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Risk-Based Approach - Consequence Analysis

An Introduction to Consequence Modeling and Identification of Outcomes from Loss of Containment Scenarios

An ioMosaic White Paper

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Abstract

The main purpose of the Consequence Analysis phase to be developed during the execution of a risk-based quantitative assessment is to answer the following question: “Which are the impacts of identified hazardous scenarios?” This step is critical for estimating reliable and accurate effects/consequences from Loss of Containment scenarios (LOCs), avoiding unrealistic results that would directly impact on the decision-making process. Additionally, it is essential that Consequence Analysis includes the identification and quantification of ALL potential outcomes that a hazardous release may cause. Event Tree Analysis (ETA) methodology is a valuable tool for identifying all these potential outcomes.

The present paper introduces the consequence analysis step by providing guidance on consequence modeling (i.e., source term characterization, dispersion of harmful gases/vapors, fires and explosions) and criteria for event trees development.

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Introduction

Consequence Analysis is formally defined as the study intended to determine the extent of consequences and effects from a given set of episodic events. An episodic event is an undesired incident or event with potentially serious consequences that occurs without warning and/or over a relatively short period of time. For example, tank and vessel failures, automobile crashes, fires, explosions and earthquakes are all considered events.

Consequences are usually stated in an expected number of injuries, casualties or in some cases, exposure to certain levels of energy or concentrations of substances. Consequence analysis results are estimates of the statistically-expected exposure of the target population to the hazard of interest and the safety/health effects related to that level of exposure. These estimates customarily use average meteorological conditions and population distribution and may include mitigating factors, such as evacuation and sheltering. Therefore, a substantial empirical database exists on the effects of fires and explosions regarding structures and equipment **[1]**.

Meanwhile, sophisticated models and correlations have been developed for consequence analysis, e.g., SuperChems™ **[2]**, providing valuable tools for the characterization of the source of the release of material or energy associated with the hazard being analyzed. They estimate the transport of the material and/or the propagation of the energy in the environment to a target of interest, identify the effects of the propagation of the energy or material on the target of interest and quantify the health, safety, environmental, or economic impacts on the target of interest. However, note that the consequence estimates can have very large uncertainties (e.g., frequency analysis). Estimates that vary by orders of magnitude can result from:

- Basic uncertainties in chemical/physical properties of the hazardous mixture
- Differences in average vs. time-dependent meteorological conditions
- Uncertainties in the release, dispersion, and effects models

For this reason, clearly defining the main purpose, scope of work and objectives of the risk-based quantitative assessment to be developed is extremely important. Based on this information, computing tools, criteria and efforts will be defined accordingly by establishing the number of different accident scenarios under scope, the number of effects the accident sequence produces and the detail with which the release, dispersion and effects on the targets of interest are estimated.

Figure 01 illustrates a simplified risk management program flowchart and the consequence analysis step is highlighted.

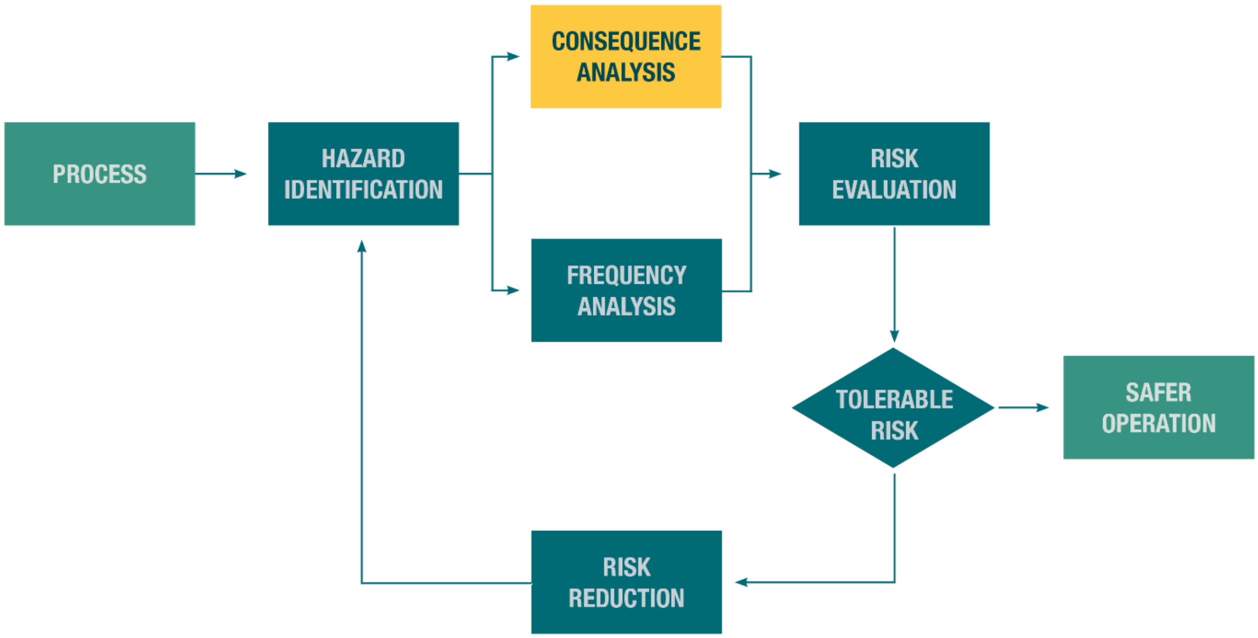

Figure 01: Risk Management Program Simplified Flowchart

The consequence analysis step for a complete risk management program aims to answer the following question: ***"Which are the impacts of identified hazardous scenarios?"*** This step is critical for estimating in a reliable and accurate way the effects and consequences, while avoiding unrealistic results that would directly impact on the decision-making process.

Consequence modeling involves the computational simulation of complex phenomena using sophisticated models. Conservatism in model application can be both friend and foe in developing solutions to real problems. The best approach is to use the most up-to-date and accurate models known **[3]**.

The present paper introduces a comprehensive approach for modeling the consequences of complex episodic phenomena. It is highlighted that treatment of the fundamentals of chemistry, physics and thermodynamics are of key importance in model formulation. Furthermore, the basic aspects of meteorology that affect episodic phenomenological consequences have to be addressed.

Finally, source term, treatment of the modeling of dispersion, fires and explosions have to be accurately characterized. Detailed information and criteria on advanced consequence modeling can be found in **[2]** and **[3]**.

Loss of Containment Scenarios, Damage Criteria and Consequences

Episodic events involving the Loss of Containment (LOCs) of hazardous materials are the focus of the consequence models to be considered during the development of a risk-based quantitative analysis. The primary areas of consequence are dispersion of a harmful vapor, fire and explosion. Each can occur in various forms and it is important to understand each type. All the cited primary areas of consequence have to be firstly characterized by source term models **[3]**.

Note that specific information on how to identify LOCs during the execution of a risk-based quantitative analysis can be found in **[4]**.

Introduction to Damage Criteria

When developing a risk-based quantitative assessment, there are mainly three damage criteria to be considered: toxic, thermal and overpressure. To evaluate toxic hazards, the impact criteria can be based on one or more of the following: percent fatality contours (probits), dosage levels and concentration levels. For thermal radiation hazards, the damage criteria can be specified by using probits, heat flux values, or time integrated heat flux (thermal dose) values. The damage caused by explosion can be defined by peak overpressure values, impulse values and probits. If a chemical has multiple hazards, e.g., flammability and toxicity, the models will determine the impact for each of the criteria separately. Therefore, there are mainly two different approaches for damage criteria: the probit analysis and well-known thresholds or doses. Further information on damage criteria for toxic, thermal radiation and overpressure hazards can be found in **[5]**.

