HyRAM+ Version 5.0 User Guide

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ABSTRACT

Hydrogen Plus Other Alternative Fuels Risk Assessment Models (HyRAM+) is a software toolkit that provides a basis for quantitative risk assessment and consequence modeling for alternative fuels infrastructure and transportation systems. HyRAM+ integrates validated, analytical models of alternative fuel behavior, statistics, and a standardized quantitative risk assessment approach to generate useful, repeatable results for the safety analysis of various alternative fuel systems. This document demonstrates how to use HyRAM+ to analyze an example system, providing tutorials of HyRAM+ features with respect to system safety analysis and risk assessment.
ACKNOWLEDGEMENTS

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<td>auto shutoff valve</td>
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<tr>
<td>AIR</td>
<td>average individual risk</td>
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<td>break-away coupling</td>
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<tr>
<td>TNT</td>
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1. INTRODUCTION

1.1. What is HyRAM+?

Hydrogen Plus Other Alternative Fuels Risk Assessment Models (HyRAM+) is a software toolkit that integrates data and methods relevant to assessing the safety of infrastructure for hydrogen and other fuels for a variety of applications, including fueling stations. The HyRAM+ toolkit uses deterministic and probabilistic models for quantifying accident scenarios, predicting physical effects, and characterizing the impact of alternative fuel hazards, including thermal effects from jet fires and pressure effects from deflagration. HyRAM+ Version 5.0 incorporates all the features of previous versions, including generic probabilities for gaseous and liquid equipment failures for multiple types of components for multiple fuels, and probabilistic models for the impact of heat flux on humans and structures, with computationally and experimentally validated models of various aspects of fuel releases [1]. Version 5.0 also includes additional capabilities: the ability to handle cryogenic fluids and blended mixtures; the addition of two extra components for different applications and the ability to customize portions of the risk analysis; and unconfined overpressure and impulse behavior for delayed ignition calculations.

1.2. Purpose of this Guide

This document provides examples of how to use HyRAM+ to conduct different types of calculations using various examples. This document will guide users through the software and how to enter and edit certain inputs that are specific to the user-defined facility. Detailed descriptions of the methodology and models contained in HyRAM+ are provided in the HyRAM+ Version 5.0 Technical Reference Manual [1].

This user guide was created with HyRAM+ version 5.0.0 and was based upon the previous HyRAM+ V2.0 User Guide [2]. Due to ongoing software development activities, newer versions of HyRAM+ may have differences from this guide. It is not the intent of this User Guide to provide an explanation as to the limitations and reference for each model, that information can be found in the HyRAM+ version 5.0 Technical Reference Manual [1].
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2. BASIC FUNCTIONS

2.1. Save/Load Workspace

The Save/Load Workspace button can be found in the File menu at the top left corner of the program window, as shown in Figure 2-1. The Save Workspace button functions as a “Save As” button. To save a workspace, click the Save Workspace option. Comments may be added to a workspace by typing in the text box in the Save Workspace pop-up window. To load a workspace that has been previously saved, click the Load Workspace option. To reset HyRAM+ to its default values and settings, the user must click File, then Exit, to close the program. After the user reopens the program, HyRAM+ will reset itself with default values and settings.

![Figure 2-1. Save/Load Workspace](image)

2.2. Changing Units

HyRAM+ contains a built-in unit conversion function. For variables with a unit, the unit must be selected before inputting a value. If a value is entered before a unit, when a different unit is selected, the software will convert the entered value into the new value corresponding to the selected unit. To change units for a variable, find the drop-down bar in the unit column, click on the Arrow next to the bar; this will reveal a List of Possible Units. Click on a new unit to select it, then click on a box within the input table to apply the unit conversion as shown in Figure 2-2.

---

* Colored text throughout this document corresponds to respectively colored indicators on associated figures to better illustrate HyRAM+ functionality and denote its features
2.3. Sorting

Some inputs are organized into tables. To change the rank or sorting of a column, click on the Title Box of the column, as in Figure 2-3. This will change the rank to numerical or alphabetical depending on the column input. Clicking the title box again will reverse the sort order.

