this author's judgment as a subject matter expert in the probabilistic risk assessment field.

3.2 Scenario analysis and sensitivity cases

3.2.1 Scenario analysis

Scenario analysis for HRS case study has been performed by comparing the risk consequences of the so-called worst-case scenario to those associated with the base case scenario. The worst-case scenario assumes that the H₂ compressor's room is not equipped with leak detection. Accordingly,

the probability of H2 leak detection and, hence, isolation before ignition is set to zero in the worst-case simulation. As such, this scenario should lead to the most severe outcomes in terms of the predicted risks of fire and explosion injuries. Similar to the base case scenario, a total of 30 million MC trials are executed to generate results for the worst-case scenario as shown in Fig. 5.

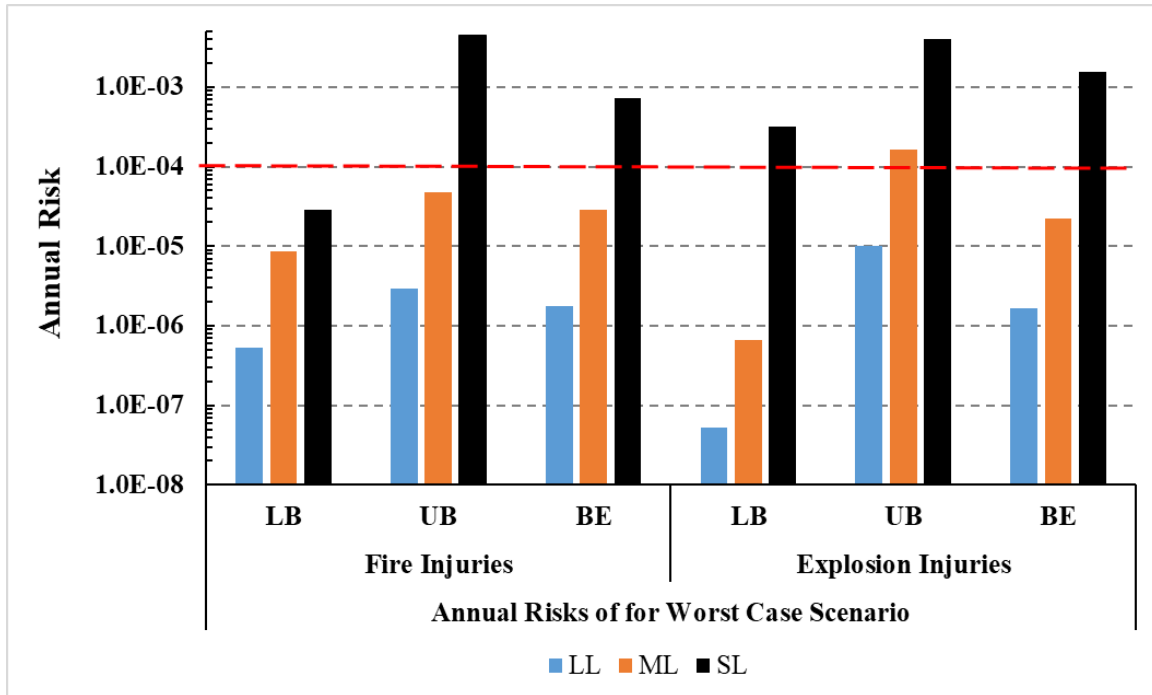


Fig. 5. Annual risks of fire and explosion injuries for the worst case scenario. Note: the horizontal dashed line represents the acceptable occupational risk level of $1.0E-4$ /year.

For the risks associated with worst-case fire injuries, the following insights can be drawn:

- The calculated LB, BE, and UB risks of worst-case LL scenario in the compressor's room remain below the acceptable risk threshold of $1.0E-4$ /year and, hence, the risk could be tolerated.
- The calculated LB, BE, and UB risks of worst-case ML scenario in the compressor's room remain below the acceptable risk threshold of $1.0E-4$ /year and, hence, the risk would be tolerable.
- With exception of the LB risk, the BE and UB risks associated with worst-case SL exceed the $1.0E-4$ /year occupational risk acceptance level and, hence, safety control measures need to be implemented in the H2 compressor's room.

For the risks associated with worst-case explosion injuries, the following insights can be drawn:

- The calculated LB, BE, and UB risks associated with LL worst-case scenario are below the risk acceptance threshold and, hence, the associated occupational risks would be tolerable.
- With exception of the calculated UB occupational risk, ML worst-case scenario leads to LB and BE occupational risk values that are below the $1.0E-4$ /year risk acceptance threshold. However, the fact that ML worst-case scenario could probabilistically lead to UB risk of explosion injuries that exceed the risk acceptance threshold would justify the need for implementation of risk control measures.

- The calculated occupational risks (LB, BE, and UB) for the SL worst-case scenario exceed the acceptable risk threshold of $1.0\text{E-}4/\text{year}$. Accordingly, risk mitigation actions would be needed to bring first-party risks to $\leq 1.0\text{E-}4/\text{year}$.

For each leak type (SL, ML, and LL), the calculated risks of fire and explosion injuries are higher for the worst-case scenario compared to the best case scenario (Figs. 6, 7, and 8, respectively). Once again, the base case scenario signifies that the compressor's room is equipped with leak detection capability whereas the worst case scenario signifies that the compressor's room is not equipped with leak detection capability.

Fig. 6 shows that in all cases, the calculated risks exceed the occupational risk acceptable level of $1.0\text{E-}4/\text{year}$. As can be seen from Figs. 7 and 8, the calculated risks of fire and explosion injuries remain below the $1.0\text{E-}4/\text{year}$ acceptable risk. Additionally, the LL risks are roughly one order of magnitude lower than those associated with the ML scenarios.

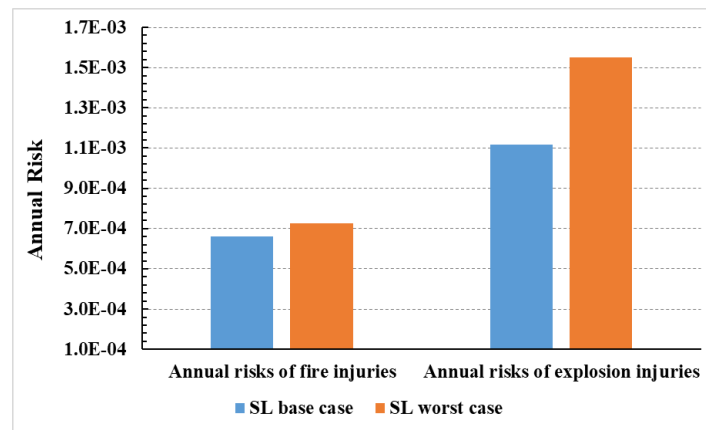


Fig. 6. Calculated annual risk of fire and explosion injuries for base case and worst-case small leak (SL) scenarios.