Probit Analysis

A popular method that is used to relate level of injury and exposure to a hazardous event of a given intensity is probit analysis (also referred to as vulnerability analysis). The use of probits or vulnerability models is recommended for risk-based quantitative assessment studies. When coupled with probits, consequence models can associate a probability of fatality (or of receiving a dangerous dose) or building damage with a specific hazard zone or isopleth. In a typical risk-based quantitative analysis, multiple contours are produced at probabilities ranging from 5 or 10% to 100% for a specific hazard outcome. A probit function (probability unit, Y) is a normally distributed random variable with a mean of 5 and a standard deviation of 1. The mortality response (percent fatality) is expressed as:

$$P = \frac{1}{\sqrt{2\pi}} \int_{-inf}^{Y-5} exp - \left(\frac{u^2}{2}\right) du = \frac{1}{2} + \frac{1}{2} erf\left(\frac{Y-5}{\sqrt{2}}\right)$$

Where Y is given by:

$$Y = A + B \ln D$$

$\boldsymbol{Y}$: Probit; i.e., value range 2.67 – 8.09 representing 1 – 99.99% fatality. It is a measure of the percentage of the vulnerable resource that might sustain damage. Fatality probability can then be determined by evaluation of $\boldsymbol{Y}$ on a probit transformation. For example:

- 1% fatality corresponds to a probit value $\boldsymbol{Y}$ equivalent to 2.67
- 25% fatality corresponds to a probit value $\boldsymbol{Y}$ equivalent to 4.33
- 50% fatality corresponds to a probit value $\boldsymbol{Y}$ equivalent to 5.00
- 75% fatality corresponds to a probit value $\boldsymbol{Y}$ equivalent to 5.67
- 99.9% fatality corresponds to a probit value $\boldsymbol{Y}$ equivalent to 8.09

These values are based on the relationship between fatality and the probit function, illustrated in **Table 01** and based on Finney **[6]**

Table 01: Relation Between Fatality and Probit

%	0	1	2	3	4	5	6	7	8	9
0	-	2.67	2.95	3.12	3.25	3.36	3.45	3.52	3.59	3.66
10	3.72	3.77	3.83	3.87	3.92	3.96	4.01	4.05	4.08	4.12
20	4.16	4.19	4.23	4.26	4.29	4.33	4.36	4.39	4.42	4.45
30	4.48	4.50	4.53	4.56	4.59	4.61	4.64	4.67	4.69	4.72
40	4.75	4.77	4.80	4.82	4.85	4.87	4.90	4.92	4.95	4.97
50	5.00	5.03	5.05	5.08	5.10	5.13	5.15	5.18	5.20	5.23
60	5.25	5.28	5.31	5.33	5.36	5.39	5.41	5.44	5.47	5.50
70	5.52	5.55	5.58	5.61	5.64	5.67	5.71	5.74	5.77	5.81
80	5.84	5.88	5.92	5.95	5.99	6.04	6.08	6.13	6.17	6.23
90	6.28	6.34	6.41	6.48	6.55	6.64	6.75	6.88	7.05	7.33
%	**0.00**	**0.10**	**0.20**	**0.30**	**0.40**	**0.50**	**0.60**	**0.70**	**0.80**	**0.90**
99	7.33	7.37	7.41	7.46	7.51	7.58	7.65	7.75	7.88	8.09

The values $\boldsymbol{A}$ and $\boldsymbol{B}$ are constants which depend on the toxic chemical (when the probit equation applied to address toxic dispersions) or on the level of damage due to fires or explosions. Finally, the parameter $\boldsymbol{D}$ is defined as the hazard dose, the product of intensity or concentration of received hazardous agent to an exponent n and the duration of exposure in seconds or minutes:

- The hazard dose of an airborne toxic gas on humans depends on the concentration of the toxic gas in the air being inhaled and the length of time an individual is exposed to this concentration. For toxic gas $\boldsymbol{D}$ equals the product of gas concentration to an exponent n and time in minutes. Concentration can be reported in parts per million (ppm) or milligrams per cubic meter ($mg \cdot m^{-3}$)

- The hazard dose of fire on humans depend on the rate at which heat is transferred from the fire to the individual and the time the person is exposed to the fire; i.e., Thermal Dose [$(kW \cdot m^{-2})^{4/3} \cdot s$]; $D = I^{4/3} t$

- The hazard dose of explosions on humans depends on the peak overpressure that reaches the individual and the explosion phase duration. Both parameters define the impulse of the explosion. For explosions, $\boldsymbol{D}$ equals the overpressure or impulse, where the impulse is approximately equal to half of the product between overpressure and duration

A summary of probit correlations for a variety of exposures is illustrated in **[7]**. **Table 02** list the most valuable probit criteria used during a risk-based quantitative assessment by type of hazard.

Note that there are many published probits for estimating fatality levels from exposure to harmful agents. Reference **[5]** provides most of worldwide recognized criteria.

Table 02: Summary of Probit Correlations

Type of Injury or Damage	D	A	B	Comments	Source
Fire – Burn deaths from flash fire	$t_e {I_e}^{4/3}/10^4$	-14.9	2.56	t_e: effective time duration [s] I_e: effective radiation intensity [kW·m^{-2}]	**[8]**
Fire – Burn deaths from pool burning	$tI^{4/3}/10^4$	-14.9	2.56	t: time duration of pool burning [s] I: radiation intensity from pool burning [kW·m^{-2}]	**[8]**
Explosion – Deaths from lung hemorrhage	p^0	-77.1	6.91	p^0: peak overpressure [N·m^{-2}]	**[8]**
Explosion – Eardrum ruptures	p^0	-15.6	1.93	p^0: peak overpressure [N·m^{-2}]	**[8]**
Explosion – Deaths from impact	J	-46.1	4.82	J: impulse [N·s·m^{-2}]	**[8]**
Explosion – Injuries from impact	J	-39.1	4.45	J: impulse [N·s·m^{-2}]	**[8]**
Explosion – Injuries from flying fragments	J	-27.1	4.26	J: impulse [N·s·m^{-2}]	**[8]**
Explosion – Structural damage	p^0	-23.8	2.92	p^0: peak overpressure [N·m^{-2}]	**[8]**
Explosion – Glass breakage	p^0	-18.1	2.79	p^0: peak overpressure [N·m^{-2}]	**[8]**
Toxic Release – Ammonia deaths	$\sum C^{2.0}T$	-35.9	1.85	C: concentration [ppm] T: time interval [min]	**[9]**
Toxic Release – Chlorine deaths	$\sum C^{2.0}T$	-8.29	0.92	C: concentration [ppm] T: time interval [min]	**[9]**
Toxic Release – Phosgene	$\sum C^{2.0}T$	-19.27	3.69	C: concentration [ppm] T: time interval [min]	**[9]**

Probit: $Y = A + B \ln D$

Well-Known Thresholds or Doses

The probit approach is one way of estimating the level of fatality for exposure to a hazardous agent and an alternative is the application of well-known thresholds or doses. Examples of those are the following when addressing toxic agents:

- **SLOT**: Specified Level of Toxicity
- **SLOD**: Significant Likelihood of Death
- **IDLH**: Immediate Dangerous to Life or Health
- **ERPG**: Emergency Response Planning Guidelines
- **AEGL**: Acute Exposure Guideline Levels

Other thresholds and dose definitions for toxic agents are available in the related bibliography **[3]**. Additionally, specific human vulnerability and structure damage criteria related to fires and explosions are available. Specific damage criteria for toxic agents, fires and explosions are out of the scope of this paper and a dedicated reference has been developed by ioMosaic Corporation with specific and detailed damage criteria **[5]**.

Atmospheric and Site Information

The definition of site properties and meteorological conditions should be addressed during the development of a risk-based quantitative assessment. This information includes the ambient conditions such as relative humidity, ambient air water, data pertaining to water temperature, mean flow velocity and depth. Geographic site location should also be defined, which translates to the respective latitude, longitude, altitude and time zone factor.

Additionally, values defining the extent of cloud cover, visual range, terrain roughness, atmospheric stability, wind velocity, wind speed reference height and lapse rate values have to be considered. The following key parameters are introduced with the aim to provide basic criteria for their definition: visual range, terrain roughness and atmospheric stability.

The visual range is the distance at which an observer can detect the contrast between an object and its surroundings. The extent of visibility can range from several kilometers on a very clear day to a few hundred meters on a foggy day **[3]**. Environmental conditions such as relative humidity, temperature, time of day and air pollution all influence the visual range (see **Table 03**).

Table 03: Visual Range Values

Typical Condition	Visual Range Value [m]
Thin Fog	2,000
Haze	5,000
Clear	10,000
Very Clear	20,000

The terrain surface roughness contributes to mixing by causing boundary layer turbulence in a cloud dispersion and it also influences the wind speed profile **[3]** (see **Table 04**).