Note: Sorting is not enabled for all columns.

2.4. Copying Tables to Paste into Other Programs

HyRAM+ tables may be copied into external programs such as Microsoft Word and Excel. To do so, select the desired cells of the table and press Ctrl+C. Tables may be pasted into external programs using Ctrl+V or pasting options defined by the external program.
3. GENERIC INDOOR FUELING SYSTEM EXAMPLE

For this document, inputs are based on a generic indoor hydrogen fueling system and the National Fire Protection Association (NFPA) Hydrogen Technologies Code (NFPA 2) requirements and industry practices. The example installation is based off the generic indoor fueling system for hydrogen-powered forklifts further documented elsewhere [3].

The system is a hydrogen dispenser located within a warehouse facility. The facility is a free-standing industrial frame structure. Interior dimensions are: 100 m (length) × 100 m (width) × 7.62 m (height). It is assumed that are 50 employees in the warehouse at any time and personnel each work 2,000 hours per year. In this example, most workers are located within 50 m of the dispenser due to building design. The vehicle fleet contains 150 vehicles (e.g., forklifts within the warehouse facility) that are operated 24 hours/day and 350 days/year. Each vehicle holds 1 kg of hydrogen and is refueled once per day.

The dispenser delivers gaseous hydrogen at 35 MPa. The dispenser operates for up to 5 minutes per fueling event, and the internal hydrogen temperature is 15°C. All piping in the storage system has an outer diameter (OD) of 3/8”, wall thickness of 0.065”, and the material is ASTM A269 seamless 316 stainless steel piping. The facility temperature is 15°C and pressure is atmospheric at sea level (101,325 Pa). Figure 3-1 illustrates the Piping and Instrumentation Diagram (P&ID) for the generic dispenser. The part count only includes components inside the building and on the main process line: one hose, 20 m of piping, five valves (ASV2, HV1, BC1, SRV1, and N1), three instruments, and 35 joints. The system also contains additional components (not pictured; within the Dispenser Appliance Boundary): 2 cylinders, 2 valves, 2 instruments, 8 joints, 10 m of piping, and 3 filters. In total, the system has 2 cylinders, 7 valves, 5 instruments, 43 joints, 1 hose, 30 m of piping, and 3 filters.

Figure 3-1. P&ID for the generic dispenser used in this example [3]
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4. **FUEL SPECIFICATION**

There are three fuel selection menus available in HyRAM+, a plume dispersion calculation (see Section 6.1.1) was done to illustrate the use of the fuel selection menu in HyRAM+ showing the different ways to select a fuel in HyRAM+.

4.1. **Pure Fuel Selection**

The Fuel selection drop down menu gives you three selection options for common fuels, click the drop down and you will be given four options; Hydrogen, Methane, Propane and Blend (described in section 4.2). Some default values in the quantitative risk assessment (QRA) mode will change when a pure fuel is selected, such as leak frequencies, ignition probabilities, and component counts; the default values are given in the HyRAM+ Technical Reference Manual [1].

![Figure 4-1. Fuel Specification Drop Down Menu](image)

Shown in Figure 4-2 is the plume dispersion calculation using Methane as the selected fuel.
4.2. Blend Specification

Within the Fuel Selection, HyRAM+ gives the user the ability to specify if they would like to select a blend of fuels. To access this option, select the three dots beside Fuel Selection drop down menu. Note: the blend must equal 100%, the user has the option to allocate the remainder of the mixture to a specific fuel in order to reach 100%.

Figure 4-3. Fuel Blend Specification
4.2.1. **Pre-Specified Blend**

The user can select pre-specified blends from the fuel specification drop down menu, this will automatically configure the fuel blend in the fuel specification table.

![Fuel Specification Table](image)

**Figure 4-4. Pre-Specified NIST1 Blend**

Shown in Figure 4-5 is the plume dispersion calculation using NIST1 mixture as the selected pre-specified fuel.