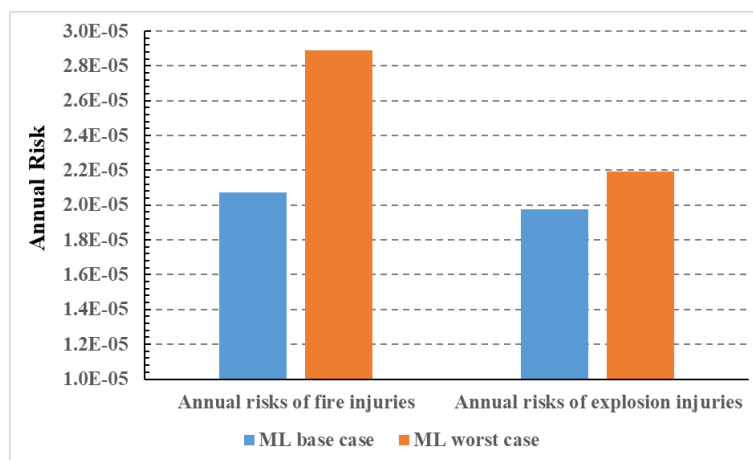


Fig. 7. Calculated annual risk of fire and explosion injuries for medium leak (ML) base case and worst-case scenarios.

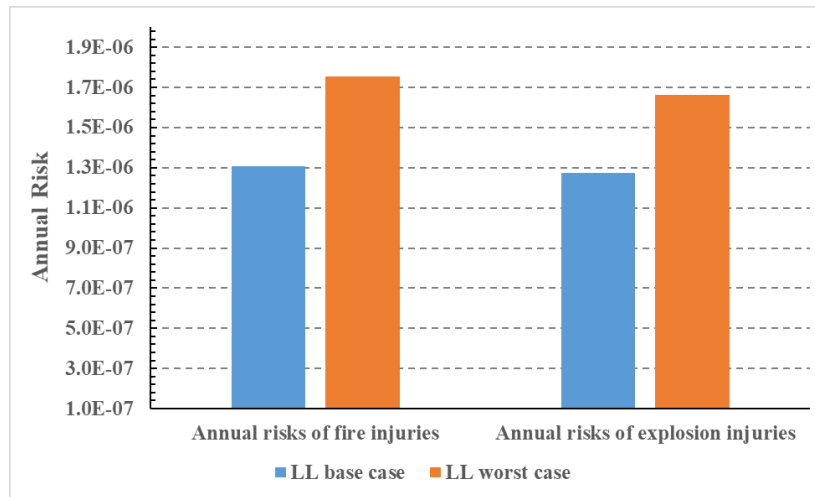


Fig. 8. Calculated annual risk of fire and explosion injuries for large leak (LL) base case and worst-case scenarios.

3.2.2 Sensitivity cases

Three sensitivity cases are simulated and their results are compared against those of the base case scenario to provide useful risk insights on how selected values of model's parameters can impact the calculated occupational risks in HRS case study. The insights to be gained from these sensitivity cases can increase risk analysts' awareness of need for safety measures to reduce the occupational risks to acceptable levels. Table 3 summarizes the probabilities used for selected model parameters.

Table. 3. Description of sensitivity cases with selected model parameters.

Model Parameters	Probabilities ⁽¹⁾ for Sensitivity cases			Base Case Probability Distributions ⁽²⁾
	1	2	3	
P(H2 Detection)	5%	20%	5%	Triangular distribution: LB: 5% BE: 50% UB: 80%
P(Fire or Explosion Ignition)	20%	40%	20%	Triangular distribution: LB: 20% BE: 40% UB: 60%
P(Personnel Present near Hazard Source)	50%	30%	10%	Triangular distribution: LB: 10% BE: 30% UB: 50%
P(Fire Ignition)	15%	50%	15%	Triangular distribution: LB: 15% BE: 50% UB: 80%
P(Explosion Ignition)	85%	50%	85%	Triangular distribution: LB: 20% BE: 50% UB: 85%

Model Parameters	Probabilities ⁽¹⁾ for Sensitivity cases			Base Case Probability Distributions ⁽²⁾
P(Injuries Fire & Personnel Present near Hazard)	30%	50%	30%	Triangular distribution: LB: 30% BE: 50% UB: 70%
P(Injuries Explosion & Personnel Present near Hazard)	10%	50%	10%	Triangular distribution: LB: 10% BE: 50% UB: 99%

- ⁽¹⁾ The selected point estimate probabilities are based on published literature (data sources are provided in Table 1) as well as this author's knowledge as a subject matter expert on probabilistic risk assessment and hydrogen safety.
- ⁽²⁾ In HRS base case scenario, triangular probability distributions (as compared to single-point estimates) are used to generate the base case occupational risks of fire and explosion injuries.

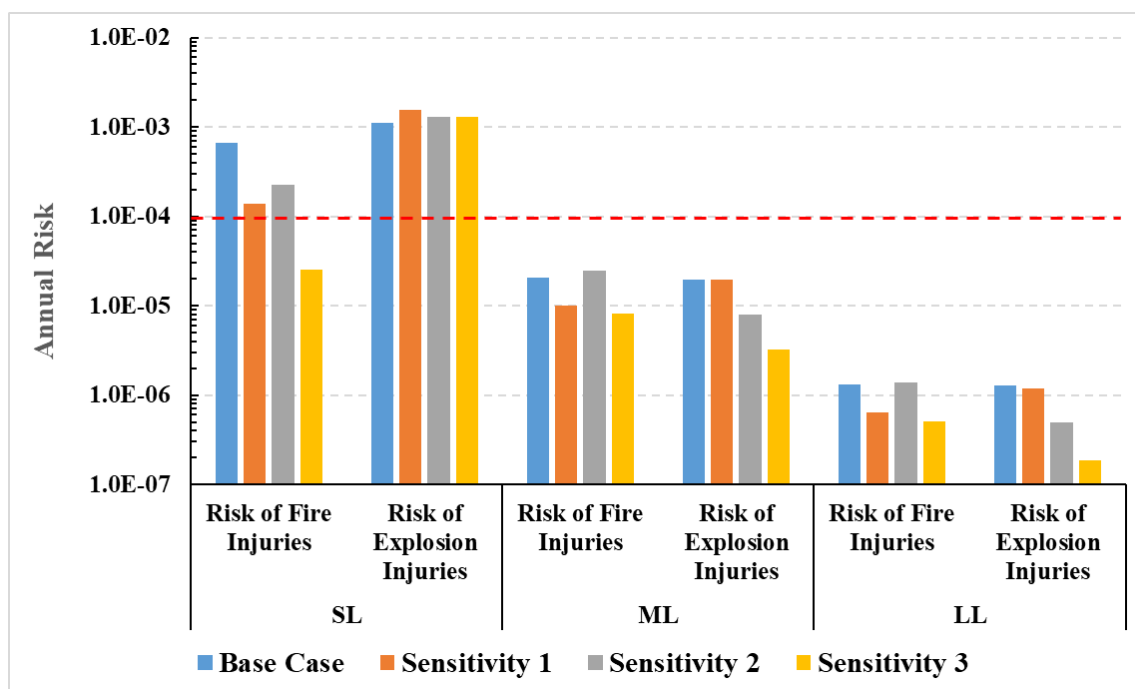


Fig. 9. Sensitivity cases: Calculated mean annual risks of fire and explosion injuries for postulated leak scenarios (SL, ML, and LL) in HRS case study. *Note that the horizontal dashed line represents the acceptable occupational risk threshold (1.0E-4/year).*

Fig. 9 compares the calculated mean annual risks of fire and explosions injuries associated with these sensitivity cases versus the base case annual risks. The following are key risk insights to be drawn from Fig. 9:

- Calculated annual risks of HRS's first-party injuries due to fires and explosions caused by SL within the H2 compressor's room exceeds (with exception of Sensitivity Case 3) the acceptable

occupational risk level (1.0E-4/year) by about one order of magnitude. It should be noted that the probability of personnel present near the hazard source is the lowest in Sensitivity Case 3 compared to Sensitivity Cases 1 and 2.