Table 04: Surface Roughness as a Function of Typical Surface

Typical Surface	Surface Roughness [m]
Water Surface	0.00001
Bare Soil	0.0005
Thick Grass, 1 cm high	0.001
Thick Grass, 5 cm high	0.01
Thick Grass, 50 cm high	0.50
Flat land with few trees	0.03
Airfield, arable land, polder with many tree	0.10
Cultivated land, glasshouse area, scattered houses, open area	0.30
Dense but low buildings, wooded area, industrial site	1.00
City with high buildings, industrial area with high obstacles	3.00

The detailed meteorological data sets have to be consistent with the facility weather conditions. Meteorological stations located in the facility or in Airports close to the location under analysis are good sources of meteorological information to be processed and used during the risk-based quantitative analysis. Detailed meteorological data is analyzed using computer tools, e.g., SuperChems™ **[2]**, which includes a powerful meteorological data processor capable to reduce massive data to representative sets of meteorological conditions. For example, it can consider the most widely used atmospheric stability categories for dispersion analysis; i.e., Pasquill Stability Classes **[3]** (see **Table 05** and **Table 06**).

Table 05: Pasquill Atmospheric Classes

Atmospheric Stability Class	Letter Designation
Extremely Unstable Conditions	A
Moderately Unstable Conditions	B
Slightly Unstable Conditions	C
Neutral Conditions	D
Slightly Stable Conditions	E
Moderately Stable Conditions	F

Table 06: Meteorological Conditions that Define Pasquill Atmospheric Classes

Surface Wind Speed	Daytime Incoming Solar Radiation			Nighttime Cloud Cover	
$[m \cdot s^{-1}]$	Strong	Moderate	Slight	>50%	<50%
<2	A	A-B	B	E	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

Note: Class D applies to heavily overcast skies, at any wind speed day or night

Consequence Modeling

Source Term

Consequence modeling is conducted to quantify the effects and consequences of identified LOCs and it entails the characterization of the sources of release of material or energy associated with the hazard being analyzed and the quantification of the impacts on a target of interest. To model the consequences of these events, the source strength, duration and phase must be accurately determined. These quantities are functions of storage conditions and the thermo-physical properties of the chemical(s) in question and can be determined from fluid flow equations: (1) Pressurized/non-pressurized liquid discharge, (2) Gas discharge, (3) Two-phase flow, (4) Flash atomization and (5) Liquid rain-out. Accuracy from the consequence models is dependent upon accuracy in the source term computation. SuperChems™ **[2]** includes the most up-to-date source term models for precise and advanced calculations for pressure relief systems, flares and consequence analysis.

Dispersions of Harmful Chemicals

Among the models required for hazard assessments, vapor dispersion models are perhaps the most complex. This is primarily because of the varied nature of release scenarios as well as the varied nature of chemicals that may be released into the environment. In dispersion analysis, gases and two-phase vapor-liquid mixtures are divided into three general classes of materials: (1) positively buoyant, (2) neutrally buoyant and (3) negatively buoyant. These classifications are based on the density difference between the released material and its surrounding medium (air). They are influenced by release temperature, molecular weight, ambient temperature, relative humidity and the presence of aerosols **[3]**.

For vapor dispersion in the atmosphere, the released vapor may rise due to the buoyancy resulting from low molecular weight or high temperature, fall because of a heavy density, or move with the surrounding air as a neutrally buoyant material. The heavy density that causes a cloud to fall or stay close to the ground may result from a relatively high molecular weight or low temperature of the released material, or it may result from a two-phase aerosol/vapor mixture which behaves as a high-density vapor. Wind conditions can also influence heavy gas behavior.

Dispersion analysis is also a function of release modes. They are usually divided into the following categories:

- Instantaneous release (puff)
- Continuous release (plume)
- Momentum-dominated continuous release (jet)
- Time-dependent continuous releases (jet/plume)

Each release mode introduces its own characteristics on the subsequent dispersion. For instance, a momentum-dominated jet will dilute much faster than a plume within a short distance of its source. In addition to the effects of initial release density, the presence of aerosols, release rate/quantity, release duration, release mode and dispersion analysis also depends on:

- Prevailing atmospheric conditions
- Limiting concentration
- Elevation of the source
- Surrounding terrain
- Source geometry

Limiting concentration, which is used to define cloud boundary, affects the dispersion distance inversely. Lower concentrations lead to larger dispersion distances. As with the source release rate, the effect is not linear. For example, a reduction factor of 10 in the limiting concentration usually doubles the dispersion distance.

Elevation of the source is attributed to the physical height of the source above ground (such as a tall stack). In general, the effect of source height is to increase dispersion in the vertical direction (since it is not ground-restricted) and reduce the concentration at ground level.

Numerous dispersion models have been published over the last three decades. Excluding jet dispersion, these models can be divided into three general classes:

- Gaussian models
- Heavy-gas box, refined box and slab models
- 3-D hydrodynamic models

The Gaussian models are simple and valid for releases of non-buoyant materials in a uniform flow field with no obstacles. The box models represent a macroscopic approach to heavy-gas dispersion. They possess empirical features and could be of questionable reliability under some release conditions. Box or refined-box models are not capable of handling terrain or the presence of obstacles. Three-dimensional models can handle complex cases with less empirical features. They require the solution of multi-dimensional, partial differential equations **[3]**.

Fires and Thermal Radiation

Fire hazards can take many forms. Building fires have been researched for many years and effective detection and protection systems are available for most occupied structures. However, this type of fire is not the most frequent or important when examining process or transportation activities. In these cases, loss of containment incidents can produce either sustained or highly transient destructive fires **[3]**. These fire types include:

- Large pool fires, usually accompanied by copious amounts of dense smoke
- Flame jets, characterized by a momentum dominated release and high levels of thermal radiation resulting from well mixed combustion
- Fireballs resulting from the rapid involvement of a large amount of flammable material, also characterized by high levels of thermal radiation
- Vapor cloud fires, wherein a flame front propagates (relatively slowly) through a flammable vapor cloud without producing significant overpressures

Explosions and Overpressure

Explosion hazards also can take different forms. The more common types include vented enclosure explosions, vapor cloud explosions, condensed phase explosions and exploding vessels **[3]**:

- The first three involve combustion of the released material and the phenomenon may be a deflagration, a detonation, or a transition from a deflagration to a detonation
- Condensed phase explosions usually involve high explosives that detonate and are characterized by very high overpressures near the epicenter of the explosion
- Vapor cloud explosions on the other hand usually have fairly low overpressures near the point of cloud ignition, but can develop high overpressures characteristic of rapid deflagrations or detonations
- The exploding vessel terminology is used to describe the rupture of an over-pressurized vessel. The material inside does not need to be flammable and if it is, does not need to be involved in combustion. The overpressure causing rupture may be produced, for example, by temperature rise from an external fire or runaway reaction, regulator failure, compressor malfunction, instrument failure, etc.

Some episodic events involve more than one type of phenomenological consequence, e.g., a BLEVE (Boiling Liquid Expanding Vapor Explosion) of a vessel containing a flammable liquid, which is accompanied by both a radiating fireball and vessel rupture. Accordingly, the identification of all potential outcomes that could lead to a LOC should be addressed.

Appendix I provides a brief description of the most used and validated mathematical models used for advanced consequence modeling:

- SuperChems™ software tool **[2]**

Outcomes Identification

It is critical that consequence analysis includes the identification and quantification of ALL potential outcomes that a hazardous release may cause. The Event Tree Analysis (ETA) methodology is a valuable tool for identifying all potential outcomes. For example, an unmitigated line release of ethylene oxide could lead (depending on the specific conditions) to a pool fire, a jet fire, a dispersed vapor cloud, or a vapor cloud explosion. The development of ETAs requires taking into account conditional probabilities of immediate ignition, probabilities and location of potential delayed ignition sources, mitigation measures such as presence of deluge systems, fire and gas detectors, etc.

Event Tree Analysis (ETA)

Event Tree Analysis (ETA) is an inductive methodology which uses a graphical representation for describing (i.e., qualitative and/or quantitative) all possible outcomes of a single LOC. The technique is able to identify the scenario sequence from the cause to the final impacts according to enabling events (e.g., safeguards, layers of protection) or conditions (e.g., presence of ignition sources). **Figure 02** illustrates a generic event tree example.