![Plume Dispersion Calculation](image)

**Figure 4-5. NIST1 Blend Plume Dispersion Calculation**
4.2.2. **Manually Specified Blend**

To manually select a specified blend of fuel, select a(n) Active fuel(s) of your choice, and type in a numerical value into the volume Percent column for the corresponding active fuel.

![Image of fuel specification interface]

Figure 4-6. Manually Specified Blend, 50% Methane, 50% Nitrogen

Shown in Figure 4-7 is the plume dispersion calculation using the mixture described in Figure 4-6 as the selected pre-specified fuel.

![Image of plume dispersion calculation]

Figure 4-7. Manually Specified Fuel mixture Plume Dispersion calculation
5. QRA MODE

5.1. Input

5.2. System Description

The System Description window, depicted in Figure 5-1, contains four tabs (Components, System Parameters, Facility Parameters, and Manual Overrides) which enable the user to input design specifications for the system.

![System Description Window](image)

**Figure 5-1. QRA Mode System Description Window**

5.2.1. Components

The Components tab contains user input for 12 types of components commonly seen in hydrogen and other alternative fuels applications and two extra component inputs for a different type of system. These extra components give the user the ability to specify a non-standard component type that does not fit well within other components; for example, it could be specified as a different type of valve, so that one type of valve uses the “Valve” component and the other type of valves uses Extra Component 1. The user should refer to a P&ID for the proper number of components. It should be noted that “pumps” and “compressors” are the treated as the same “component” in HyRAM+, the difference is pumps are for liquids and compressors are for gas. Piping is specified per unit length, and so the unit of length is user-selectable. The Components Input, based on the preceding example, is portrayed in Figure 5-2.
5.2.2. **System Parameters**

The System Parameters tab contains Piping and Vehicle input. This information can be found in the P&ID and the description of the facility.

5.2.2.1. **Piping**

The Piping tab contains inputs for **Fluid phase** as well as pipe dimensions of the system and the operating conditions (both internal to the system and in the surrounding external environment). The user can select one of the following fluid phases; Gas, Saturated Vapor, or Saturate Liquid from the fluid phase drop down menu. If Saturated Vapor or Saturated Liquid are selected, the fluid temperature input will disappear, and the temperature of the fuel is calculated based on the fluid pressure. This information is used in calculations for release sizes and characteristics. Based on the preceding example, the Piping tab Input is shown by Figure 5-3.
5.2.2.2. Vehicles

The Vehicles tab contains inputs that establish the use conditions of the station. Users input the Number of Vehicles, the number of times a vehicle is fueled per day (Number of Fuelings Per Vehicle Day), and the number of operating days of the vehicles (Number of Vehicle Operating Days per Year). HyRAM+ calculates the annual demands (number of fuelings per year) as the product of those three inputs. Based on the preceding example, Vehicles Input is depicted by Figure 5-4.

Note: The annual number of demands is used in the calculation of the frequency of releases from elements contained in a fault tree (FT) (i.e., a diagram that presents theoretical scenarios on which a component fails, and what events that might lead to). If the user decides to not use this FT, the user should input zero for one of the inputs. If the user puts zero for any variable, the code will result with an annual demand of zero. This implies that the “100% Release FT” will not be used. For example: if the user inputs zero on "Number of Vehicles", the code will produce an “Annual Demands (calculated)” of zero. The manual override (see Section 5.2.4) for “100% H2 Release (accidents and shutdown failures)” will also override this.

5.2.3. Facility Parameters

The Facility Parameters tab contains the Facility and Occupants tabs.

5.2.3.1. Facility

The Facility tab contains measurements for the facility, as shown in Figure 5-5. Based on the preceding example, Facility Input would be as shown:

Note: In HyRAM+ 5.0, the input values for Width and Length will not affect risk calculations. Future HyRAM+ versions may use these numbers to assess further risk characteristics. For now, they are only used to make the plot of occupant positions (see Section 5.7.5).
### 5.2.3.2. Occupants

The Occupants tab contains input details for number of persons on site (e.g., exposed employees) and a function to randomly distribute workers based on a uniform or normal distribution, or defines a specific location using the deterministic value. These distributions are used to determine personnel locations (i.e., the distance from the system for use in harm calculations).