- Calculated annual risks of explosion injuries for the SL base case as well as the three sensitivity cases exceed the acceptable risk level by about one order of magnitude.
- For the selected sensitivity cases as well as the base case scenario, ML and LL scenarios lead to risks of fire and explosion injuries below the acceptable occupational risk level.

Based on the aforementioned insights and given the selected sensitivity cases, SL scenarios in the H2 compressor's room can pose unacceptable first-party risks compared to ML and LL scenarios. This observation can be attributed to the following risk-based argument:

The risk (R) function is defined by the product of two risk factors, namely, probability of occurrence of the undesired event (O) times the consequences (C) should the event occur. In the HRS case study, the H2 compressor's SL frequency is about two orders of magnitude higher than that of ML and LL (Zhiyong et al., 2010). Hence, even if the consequences of ML and LL scenarios could be more severe compared to that of the SL scenario, the risk (*i.e.*, product of $O \times C$) associated with SL could be higher as it is in the case here.

3.3 Economic cost of injuries

Economic risk assessment can be performed by framing the calculated probabilistic risks of postulated accident scenarios in monetary terms. The resulting economic cost of injury can be used to support cost-to-benefit analyses of proposed safety measures designed to eliminate, or mitigate, the identified risks.

The economic cost of fire and explosion injuries can be calculated by multiplying the calculated risk frequency times a fraction of the value of statistical life (VSL) that is commensurate with injury's severity level. To account for inflation and real income growth, the VSL can be adjusted as shown by Eq. (2).

$$(VSL)_T = (VST)_0 * \left(\frac{P_T}{P_0}\right) * \left(\frac{I_T}{I_0}\right)^\varepsilon \quad \dots \dots (2)$$

The parameters shown in Eq. (2) can be defined as follows: Subscript 0 signifies the base year and T signifies the year (T) of interest. Parameter P_T signifies the price index in year T , I_T signifies the real income in year T , and ε represents the income-elasticity of VSL. Costa and Kahn (2004) proposed values between 1.5 and 1.6 for the income-elasticity of VSL. Moran and Monje (2016) discussed Eq. (2) and described a procedure (currently used by the U.S. Department of Transportation) to assign a fractional value of VSL to each injury class based on its severity level.

In the U.S., for example, the VSL for occupational risk was \$7.17 million (Viscusi, 2003; 2005). In 2016, however, the VSL has been revised to \$9.6 million using a 2015 base year (Moran and Monje, 2016). To put the meaning of VSL into perspective, a VSL of \$9.6 million denotes that an

organization is willing to pay (WTP) \$960 to reduce the annual risk of fatality by one in 10,000 (where $\$960/1.0\text{E-}4 = \9.6M).

For the purpose of this research, we propose to use the following VSL multipliers as shown in Table 4. As depicted in this table, fire and explosion injuries are classified into three classes and each class is assigned a VSL multiplier. These multipliers are derived from the fractions proposed by Moran and Monje (2016) for six classes in injuries.

Table 4. Proposed multipliers of VSL for injury classes with different severity levels (this work).

Injury Classification (Based on Severity Level)	Proposed VSL Multiplier	Adjusted VSL by Injury Class (Based on 2016 VSL of \$9.6M)
Minor to Moderate <i>Example: first-degree burns</i>	0.025	\$0.240M
Serious to Severe <i>Example: Second-degree burns</i>	0.186	\$1.786M
Critical <i>Example: Third-degree burns</i>	0.593	\$5.693M

The following quantitative example illustrates the proposed methodology for calculating economic costs of injuries associated with the leak scenarios described in this research:

Based on HRS case study, the calculated mean occupational risk of a fire injury that resulted from the SL base case scenario is $6.62\text{E-}4/\text{year}$ (refer to Fig. 4). Assuming that third-degree burns sustained by the impacted station's workers represent 20% of the calculated risk of fire injuries, then the cost of injury (in 2016 dollars) of an impacted HRS's worker who sustained a third-degree burn can be calculated using Eq. (3) as follows:

$$(20\%).(6.62\text{E-}4/\text{year}).(\$5.693\text{M}) \approx \$754/\text{year} \quad \dots\dots (3)$$

The corresponding upper bound (UB) of cost associated with a fire injury caused by the base case SL scenario can be calculated by Eq. (4):

$$(20\%).(4.26\text{E-}3).(\$5.693\text{M}) \approx \$4,850/\text{year} \quad \dots\dots (4)$$

Where $4.26\text{E-}3/\text{year}$ is the calculated UB risk of a fire injury (see Fig. 4).

4. Conclusions, recommendations, and future work

4.1 Conclusions

The proposed probabilistic model is a robust simulation tool for training relevant stakeholders to better understand potential occupational risks associated with ignition of leaked flammable gases within confined spaces in a broad range of industrial settings. Users of this tool can simulate *what-if* accident scenarios and quantify sensitivities of the predicted frequencies of occupational risks to different values of inputs to this model. The predicted risks can then be compared to occupational risk acceptance threshold of $1.0\text{E-}4/\text{year}$ to determine conditions under which the calculated risks exceed this threshold. The results of scenario analysis and sensitivity cases should raise awareness

of model's users about the importance of compliance with safety regulations and actions required to mitigate those risks to acceptable levels.

The HRS case study showed that postulated accidents involving H₂ small leaks (SL) in the compressor's room could lead to unacceptable occupational risk frequencies that exceed the 1.0E-4/year acceptance criterion and in excess of the 2.0E-5/year risk value proposed by NFPA as a guideline driven by the comparative risk to gasoline refueling stations. For example, the predicted frequencies of risks associated with the base case SL scenario can be summarized as follows:

- Fire-related injuries: 6.62E-4/year (BE) and 4.26E-3/year (UB)
- Explosion-related injuries: 1.12E-3/year (BE) and 3.85E-3/year (UB)

Our finding that occupational risk frequencies of SL scenario are greater than those associated with LL and ML scenarios (Figs. 4 and 5) can be attributed in part to the fact that the compressor's SL frequencies are at least two orders of magnitude greater than LL and ML leak frequencies. This finding is also consistent with qualitative and quantitative conclusions made by other researchers as previously discussed in Subsection 3.1.

4.2 Recommendations

Based on the risk insights generated from HRS case study, the following set of best practices is recommended to manage occupational risks caused by ignition of potential leaks of flammable gases into confined spaces:

- Design failsafe configurations for systems that handle flammable gases. For example, install a dedicated circuit breaker on H₂ compressor's power supply line such that the breaker automatically opens when H₂ leak is detected in the compressor's room. Also, install a dedicated isolation valve on compressor's outlet so that it automatically closes to stop a downstream H₂ leak.
- Prevent H₂ backflow from higher to lower pressure by installing a check valve at the interface between high- and low-pressure lines.
- Perform visual inspection of flammable gas flow pipes and connections only during systems' shutdown.
- Employ pressure and temperature sensors in all confined spaces containing flammable gases. These devices should be designed to activate high-speed emergency ventilation when over-pressure or over-temperature conditions are detected. Increased ventilation (air changes per hour) helps preventing buildup of leaked flammable gases to their LFL concentrations.
- Use high-sensitivity detection devices that can detect leaked flammable gases far before reaching their LFL concentrations. To eliminate single-point failure of detection capability, use redundant (at least two) detection devices.