It is important to mention that the ETA methodology is valid for the identification of all potential outcomes of a given LOC and is also advantageous for estimating the final outcomes frequencies of occurrence when a risk-based quantitative assessment is developed. The following parameters have to be characterized:

- Frequency of occurrence of the LOC under analysis
- Probabilities of success of conditions, enabling events considered in the event tree

Frequencies of occurrence of LOCs and probabilities of success of conditions enabling events are out of the scope of this paper and detailed information and criteria can be found in reference **[10]**.

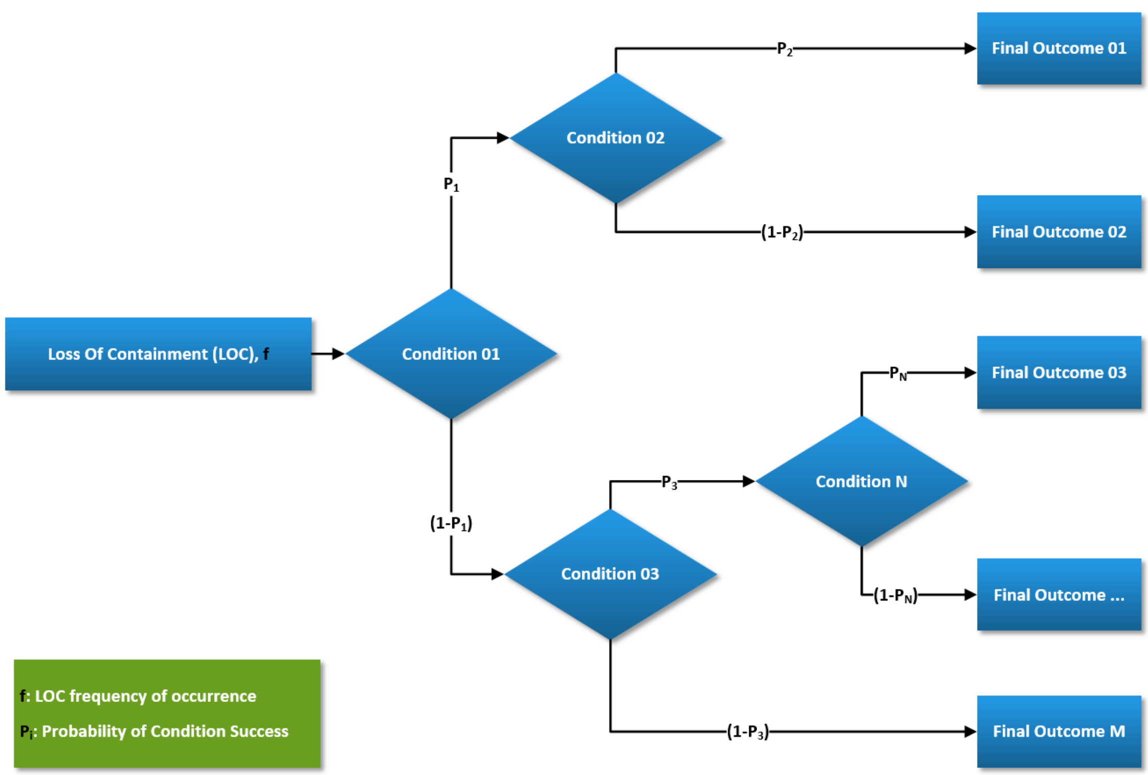

Figure 02: Generic Event Tree Structure Example

As an illustrative example of event tree development, consider a release of refrigerated LNG from a large vessel. The following scenario outcomes should be considered (see **Figure 03**):

- The formation of a liquid pool which spreads and vaporizes as a function of time
- If ignition is immediate, the pool results in a pool fire and thermal hazard radiation footprints are established
- If ignition is delayed, the pool vaporizes and leads to the formation of a flammable cloud. If ignition is encountered downwind, the vapor cloud can ignite and burn back to the source in the form of a vapor cloud fire and, if the release is still continuing, will cause a pool fire
- If the flame encounters turbulence or significant blockage as it burns back to the source, an unconfined / semi-confined vapor cloud explosion can result

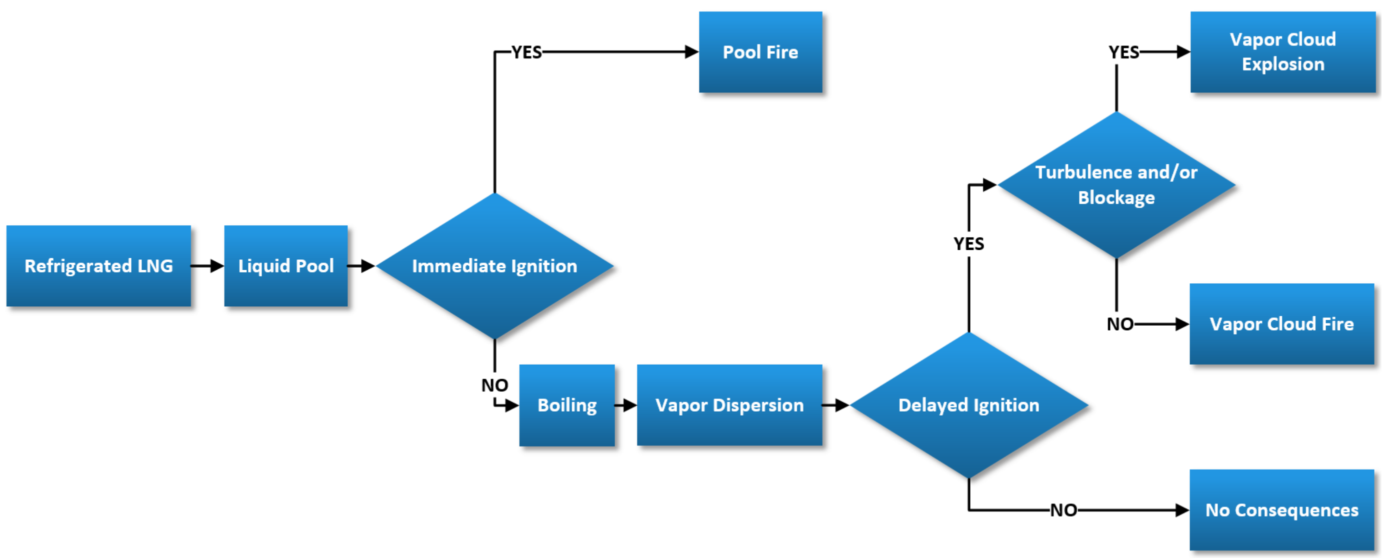

Figure 03: LNG LOC Event Tree Example

Appendix II provides generic event trees for typical LOCs leading to fire and flammability hazards, vapor dispersion hazards and explosion hazards assuming the material released is both toxic and flammable. The illustrated event trees mainly represent the following four (4) typical types of LOCs:

- Finite duration liquid spill at or below its bubble point at atmospheric pressure
- Finite duration release of a subcooled, saturated, or two-phase liquid at a temperature above its bubble point at atmospheric pressure
- Finite duration release of a gas/vapor from a vessel/source containing gas or a two-phase mixture
- Catastrophic failure of a vessel containing a two-phase/saturated liquid or gas/vapor under pressure

The availability of these event trees in consequence analysis allows the user to perform efficient sensitivity and what-if analyses as well as mitigation effectiveness assessment. For example, the SuperChems™ **[2]** tool helps automatically conduct this analysis in an effective and efficient time manner.

Conclusions

Episodic events involving Loss of Containment (LOCs) of hazardous materials are the focus of the Consequence Analysis step to be developed during the execution of a risk-based quantitative assessment. The primary areas of consequence are dispersion of a harmful vapor, fire and explosion.

The main purpose of the Consequence Analysis phase to be developed during the execution of a risk-based quantitative assessment is to answer the following question: "Which are the impacts of identified hazardous scenarios?" This step is critical for estimating reliable and accurate effects/consequences from Loss of Containment scenarios (LOCs), avoiding unrealistic results that would directly impact on the decision-making process. Additionally, it is essential that Consequence Analysis includes the identification and quantification of ALL potential outcomes that a hazardous release may cause. The Event Tree Analysis (ETA) methodology is a valuable tool for identifying all these potential outcomes.