Several scenarios can be defined for personnel. For each scenario, the user defines the Number of Occupants (i.e., the number of personnel) and provides a description of the scenario in the Description field. The user can then choose between the Normal, Uniform, or Deterministic Location Distribution Types for each of the X, Y, and Z coordinate values. If the user selects a Normal or Uniform Distribution Type, the user will need to enter parameter values for Location Distribution Parameters A and B. If the user selects the Deterministic Distribution Type, only coordinate values for Location Distribution Parameter A are required. The units (Location Parameter Unit) correspond to the distribution parameters. The Exposed Hours Per Year for a single target is also assigned by the user.

To delete a row in the Occupants tab, the user must click on the Arrow (see Figure 5-6) next to the row to highlight the entire row, and then press the keyboard Delete button. To add a row in the Occupants tab, the user must enter a new value in the last row for Number of Occupants and press Enter on the keyboard, then a new row will be created.

When selecting a Normal Location Distribution Type, Location Distribution Parameter A corresponds to the mean \( \mu \) and Location Distribution Parameter B corresponds to the standard deviation \( \sigma \). For a Uniform distribution, Location Distribution Parameter A and Location Distribution Parameter B correspond to the minimum \( a \) and maximum \( b \) values, respectively. Deterministic distribution corresponds to a constant value for the location and is entered in Location Distribution Parameter A. Distributions are applied with respect to the fuel system; that is, the fuel system is at the origin of the coordinate space \((0, 0, 0)\), which effectively occurs at the lower left corner of a Cartesian coordinate system in a top-view of the facility.

Worker positions relative to the storage system could be randomly assigned by sampling from a normal distribution. For the example case [3], the 50 workers are assumed to be within 50 m of the storage system. The authors translate this assumption into a normal distribution centered at the dispenser \((\mu = 0 \text{ m})\) and a standard deviation of \(50/3 = 16.67 \text{ m}\) \((\mu = 0 \text{ m}, \sigma = 16.67 \text{ m})\). The authors recommend using the shortest dispenser-to-wall distance and dividing by three since three standard deviations account for 99.7% of the possible positions. Based on the preceding example, the Occupants tab Input is shown by Figure 5-6.

![Figure 5-6. Example Input for Occupants Tab](image)

The location distributions (described above) are used to generate possible positions. However, all generated positions must be some minimum distance away from the leak; this is the Exclusion Radius (in meters). Additionally, the pseudo-random number generator requires a “seed” from
which to generate positions; the user is given the ability to set whatever Random Seed value they wish; this will help generate reproducible results from session to session. By default, a new random seed value will be generated each time the HyRAM+ software is launched; if repeatable results are desired, this value should be noted and used in future calculations. Figure 5-7 shows the default random seed and exclusion radius values used for this example.

![Image of boundary conditions input](image)

**Figure 5-7. Boundary Conditions Input**

### 5.2.4. Manual Overrides

There are six different Manual Overrides available for the user in HyRAM+: one for the fault tree results for each leak size and one for Gas Detection and Isolation Credit (the probability of successful release detection and isolation before ignition). For each of the five leak sizes (0.01%, 0.1%, 1%, 10%, and 100%), there is an associated fault tree (FT; see Section 5.3.2) based on the equipment around the user-described facility and how likely each leak size will occur. If the user wants to use another FT to calculate different leak frequencies, HyRAM+ gives the option to customize results of the FT. The Manual Overrides tab lets the user directly specify an annual leak frequency (e.g., for a 1% leak size, there is a 0.003 leaks/year) from a customized FT. It is important to note that HyRAM+ does not enable substitution of the default FTs for a user-defined one, rather HyRAM+ lets the user by-pass the default FT to directly input user-specific FT results. A value of -1 means that the default HyRAM+ FT will be used for each leak size.