4.3 Future work

New features will be added to the proposed model as follows:

- Risk of property damage and other collateral financial consequences to the industrial facility that sustains an accident involving ignition of a leaked flammable gas into a confined space.
- Capability to quantify first-party human toxicity risk caused by accident scenarios that involve ignition of leaked R1234ze(e) from a chiller located in a confined space to a building's machine room. In such case, combustion gases emitted from burning of this mildly-flammable refrigerant contains hydrogen fluoride (HF), which a toxic gas.

Glossary

AHRI	Air Conditioning, Heating, and Refrigerating Institute
ASHRAE	American Society of Heating, Refrigerating, and Air Conditioning Engineers
BE	Best estimate
BN	Bayesian Networks
CFD	Computational fluid dynamics
CHG	Compressed hydrogen gas
CNG	Compressed natural gas
DDT	Deflagration to detonation transition
GWP	Global warming potential
HAZID	Hazard identification
HAZOP	Hazard and operability analysis
HIAD	Hydrogen incidents and accidents database
HIRD	Hydrogen incidents reporting database
HRS	Hydrogen refueling station
LB	Lower bound
LL	Large leak
MCS	Monte Carlo sampling
MIE	Minimum ignition energy
ML	Medium leak
NFPA	National Fire Protection Association
ODP	Ozone depletion potential
QLRA	Qualitative risk assessment
QRA	Quantitative risk assessment
SL	Small leak
UB	Upper bound
VCE	Vapor cloud explosion
VSL	Value of statistical life

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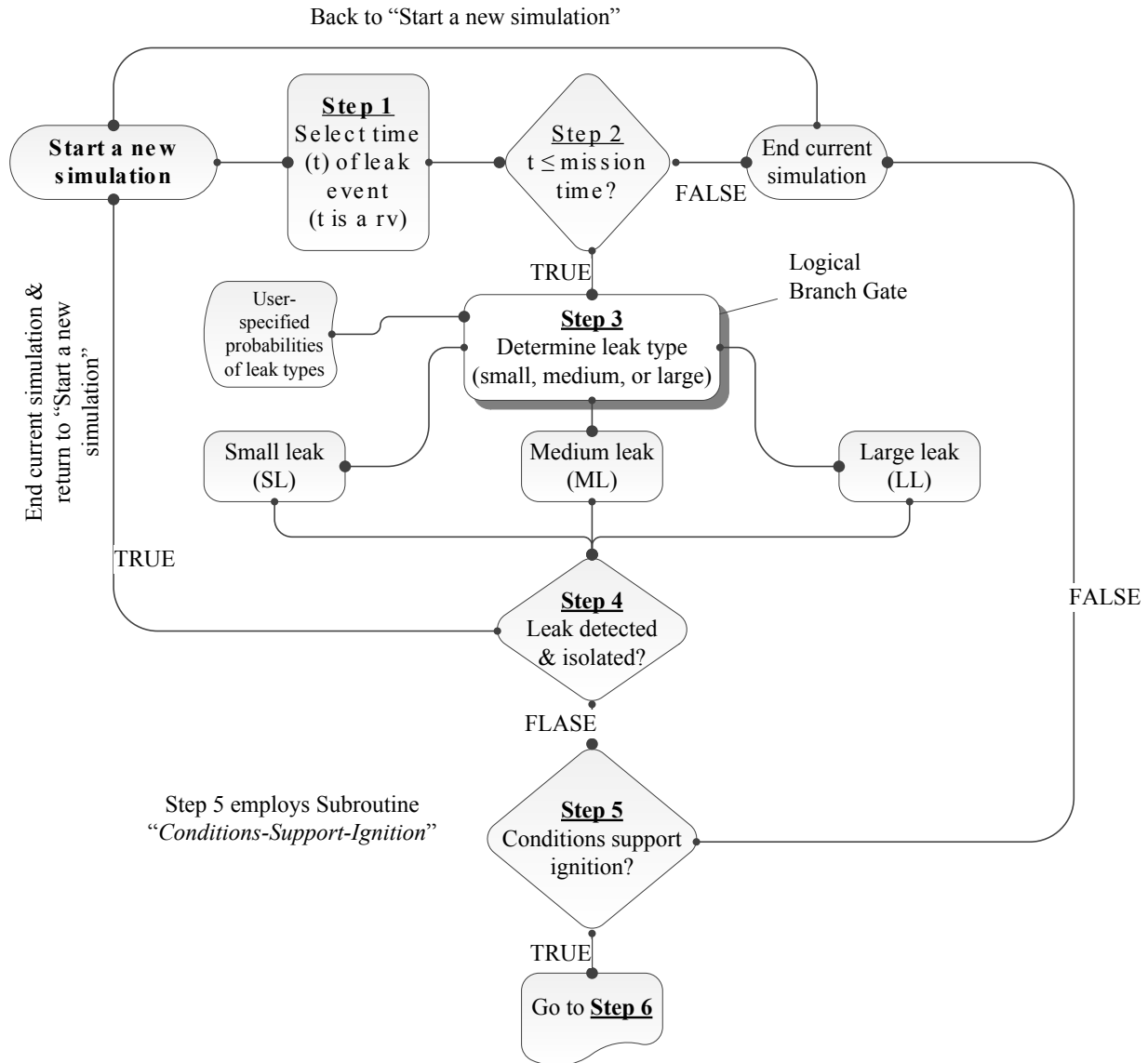


Fig. 1a. A probabilistic visual-flowcharting-based model for safety consequence assessment of fire and explosion events involving leaks of flammable gases within enclosures:
MainChart.