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Appendix I: Mathematical Models for Consequence Analysis

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Table I.01: Source Term Modeling

Source Term Models	Description / Purpose
Droplet Evaporation / Trajectory	The model simulates the trajectory and behavior of a droplet. This model is often used in conjunction with the Two-phase jet dispersion model to calculate rainout.
Gas / Vapor Expansion	The model simulates the behavior of the gas release in the zone just after the material is released from containment. It performs the necessary calculations to drop the pressure from the release pressure to the atmospheric pressure. Note that this model works alongside the gas jet dispersion model. When the gas jet dispersion model is submitted, it automatically runs this model if the release pressure is higher than ambient.
Liquid Pool	The model integrates spill liquid spreading and dynamic evaporation of material from the liquid pool. As the spilled liquid spreads over the surrounding surface, it evaporates or exhibits boil-off/vaporization. Emission rates from spilled liquids depend upon their volatility, composition, meteorological / ambient conditions, storage conditions, spill geometry, etc. For liquids with high boiling points, the emission rate is a strong function of solar heat flux and convective heat transfer from the atmosphere. For liquids with low boiling points, such as most liquefied gases, the emission rate is normally driven by the rate of heat transferred from the spill surface by conduction.
Steady Liquid Flow from Pipes	The model enables advanced simulation of liquid steady flow. Practical applications range from piping flow capacity calculation to piping network and headers simulation.
Steady Liquid Flow from Headers	This model performs liquid header rating calculations. It analyzes all the lines connecting and feeding to the header. Note that each line connecting and feeding the header requires the user to create a separate scenario. The user must then rate the piping layout associated with that scenario for two-phase, gas phase and/or liquid flow.
Steady Gas / Vapor Flow from Pipes	The model enables advanced simulation of gas steady flow. Practical applications range from piping flow capacity calculation to piping network and headers simulation.
Steady Gas / Vapor Flow from Headers	The model performs gas header rating calculations. It analyzes all the lines connecting and feeding the header. Note that each line connecting and feeding the header requires the user to create a separate scenario. The user must then rate the piping layout associated with that scenario for two-phase, gas phase and/or liquid flow.
Steady Two-Phase Flow from Pipes	The model enables advanced simulation of two-phase steady flow. Practical applications range from piping flow capacity calculation to piping network and headers simulation.
Steady Two-Phase Flow from Headers	The model performs two-phase header rating calculations. It analyzes all the lines connecting and feeding the header. Note that each line connecting and feeding the header requires the user to create a separate scenario. The user must then rate the piping layout associated with that scenario for two-phase, gas phase and/or liquid flow.
Two-Phase Expansion / Aerosol Formation	The model simulates the behavior of the two-phase release in the zone just after the material is released from containment. It performs the necessary calculations to drop the pressure from the release pressure to the atmospheric pressure.
Vessels Containing Liquids	The model simulates the time varying releases from vessels containing liquids. Its main application is for non-flashing releases from atmospheric or near atmospheric storage tanks.
Vessels Containing Gases / Vapors	The model enables advanced dynamic simulation of vessels containing gases/vapor. This includes supercritical flow where fluid temperature is at or higher than its critical point.
Vessels Containing Two-Phases	The model enables advanced simulation of vessels containing two-phases, a liquid and a vapor phase. This model fully supports the DIERS two-phase technologies including the DIERS coupling equation as evident when appropriate flow types (such as churn turbulent and bubbly flows) and disengagement parameters are specified.

Table I.02: Dispersion Modeling

Dispersion Models	Description / Purpose
Continuous Heavy Gas with Aerosol Effects	The model simulates the dispersion of a continuous release of a gas that is heavier than air. It is suitable for modeling low momentum release.
Finite Duration Gaussian	The model simulates the dispersion of a neutrally buoyant material based on Gaussian dispersion. It is best suited for low momentum releases to provide quick estimates.
Indoor Dispersion	The model calculates concentration variations of airborne toxic and flammable materials within indoor compartment(s) and the surrounding. It handles multiple compartments and is able to process inlet streams as well as gas releases from other source-term models. All mass and energy balance-including those contributed from natural ventilation-are accounted for. Air infiltration is also considered.
Instantaneous Heavy Gas with Aerosol effects	The model simulates the dispersion of an instantaneous release of a gas that is heavier than air. It is suitable for modeling low momentum release. The model assumes the cloud mass is known.
Integrated Transient Gaussian Puff	The model is used to simulate the effect of Gaussian dispersion of a series of releases of different source strengths and geometries. It can be thought of as a series of Finite duration Gaussian runs. The model is useful for modeling the dispersion of neutrally buoyant, low momentum and time-varying releases.
Gas Jet Dispersion	The model simulates the dispersion behavior of a gas release, which results in the formation of a jet. It is generally suitable for modeling high pressure releases. Gas expansion model is automatically activated if release pressure is higher than ambient pressure. If the gas jet hits ground, dispersion calculations automatically switch to the Gaussian model.
Plume Rise	The model simulates the momentum or buoyancy rise of gases leaving stacks at velocities higher than that of the surrounding air or at densities lower than that of ambient air. Its primary purpose is to estimate the effective release height before the plume is entrained with air.
SLAB Model	The SLAB model (developed by US department of Energy and supported by the USAF Engineering and Services Center and American Petroleum Institute) was designed to simulate the atmospheric dispersion of denser-than-air releases. The types of releases treated by the model include a ground-level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet and an instantaneous volume source. Except for the evaporating pool source, which is assumed to be vapor, all the remaining sources may be either pure vapor or a mixture of vapor and liquid droplets.
Two-Phase Jet Dispersion	This model simulates the dispersion behavior of a two-phase release, which results in the formation of a jet. It is generally suitable for modeling high pressure releases. Two-phase expansion model is automatically activated if release pressure is higher than ambient pressure. If the two-phase jet hits the ground, dispersion is automatically switched to the Gaussian model.
Water Sprays / Curtains	This model calculates the effect of water spray/curtain mitigation on releases. It calculates both the dilution effects due to mixing and the solubility effects. This model integrates with the Gaussian model to perform relative effectiveness of the toxic impacts to user-specified limiting concentration.

Table I.03: Fire Modeling

Fire Models	Description / Purpose
Fireball	The model simulates the effects of fireballs, which occur following immediate ignition of instantaneous vessel failures containing flammable materials. They are typically observed following a Boiling Liquid Expanding Vapor Explosion (BLEVE) caused by external fires. Since fireballs are a time-dependent phenomenon, it is useful to also look at the thermal radiation dosage in addition to the thermal radiation levels.
Gas Flame Jet and Flare	The model simulates the thermal effects due to a jet fire, which occurs following the ignition of a flammable gas or flare release. It is generally suitable for modeling high pressure releases. Gas expansion model is automatically activated if release pressure is higher than ambient pressure.
Pool Fire	The model simulates the thermal effect due to a pool fire, which occurs when a liquid pool is ignited following a spill on land or water. It is directly integrated with the Liquid pool model. The model assumes that the ignition takes place after the liquid discharge duration. The pool ignition time and spreading behavior are key parameters to be defined.
Two-Phase Flame Jet	This model simulates the thermal effects due to a jet fire, which occurs following the ignition of a flammable two-phase release. It is generally suitable for modeling high pressure releases. Two-phase expansion model is automatically activated if release pressure is higher than ambient pressure.
Vapor Cloud Fire	This model predicts the zone of hazard for fire by dispersing the released material to specified limiting concentrations. It uses Gaussian dispersion model to estimate the fire hazard zone. Model assumptions and data inputs are essentially the same as those required in the Gaussian model.