While following the ESD (Event Sequence Diagram; see Section 5.3.1) in HyRAM+, the Gas detection credit probability input works by establishing the probability that the leak will be isolated and detected. For example, if the user inputs a credit of 0.9, then HyRAM+ runs by calculating that when a fuel leak occurs, there is a 90% chance that it is detected and isolated. This means that there is a 10% chance said detection and isolation does not happen, therefore the rest of the ESD (ignition branches) will be considered. This gives the user an option to override it to any number, like zero (i.e., no gas detection or isolation whatsoever).
5.3. Scenarios

The Scenarios window contains an event sequence diagram (ESD), which models the fuel release scenarios, and fault trees (FTs), which model likelihood of fuel releases.

5.3.1. Event Sequence Diagrams

The Event Tree tab illustrates the scenarios that could occur after a fuel release, depending on the success of detection/isolation and the time of ignition.

There are three possible outcomes that may result if a fuel release is not detected and isolated: jet fires, explosions, and unignited releases. If fuel is not ignited (either due to successful detection/isolation of the release or due to lack of ignition), there are no risk-significant consequences considered.† When a high-pressure release of fuel is immediately ignited near the source, the result is a classic turbulent-jet flame. If the fuel does not ignite immediately but is subsequently ignited (delayed ignition), the result is an explosion.

The event tree coded in HyRAM+ models these scenarios. The user may input a value (between 0.0 and 1.0) for gas detection credit, as shown in Section 5.2.4. This value is probabilistically associated with the event tree event yes/true (upper branch) for the single node “Leak detected and isolated”. If the user has separate probabilities for leak (release) detected and leak (release) isolated, simply multiply the two probabilities together and enter this product into the gas detection credit input.

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† Asphyxiation, hypoxia, and frostbite are not considered in HyRAM+. 

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Each leak size has an associated FT, on which the top event probability from each FT is calculated according to the system description, system parameters, and data/probabilities (i.e., leak size scenario, number of pieces of equipment/components, and data/probabilities). For the 100% leak size, there is an additional sub-FT where other accidental failures for a dispenser are considered. If the user does not want to include this sub-FT, then input zero in the “Number of Fuelings Per Vehicle Day” or “Number of Vehicles” as described in Section 5.2.2.2. If the result for any leak size from another FT (e.g., for a different application) is calculated externally to HyRAM+, that value can be entered as per Section 5.2.4 to override any of the default FTs.

5.4. Data/Probabilities

The Data/Probabilities window contains the data for Component Leaks, Component Failures, and Ignition Probabilities.
5.4.1. Component Leaks

The Component Leaks tab contains assumptions about the frequency of leaks of five size categories for 12 types of components used in gaseous and liquid fueled systems. The size categories are percentages (0.01%, 0.1%, 1%, 10%, and 100%) of the pipe area which is calculated from the user input described in Section 5.2.2.1.

HyRAM+ contains default values for the gaseous and liquid leak frequencies from each type of component for each fuel and phase combination [1]. The values in HyRAM+ are encoded as parameters of a lognormal distribution (\(\mu\) and \(\sigma\)). HyRAM+ automatically calculates the mean and variance from a given \(\mu\) and \(\sigma\). Users may modify a component’s leak probabilities by entering new values for \(\mu\) and \(\sigma\). Users may also enter a value for the median leak frequency, and the graphical user interface will calculate the associated \(\mu\) value. Figure 5-11 portrays the default Component Leaks values for Compressors for gaseous hydrogen. These default values are updated as the fuel or phase of the fuel changes. Note that there is no default data for some components for certain combinations of fuel and phase. In this case, \(\mu\) and \(\sigma\) are by default 999, leading to an infinite mean and median leak frequency. This will result in infinite risk if that component is included in the system, in order to alert the user that different values should be selected.