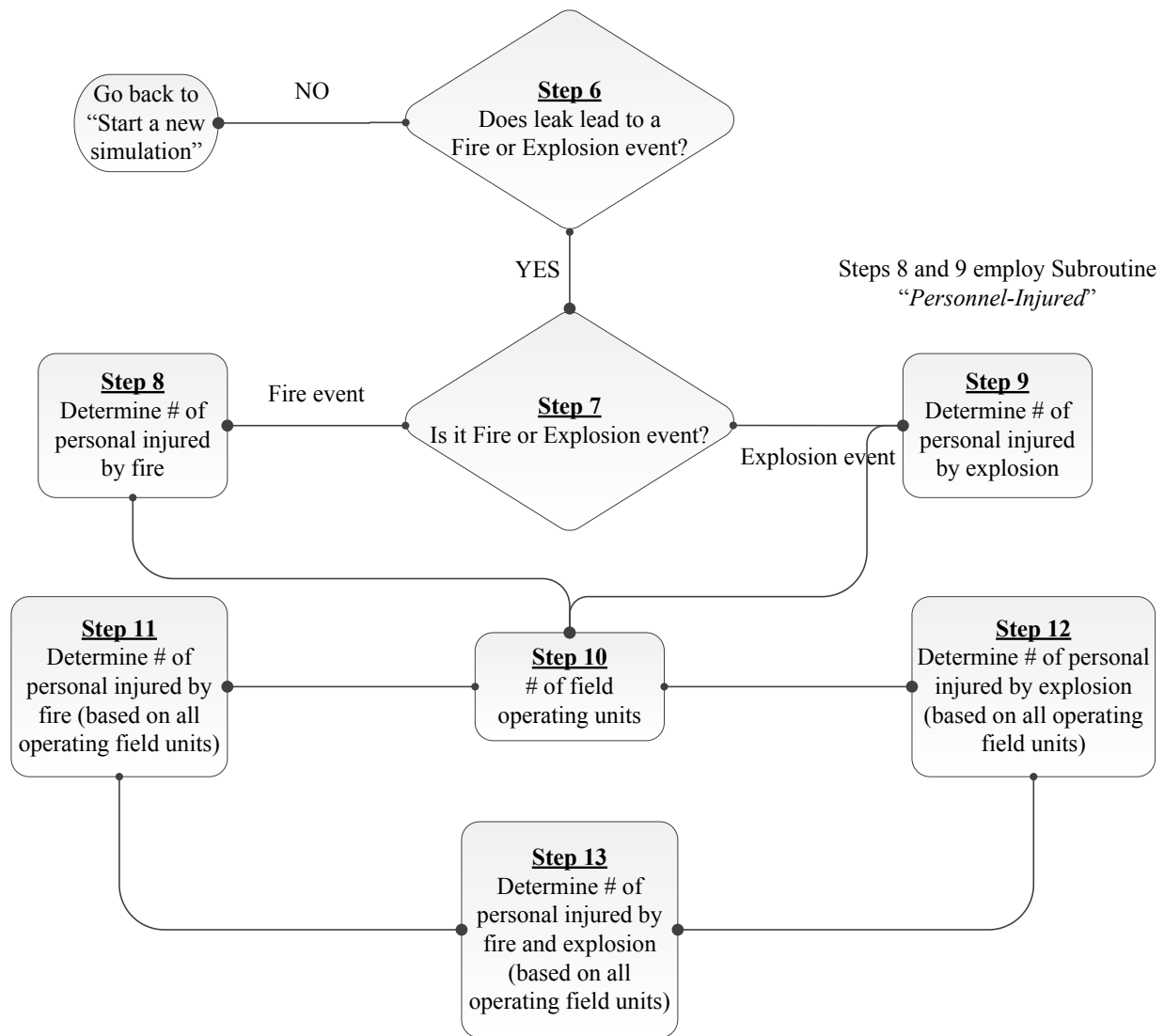


Fig. 1b. A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases within enclosures: *MainChart* (cont'd).

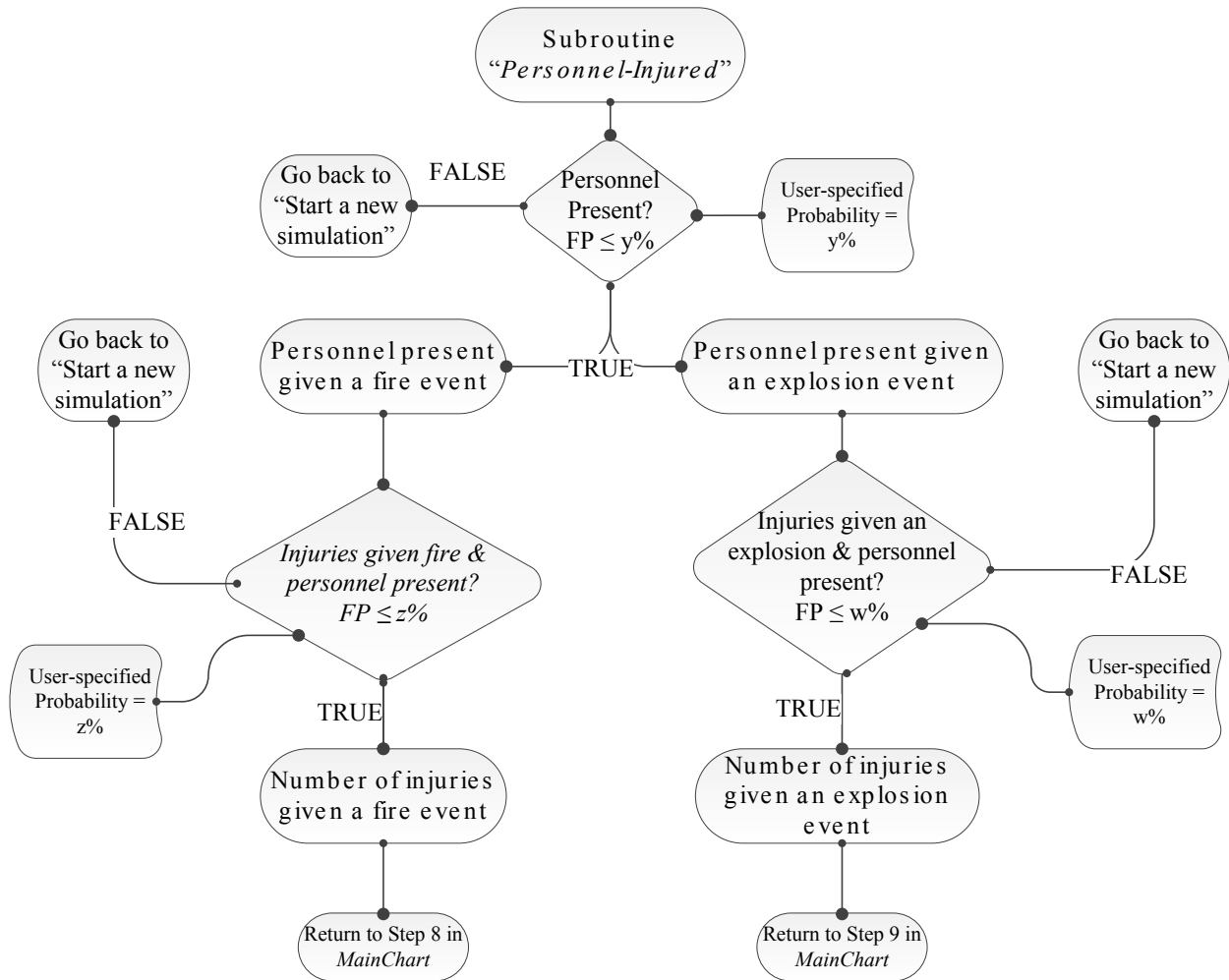


Fig. 2. A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases with enclosures: Subroutine "Personnel-Injured."