Table I.04: Explosion Modeling

Explosion Models	Description / Purpose
Vessel Burst	The model estimates the overpressure footprint cause by vessel rupture / PV energy.
Fragments / Projectiles Trajectory	The model calculates the distance and path to which a vessel fragment would travel as a result of a vessel explosion. It is particularly useful for incident investigations and estimating safe separation distances.
Vented Deflagrations (Semi-Confined Deflagrations / Transient)	The model calculates the effects of fuel-oxidizer explosive reactions in enclosures. The Metghalchi and Keck model is used to calculate burning velocities
Vapor Cloud Explosion: Baker-Strehlow	The model uses a series of curves generated by Strehlow (1979) during numerical studies to analyze the structure of blast waves generated by both constant-velocity and accelerating flames propagating in a spherical geometry.
Vapor Cloud Explosion: TNT Equivalence	The model calculates the effects of an explosion by establishing an equivalent "TNT yield" for the vapor cloud explosion.
Vapor Cloud Explosion: TNO Shockwave Model	The model calculates the effects of an explosion by using the TNO shockwave method; i.e., the cloud is assumed hemispherical, homogenous in composition and centrally ignited. The formation of the shock wave is caused by expansion of the cloud following due the energy addition by combustion.
TNO Multi-Energy Method	The Multi-Energy Explosion method treats a vapor cloud explosion as a number of sub-explosions. These sub-explosions are centered on parts of the cloud that are either in intensely turbulent motion or are partially confined or obstructed.
Hugoniot and One-Dimensional Flow with Chemical Reactions	Automated method for calculating an entire Hugoniot using direct Gibbs free energy minimization.