![Data/Probabilities](image)

**Figure 5-11. Component Leaks Frequencies Input for Compressors**

5.4.2. Dispenser Failures

The Dispenser Failures tab, depicted by Figure 5-12, contains generic parameters about the likelihood of failure mechanisms of specific components within a fueling dispenser, and about the likelihood of different accident-related events such as drive-offs (i.e. the event where the user “drives away” with the refueling station’s nozzle still connected to the vehicle). It is important to note that the user can edit the Component Failures input values. These values are used in the calculation of the frequency of releases along with the vehicle demands as described in Section 5.2.2.2.

Note: For each different leak size there is a specific FT, all of which are the same with the exception of the 100% leak size. The 100% leak size includes other accidental scenarios involving the system’s dispenser. This section of the FT is emphasized because it involves not only a leak, but the possibility of a component failure and human error. It is important to include human error in the analysis because the dispenser is the part of the fueling station which involves the most frequent and direct interaction with the user.
5.4.3. Ignition Probabilities

The Ignition Probabilities tab is portrayed by Figure 5-13 and contains ignition probabilities associated with different release flow rate thresholds [1]. The probabilities are associated with two ignition event classes: either that the fuel ignites immediately (leading to a jet fire) or ignites with a delay (leading to an explosion).

The default values are based on published values for probabilities of fuel ignition and are specific to the fuel selection [1]. Users may input different values for Immediate and/or Delayed Ignition Probabilities for any of the defined release rates. Users may also add new release rate categories and remove the current categories.

To add a new Ignition Flow Rate Threshold, enter the value in the kg/s box and click the Add button. The addition of a new release rate requires the new input of ignition probabilities. To delete an Ignition Flow Rate Threshold, click on the value you want to delete in the Ignition Flow Rate Threshold box and click the Delete button.

5.5. Consequence Models

The Consequence Models window contains a selection of models used to calculate the physical effects of ignited releases and the probability of harm from a known physical effect.
5.5.1. **Physical Consequence Models**

The Physical Consequence Models tab contains input parameters for the Notional Nozzle Model, Overpressure method, and Mach flame speed as shown in Figure 5-14.

The default selections for physical effect models are the *Yuceil/Otugen* notional nozzle model, BST overpressure method, and 0.35 Mach flame speed. The default options can be changed by selecting any option from the drop-down menus. The user also has the ability to change the overpressure calculation method along with their respective parameters: if BST is selected, the default Mach flame speed is 0.35; if TNT is selected the user can input a TNT equivalence factor; while options unavailable for specific overpressure calculation methods are grayed out and cannot be edited. Description of the different physical consequence models can be found in the HyRAM+ Technical Reference Manual [1].

![Figure 5-14. Physical Consequence Models Input](image)

5.5.2. **Harm Models**

The Harm Models tab, shown by Figure 5-15 contains the **Thermal Probit Model** and the **Overpressure Probit Model**. Users may select the preferred probit models by clicking the drop-down menu next to the model name. Input values for the **Thermal Exposure Time** can also be entered in the Thermal Probit section. Description of the different harm models can be found in the HyRAM+ Technical Reference Manual [1].

![Figure 5-15. Harm Model Selection Window](image)
5.6. Output

5.7. Scenario Stats

The Scenario Stats window output provides a single sheet divided into two sections: Risk Metrics, and the six tabs: Scenario Ranking, Scenario Details, Cut Sets, Thermal Effects, Overpressure, and Impulse, which are collectively called Importance Measures.

5.7.1. Risk Metrics

The Risk Metrics window contains the results of the calculated risk in terms of potential loss of life (PLL), fatal accident rate (FAR), and average individual risk (AIR). Details of the risk metric calculations can be found in the HyRAM+ Technical Reference Manual [1]. Based on the preceding example, the Risk Metric output for the entire system is portrayed by Figure 5-16.