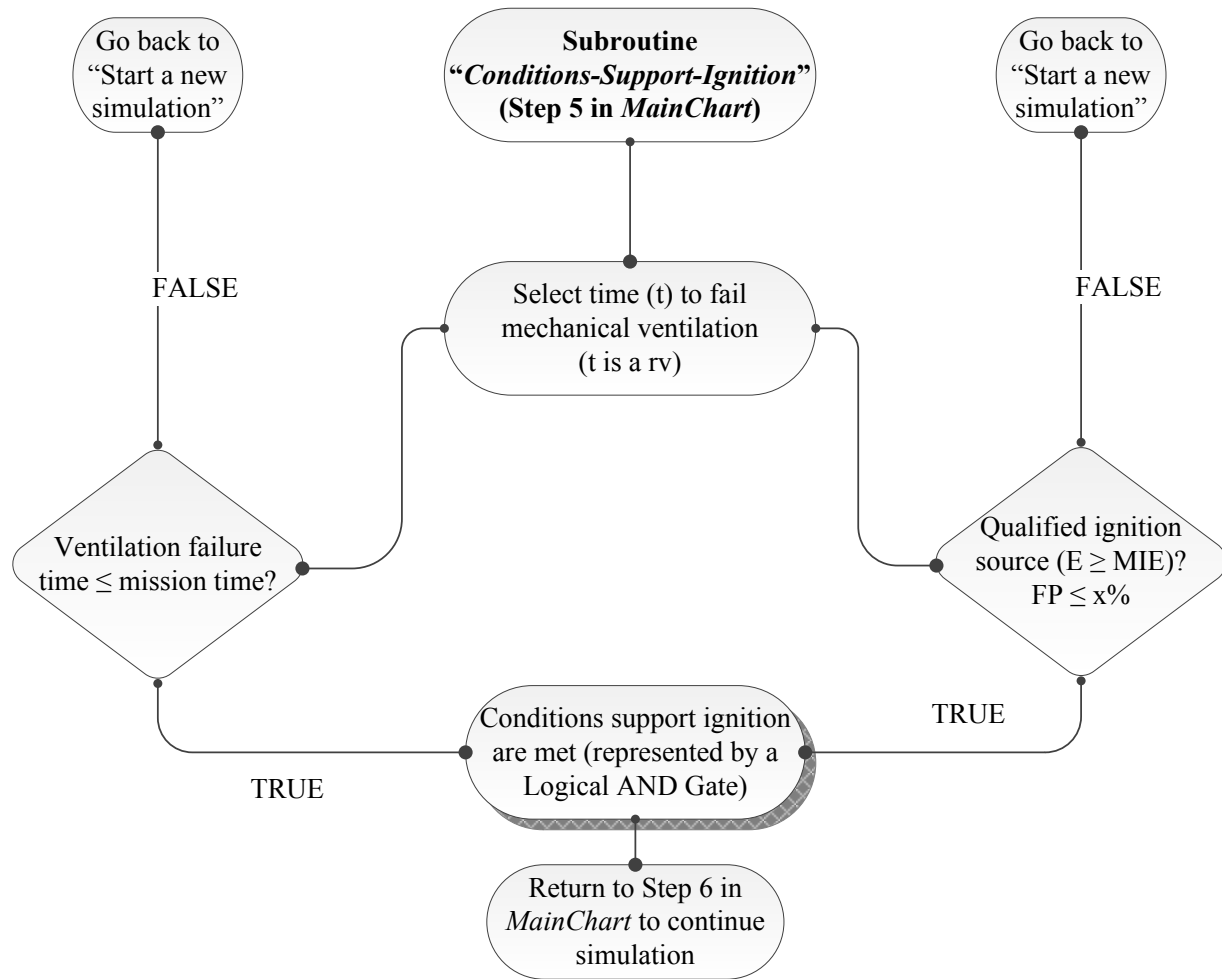


Fig. 3. A probabilistic visual-flowcharting-based model for consequence assessment of fire and explosion events involving leaks of flammable gases: Subroutine “*Conditions-Support-Ignition*.”

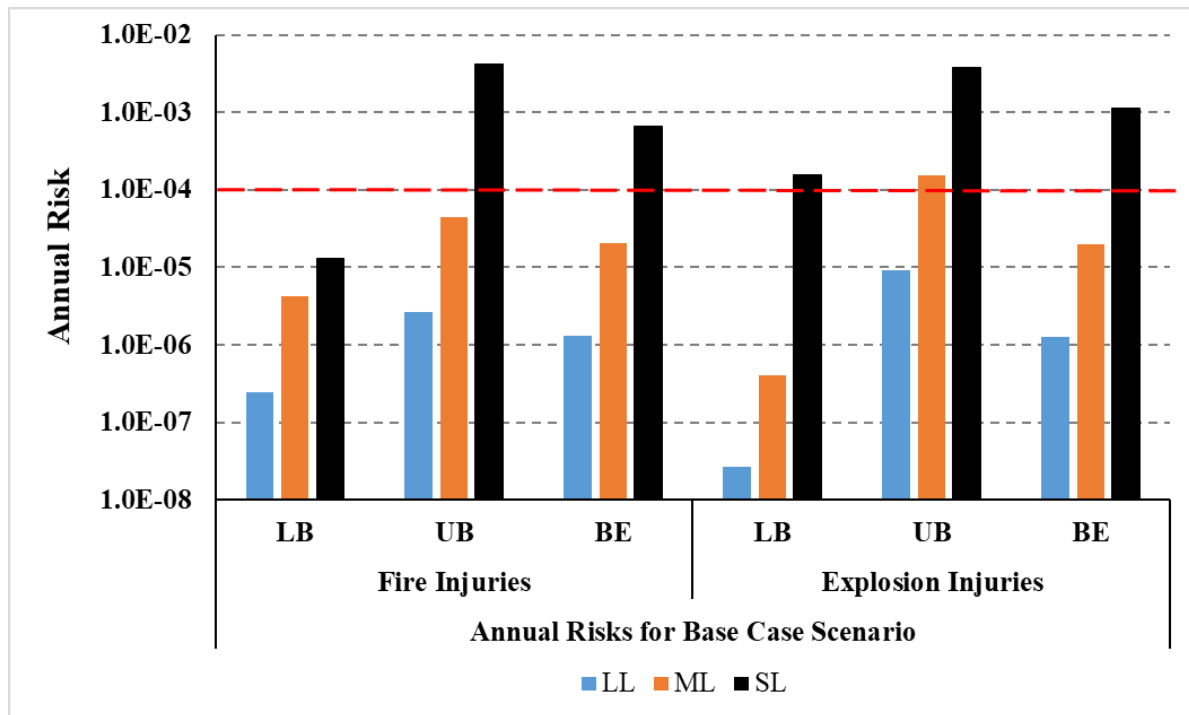


Fig. 4. Calculated annual risks of fire and explosion injuries for the base case scenario.
Note: the horizontal dashed line represents the occupation risk acceptance threshold of 1.0E-4/year.

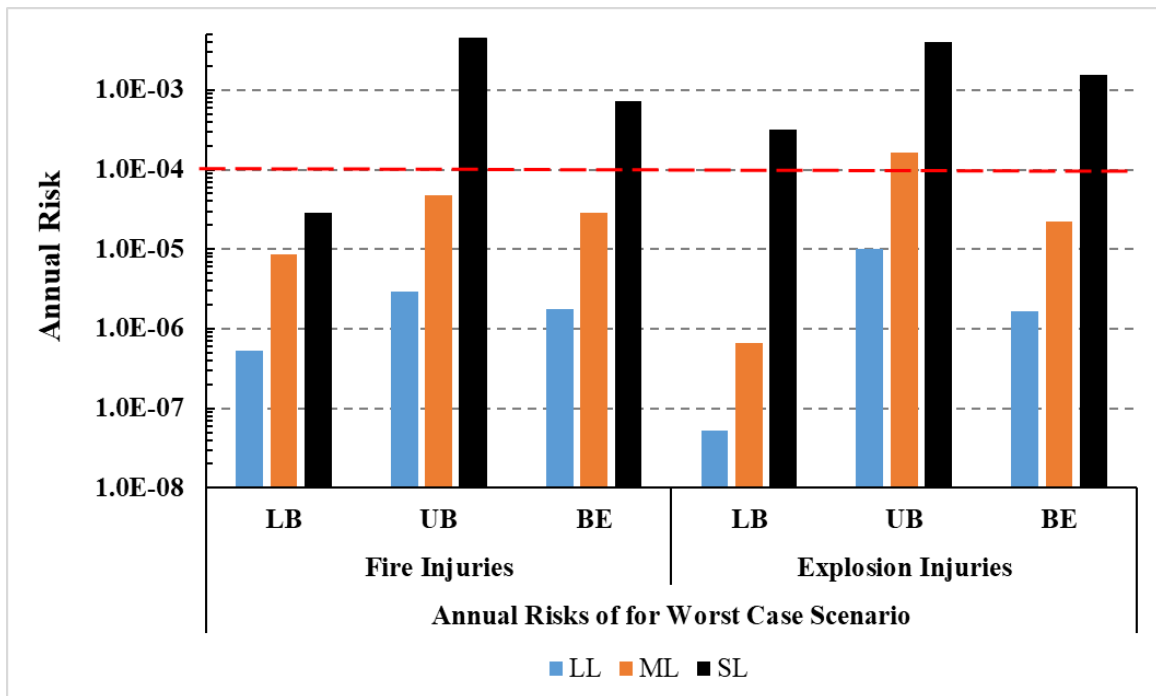


Fig. 5. Annual risks of fire and explosion injuries for the worst case scenario. *Note: the horizontal dashed line represents the acceptable occupational risk level of $1.0E-4$ /year.*