Appendix II: Outcomes Identification – Generic Event Trees

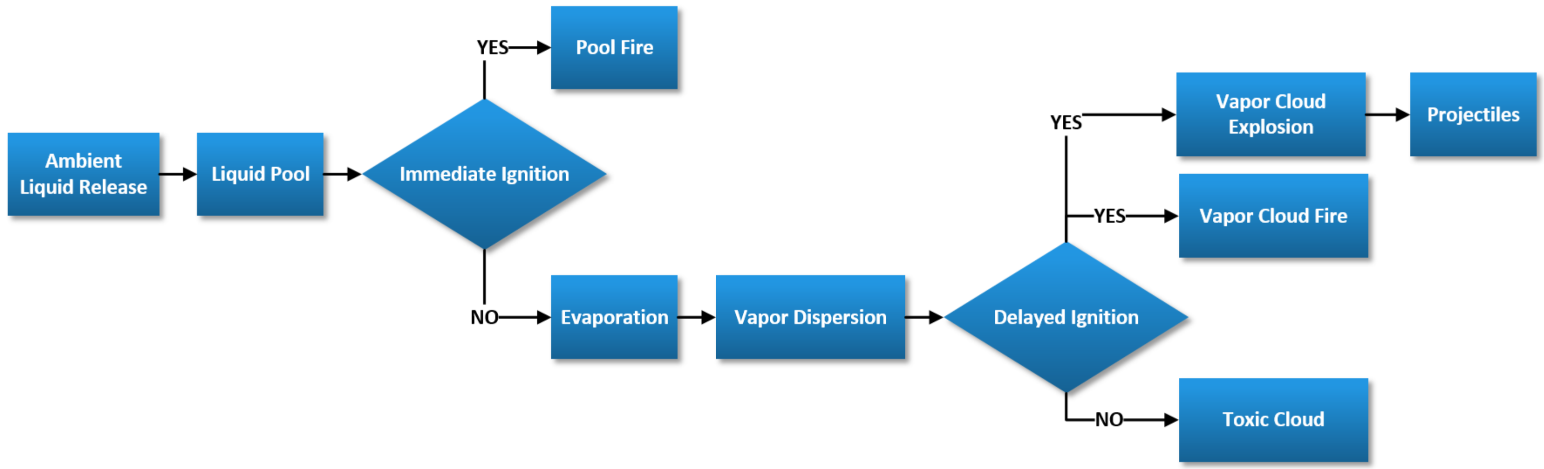

Figure II.01: Ambient Liquid Release Event Tree

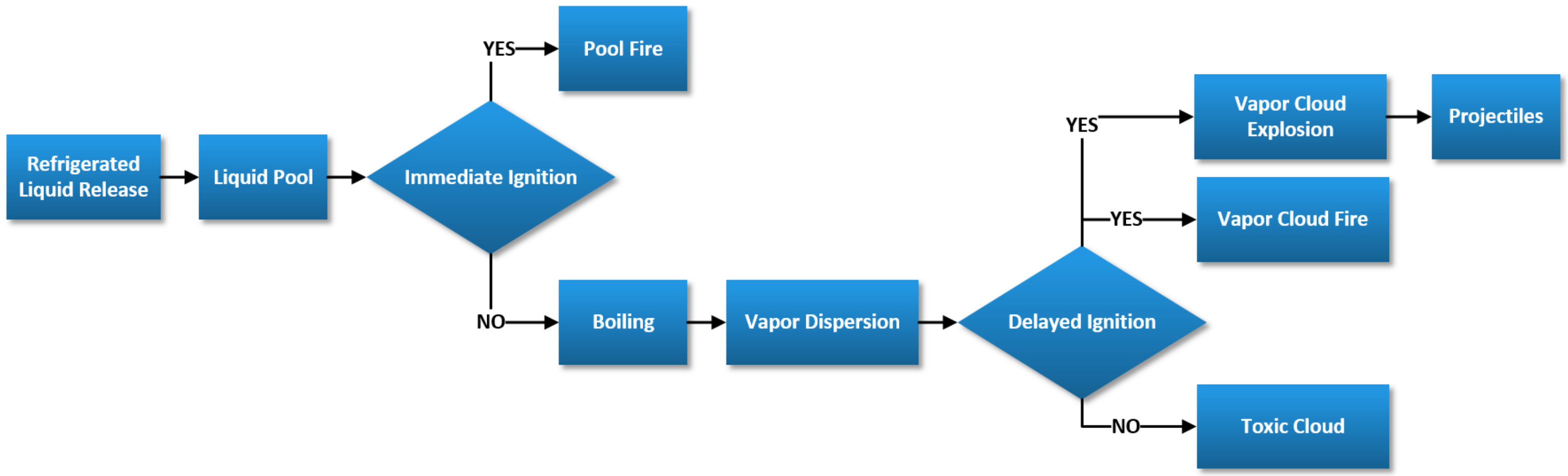

Figure II.02: Refrigerated Liquid Release Event Tree

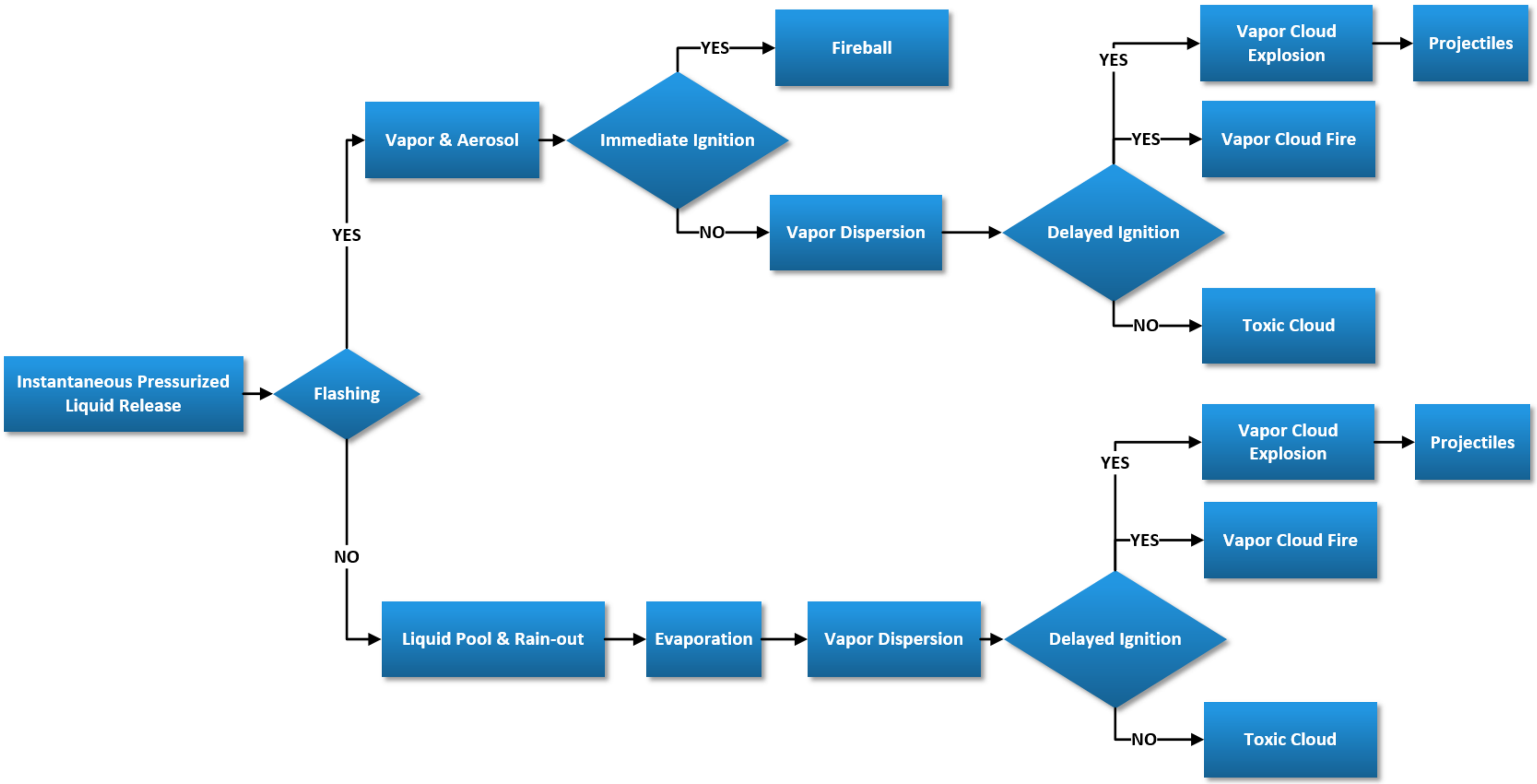

Figure II.03: Pressurized Instantaneous Liquid Release Event Tree

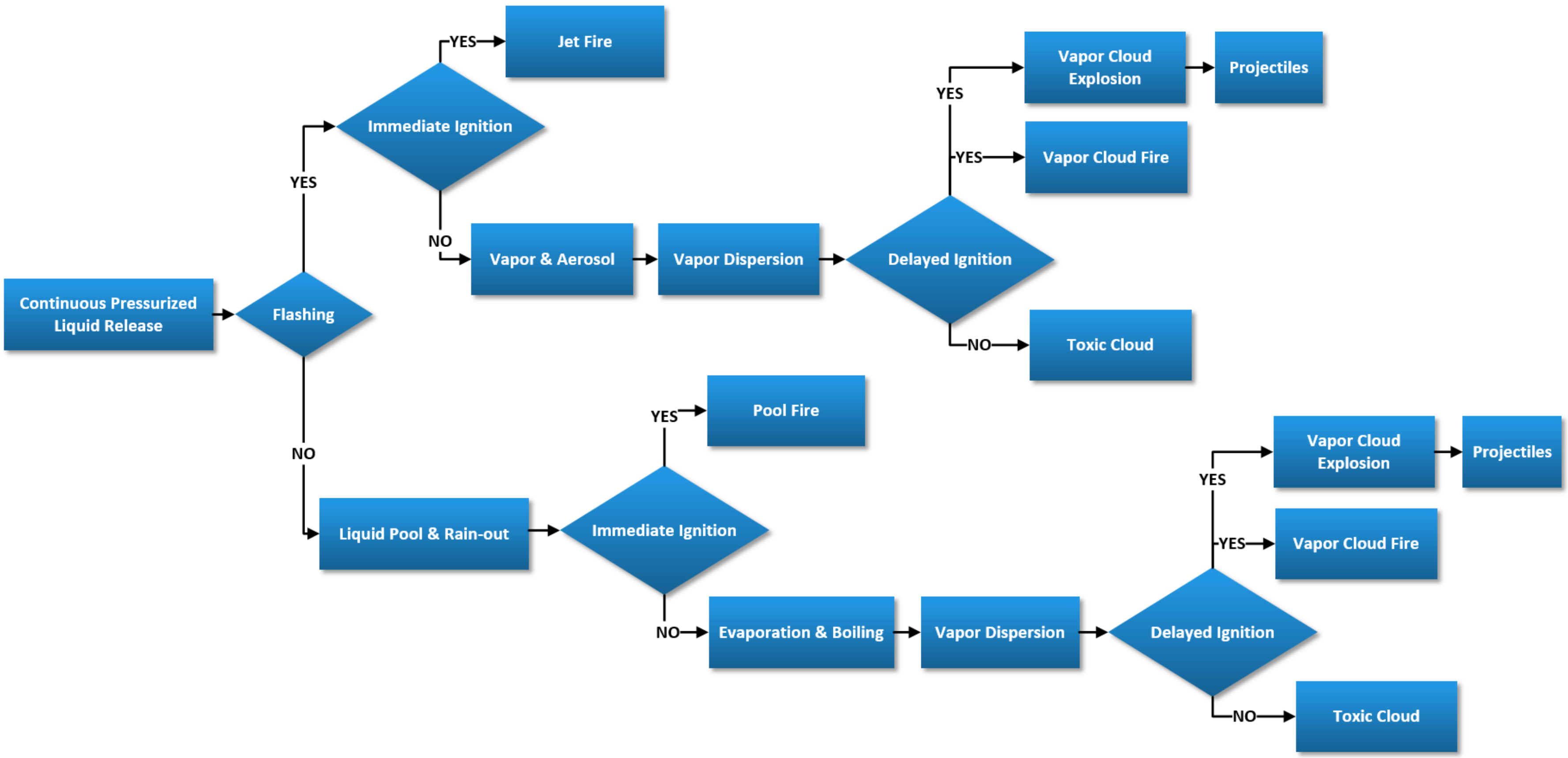

Figure II.04: Pressurized Continuous Liquid Release Event Tree

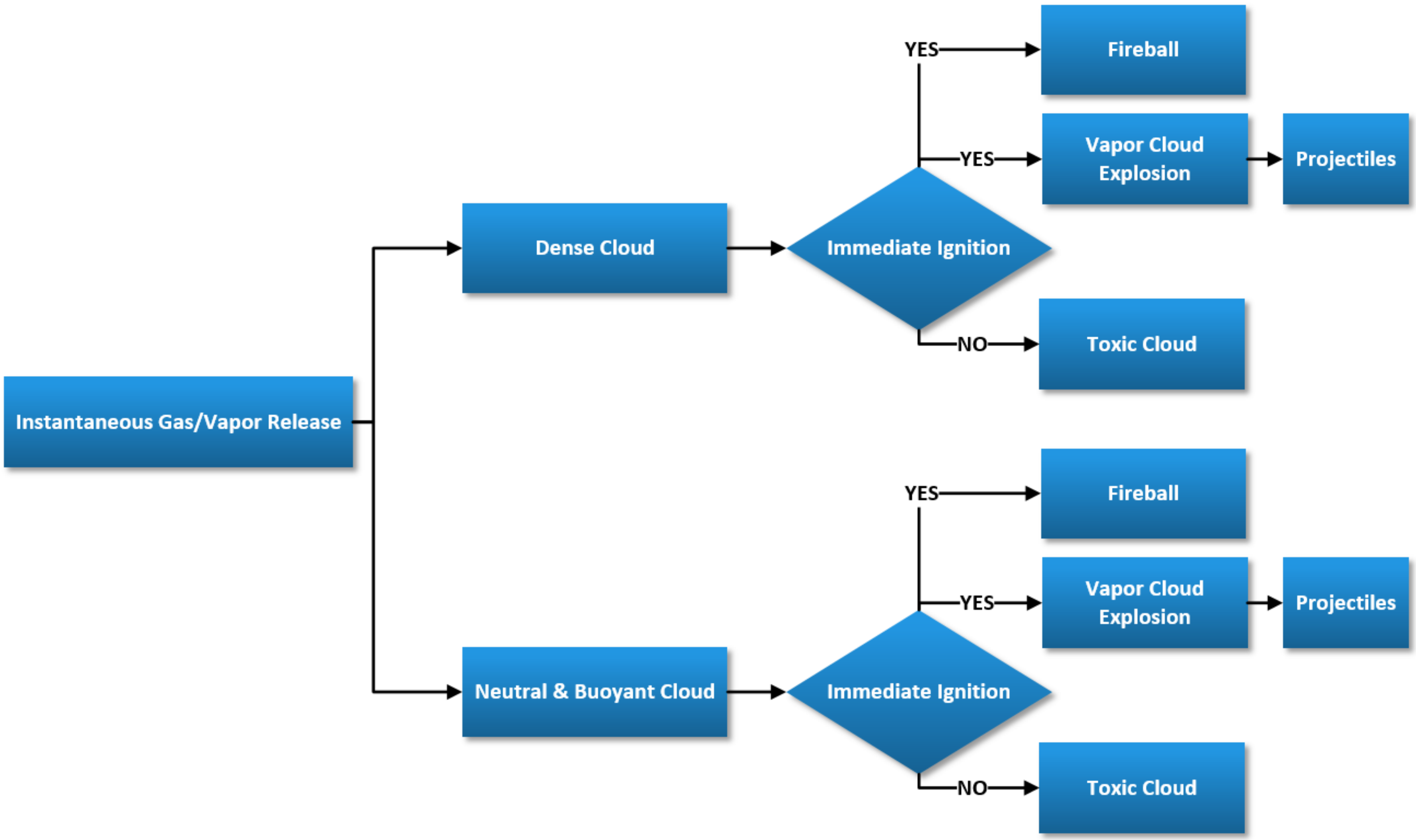

Figure II.05: Instantaneous Gas/Vapor Release Event Tree

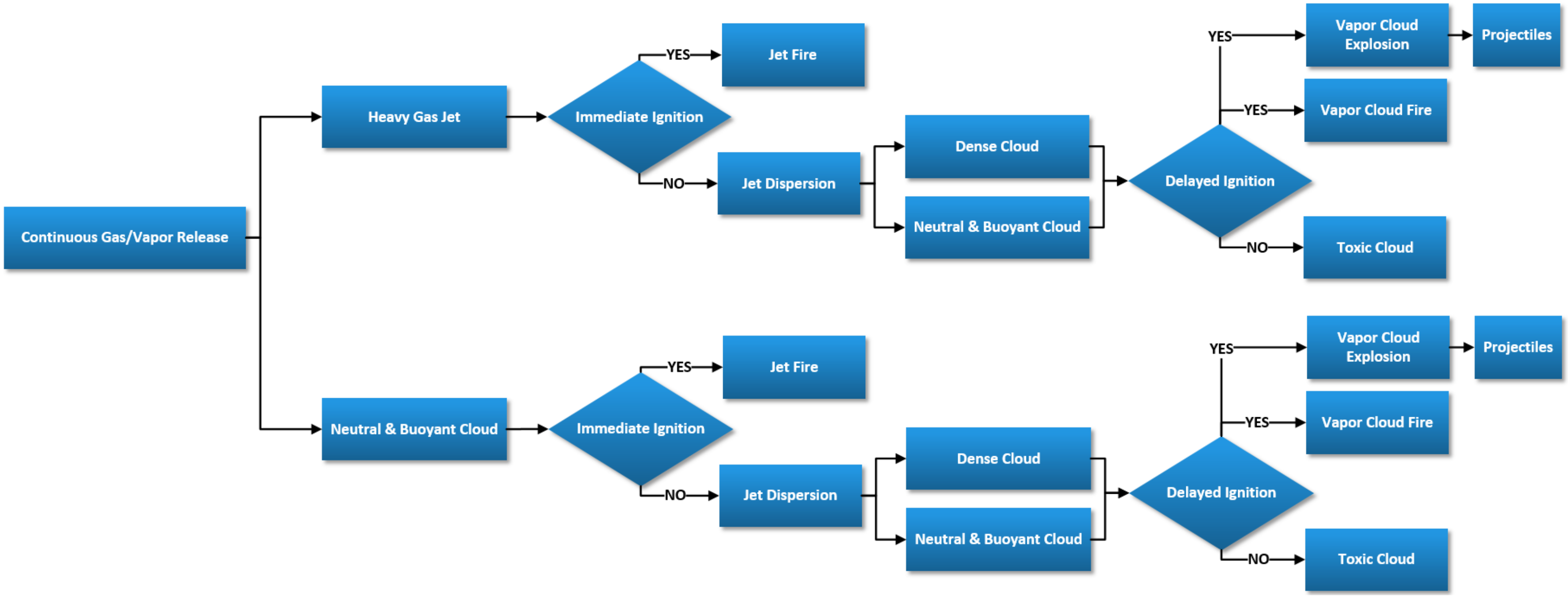

Figure II.06: Continuous Gas/Vapor Release Event Tree