![Figure 5-16. Risk Metrics Output](image)

5.7.2. Scenario Ranking

The Scenario Ranking tab contains the end state types, frequencies, and risk contribution (based on PLL metric calculations) for all release sizes. By default, the results are sorted by release size. These results can be sorted by any of the headings by clicking on the heading name (e.g., to sort by Avg. Events/Year or by Risk (PLL) Contribution). Based on the preceding example, Figure 5-17 shows the Scenario Ranking output tab.
5.7.3. Scenario Details

The Scenario Details tab, shown in Figure 5-18, provides details for each leak size; including its respective mass flow rate and leak diameter. In the table below the user is also provided with corresponding outcome probabilities to those various leaks mentioned above in the event tree, including shutdown, jet fire, explosion, and no ignition. The leak scenario details are calculated based on pipe size, pressure, and fractional leak sizes. The leak outcomes are calculated by isolation and ignition probabilities.
5.7.4. **Cut Sets**

The Cut Sets tabs, shown in Figure 5-19, represent the expected frequency of failure for each system component. Specifically, a cut set is the influence a component failure will have on a particular, potential leak size. This calculation takes into account the expected leak frequency for each leak size for each possible system component and weights these leak frequencies by the number of those specific components in the system. These calculations can tell the user which component is more likely to contribute to a leak of a particular size. This can provide insight to decision-makers on whether to limit the usage of particular components to minimize leaks.

![Figure 5-19. Cut Sets Output Tab](image)

Make note that the Cut Sets tabs for a 100% leak size has more information as an output due to its expanded FT, as shown in Figure 5-20.
5.7.5. **Plots**

Visual representations are generated of the Radiative Heat Flux, Peak Overpressure, and Impulse that the system occupants may experience while in the presence of varying leak sizes (0.01%, 0.1%, 1%, 10%, and 100%). They are located in the following three tabs respectively: Thermal Effects, Overpressure, and Impulse. In addition, position data for the plots is also available within the perspective tabs.

The facility in the following example Figures uses the parameters set in the previous input examples with length and width facility dimensions of 100 meters, however, the occupants tab was altered to demonstrate the plots tab functionality. The occupants tab within facility parameters of the system description will allow the user to set the plots location of facility occupants relative to a leak.

In Figure 5-21, Figure 5-22, and Figure 5-23 there are 9 occupants in the facility with Uniform X location Distribution A and B Parameters set to 1 and 20 meters, respectively, to represent the length at which the occupants may be in the plot. The width that facility occupants may be located in is represented by the Uniform Z location Distribution A and B Parameters set to 1 and 12 meters (see Section 5.2.3.2).

The Radiative Heat Flux sustained by the occupants (see Figure 5-21) is the potential harm associated with the immediate ignition jet fire scenario. The height from the ground at which the facility occupants would experience heat flux, relative to the leak, was set at a Deterministic Y Location Distribution A Parameter of 1 meter. After the user clicks on the Scenario Stats to generate data, they have the option to choose plots with varying leak sizes.
The blue square in the corner of the generated facility plot represents the fuel leak point while the blue line on the bottom, x-axis, is the coordinate direction of the leak.

The dots represent locations of the 9 facility occupants and respective dot colors indicate the radiative heat flux (in kW/m²) that those facility occupants would experience relative to their locations to the hydrogen leak. A similar plot is shown in Figure 5-22, but this is representative of the Peak Overpressure (in kPa) experienced at the same occupant positions.

Figure 5-23 is a plot representative of the impulse (in kPa*s) experienced at the same occupant positions.
Figure 5-23. Impulse plot
6. PHYSICS MODE
The physics models are included as stand-alone fuel release behavior models.

6.1. Gas Plume Dispersion
The Gas Plume Dispersion window contains variables that calculate the characteristics of an unignited fuel plume. Before clicking the Calculate button located at the bottom right of the window, the user should input values for each of the variables.

6.1.1. Gas Plume Dispersion Input
The Gas Plume Dispersion Input tab, depicted by Figure 6-1, contains the characteristics of the output plot for the unignited fuel plume. The user can alter the Plot Title, Notional nozzle model, and fluid phase as well as distinct environment and physical conditions Inputs to generate the appropriate plume characteristics.

![Figure 6-1. Plot Properties Input](image)

To generate the Output plot, click the Calculate button located at the bottom right of the window.