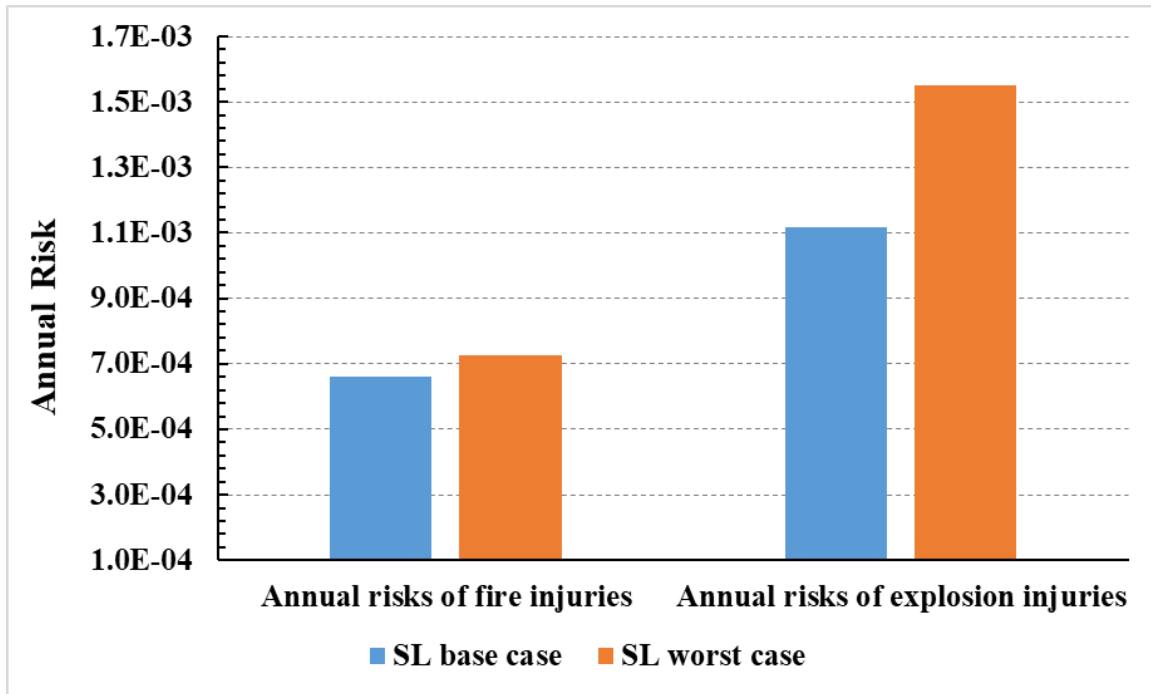


Fig. 6. Calculated annual risk of fire and explosion injuries for base case and worst-case small leak (SL) scenarios.

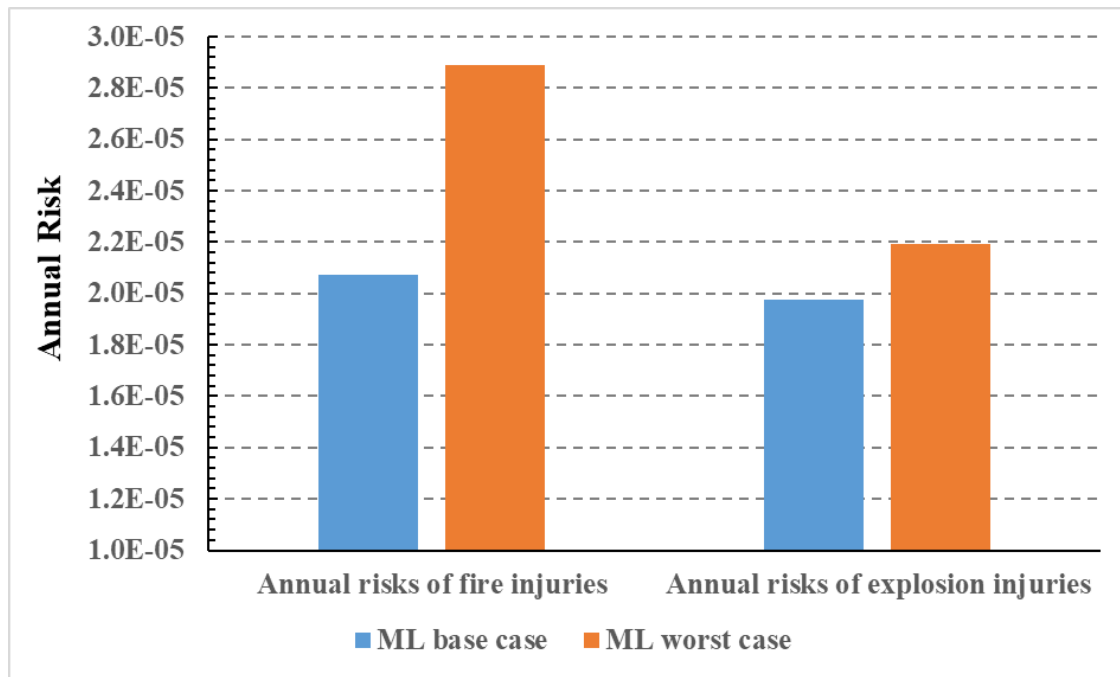


Fig. 7. Calculated annual risk of fire and explosion injuries for medium leak (ML) base case and worst-case scenarios.