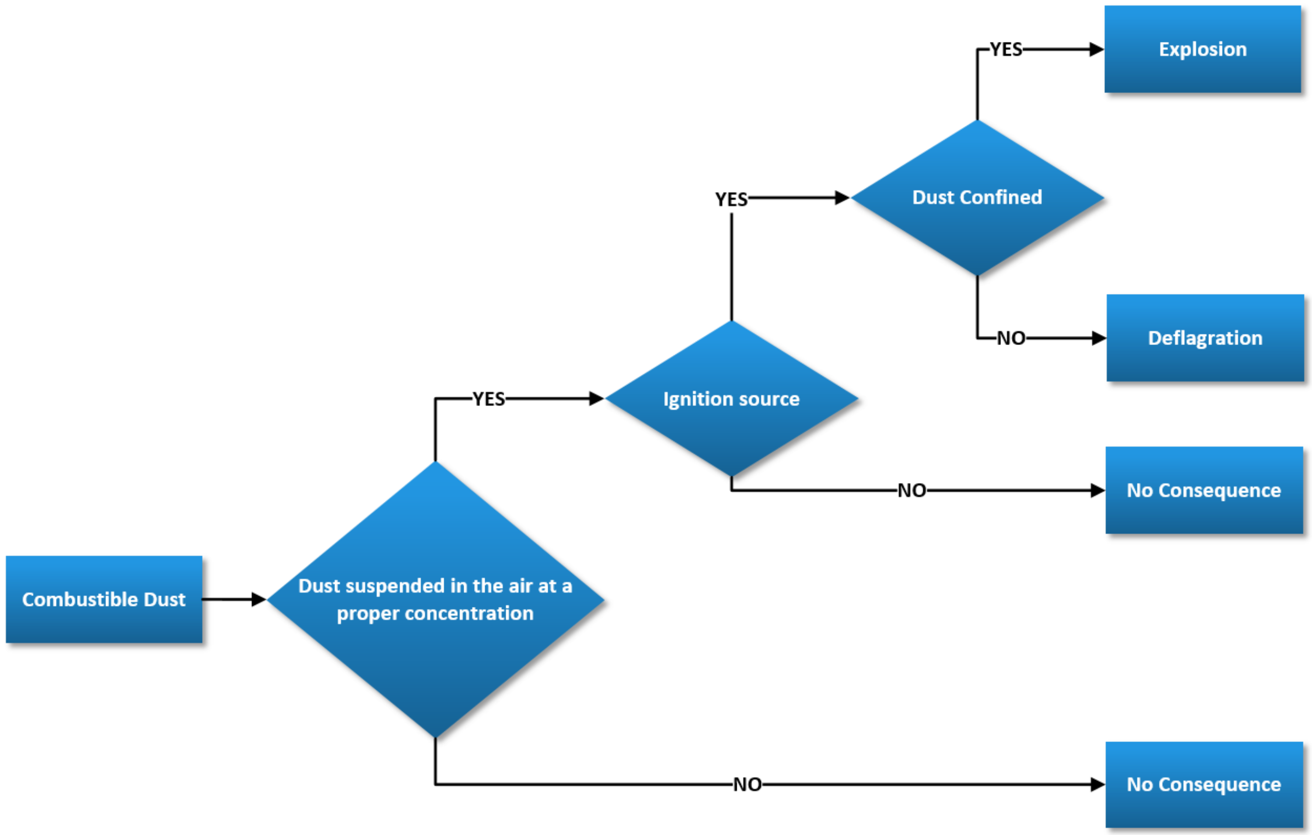

Figure II.07: Combustible Dust Event Tree

Note: five (5) key elements have to be accounted for when characterizing potential dust explosions: (1) combustible dust, (2) dispersion of dust particles, (3) ignition source, (4) confinement of dust cloud and (5) oxygen in air. When all these elements are in place, rapid combustion known as deflagration (a rapid burning slower than the speed of sound) can occur. If this event is confined by an enclosure such as a building, room, vessel or process equipment, the resulting pressure rise can cause an explosion (a rapid burning faster than the speed of sound).