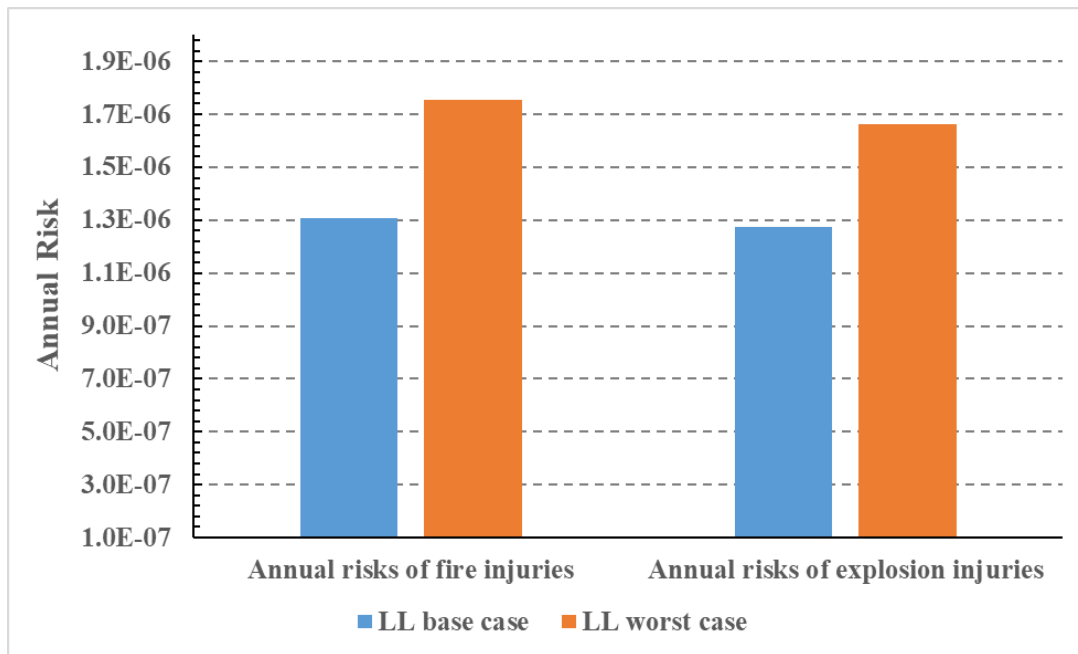


Fig. 8. Calculated annual risk of fire and explosion injuries for large leak (LL) base case and worst-case scenarios.

Table. 1. User-specified probability data (base case) as used in the HRS case study.

Model's Inputs	User-Specified Probabilities	Sources of probability data
<p>Leak type:</p> <p>Large leak (LL)</p> <p>Medium leak (ML)</p> <p>Small leak (SL)</p> <ul style="list-style-type: none"> The LL type represents catastrophic, instantaneous rupture of pressure boundaries of systems containing the flammable gas. Examples LL include compressed gas storage tanks and full-bore (i.e., double-ended guillotine) rupture in compressors' connecting pipes, etc. The ML and SL leak types represent gradual gaseous discharge over time from pipe connections, flanges, seals, valves, etc. 	<p>0.6%</p> <p>4.8%</p> <p>94.6%</p>	<ul style="list-style-type: none"> IAEA (1988). Cox et al. (1990). E&P Forum (1992). Spencer and Rew (1996). Purple Book (1999). Lees (1006). Spencer and Rew (1997). Daycock and Rew (2004). Energy Institute (2006). LaChance (2008; 2009). Zhiyong et al. (2010). HSE (2012). Sun et al. (2014). Sakamoto et al. (2016).
Fire or explosion event given ignition of formed gas cloud.	40%	
Fire event given ignition of undetected SL.	80%	
<p>Presence of a qualified ignition source (IS) in the confined space.</p> <p>A qualified ignition source means:</p> $E_{IS} \geq (MIE)_{\text{Flammable gas-air-mixture}}$	20%	
Fire event given ignition of LL	99%	
Explosion event given ignition of LL	1%	
LL detection in the confined space	90%	
Fire event given ignition of undetectable ML	80%	
Explosion event given ignition of undetectable ML	20%	
Personnel presence near the hazard source	30%	
Personnel injury given a fire event	50%	
Personnel injury given an explosion event	99%	

Table 2. User-specified (assumed) probability distribution functions.

Model Parameter	Assumed Probability Distribution Function
In <i>MainChart</i> (Fig. 1a): Flammable gas leak initiation time within the confined space.	<p>Weibull probability distribution function with $\beta = 2$ and $\eta = 24,000$ hours</p> <p>A function <code>rvm(WB(2, 2400))</code> returns a random time which is then checked against the user-specified mission time. If selected time is within the mission time, a value of 1 (signifying TRUE condition) is then passed on to the next step in the model to determine the leak type (SL, ML, or LL).</p>
In <i>MainChart</i> (Fig. 1a): Leak type (SL, ML, or LL)	<p>Leak type (SL, ML, or LL) is determined using a random variable (rv) selected from a uniform probability distribution (<code>rv_uniform(rand, 0, 1)</code>) in conjunction with the user-specified probability range for each leak type. In the uniform distribution, the argument '<i>rand</i>' is a random number generator.</p>
In <i>PersonnelInjured</i> Subroutine (Fig. 2): Number of personnel injured by fire (explosion) within the confined space.	<p>Normal distribution function with mean (μ) = 5 persons and standard deviation (σ) = 1 person</p> <p>The embedded function <code>rvm(NOR(5, 1))</code> returns a random value of the number of injured personnel, given a fire (or an explosion).</p>
In <i>Conditions Support Ignition</i> Subroutine (Fig. 3): Confined space mechanical ventilation failure time.	<p>Exponential distribution function with mean time between failure (MTBF) = 24,000 hours</p> <p>A random time to failure of the installed ventilation system in confined space is generated from the user-specified exponential probability distribution using the following embedded function: <code>rvm(EX2(1000, 0))</code></p> <p>If the determined time is within the specified mission time, a 1 (signifying TRUE) is passed to the next step in the model.</p>
<p>Conditional function <code>PF <= %</code></p> <p>This conditional function, which is one of RENO's internal functions, has been used in several steps defined in the proposed probabilistic model. The function draws a random number that is uniformly distributed (between 0 and 100) and then evaluates whether the value of the input variable to this function</p>	

Model Parameter	Assumed Probability Distribution Function
<p>is \leq the user-specified value for this variable. If the condition (TRUE), the function's output is 1 and if the condition is not met (FALSE), the output of this function is 0.</p> <p>For example, PF \leq% is used to check whether the specified probability of personnel presence near the hazard source is met. The function generates a random value and compares it against the specified probability value. If the condition is met, then 1 (signifying TRUE) is passed on the next step.</p>	

Table. 3. Description of sensitivity cases with selected model parameters.

Model Parameters	Probabilities ⁽¹⁾ for Sensitivity cases			Base Case Probability Distributions ⁽²⁾
	1	2	3	
P(H2 Detection)	5%	20%	5%	Triangular distribution: LB: 5% BE: 50% UB: 80%
P(Fire or Explosion Ignition)	20%	40%	20%	Triangular distribution: LB: 20% BE: 40% UB: 60%
P(Personnel Present near Hazard Source)	50%	30%	10%	Triangular distribution: LB: 10% BE: 30% UB: 50%
P(Fire Ignition)	15%	50%	15%	Triangular distribution: LB: 15% BE: 50% UB: 80%
P(Explosion Ignition)	85%	50%	85%	Triangular distribution: LB: 20% BE: 50% UB: 85%
P(Injuries Fire & Personnel Present near Hazard)	30%	50%	30%	Triangular distribution:

Model Parameters	Probabilities ⁽¹⁾ for Sensitivity cases			Base Case Probability Distributions ⁽²⁾
				LB: 30% BE: 50% UB: 70%
P(Injuries Explosion & Personnel Present near Hazard)	10%	50%	10%	Triangular distribution: LB: 10% BE: 50% UB: 99%

⁽¹⁾ The selected point estimate probabilities are based on published literature (data sources are provided in Table 1) as well as this author's knowledge as a subject matter expert on probabilistic risk assessment and hydrogen safety.

⁽²⁾ In HRS base case scenario, triangular probability distributions (as compared to single-point estimates) are used to generate the base case occupational risks of fire and explosion injuries.