6.1.2. Gas Plume Dispersion Output
Figure 6-2 shows the Gas Plume Dispersion Output based on the preceding example. The mass flow rate through the leak orifice is also given in the Output tab.
If the user wishes to save the output, click the Save Plot button located at the bottom right of the window.

6.2. Accumulation

6.2.1. Indoor Release Parameters

The Indoor Release Parameters tab contains measurements to calculate the accumulation of the storage system following an indoor release. The default window for the Indoor Release Parameters tab is shown below. A general sketch is provided to the right of the variable inputs to help the user visualize the enclosure and identify the variables related to the enclosure and the release. Once the user has entered all Inputs and selected the desired Output Options (see Section 6.2.2), then the user must click the Calculate button to produce the Overpressure Output, as shown in Figure 6-3. Within the inputs the user has the ability to select between either a blowdown (transient process of the tank emptying) or steady state release type.
6.2.2. **Output Options**

The Output Options tab, portrayed by Figure 6-4 allows the user to specify *Times* for calculating pressure, specify the *Maximum Time* for overpressure data generation, specify *Pressures* to be drawn across the plot with a horizontal line, and place dots where *Pressure* and *Time* intersect. After providing input parameters, the user must click *Calculate* (as shown in Figure 6-3) in the bottom of the input window to produce the output.
6.2.3. **Accumulation Output**

The Output tab contains a Pressure plot, Flammable Mass plot, Layer plot, Trajectory plot, Mass flow plot, and Data table for results. Based on the default inputs, the Pressure plot is shown by Figure 6-5.

In the Overpressure plot, the Layer line represents the overpressure that would develop if the accumulated layer were ignited. The Combined plot line represents the overpressure that would develop if both the layer and the gas plume were to be ignited. The pressures specified in Section 6.2.2 (13.8 kPa, 15 kPa, and 55.2 kPa) are also shown on this plot. If the user wishes to save the output, click the Save Plot button located at the bottom right of the window.

Figure 6-6 shows the Flammable mass plot based on default inputs.
Figure 6-6. Overpressure Output Flammable Mass Plot

The Flammable Mass Plot shows the amount of hydrogen that exists in a flammable concentration over the time-period of interest. This includes both the accumulated layer as well as the plume from the leak; also plotted is the combined flammable mass that combines the flammable masses from both the layer and the plume.

Figure 6-7 shows the Layer plot based on the default inputs.

Figure 6-7. Overpressure Output Layer Plot

The fuel mole fraction of this layer is represented by the graph on top by the left vertical axis % Fuel in Layer. At 30 seconds the mole fraction is about 5%. The Layer Thickness represents the layer of gas formed along the ceiling (due to buoyancy); this is represented by the vertical axis left of the graph on the bottom. At 30 seconds the layer thickness from the ceiling is about 1.2 m.
Furthermore, in the Pressure plot (Figure 6-5), overpressure is non-zero from 0 seconds to 30 seconds. Comparing the time range to the Layer plot above, we see that the hydrogen mole fraction is greater than or equal to the lower flammable limit of hydrogen (4% by volume) in this timeframe. To save the output, the user must click the Save Plot button located at the bottom right of the window.

The Trajectory plot (Figure 6-8) shows the hydrogen leak jet plume’s travel trajectories over time, dark blue indicating moments early in the blowdown, and yellow later on in the duration. User-defined parameters (see Figure 6-3) will influence how the jet plume will behave, specifically whether the plume will be momentum-dominant or buoyancy-dominant, and how the transition occurs on the interval of time as the hydrogen depletes from the tank. This plot shows the unignited gas jet plume getting re-directed by the wall of the enclosure at 2 m at early times because the length of the jet exceeds the distance from leak to wall input; this is shown on the right-hand side of the plot.

![Release Path Trajectories Over Time](image)

**Figure 6-8. Overpressure Output Trajectory Plot**

Figure 6-9 shows the Mass Flow plot tab based on the default inputs. The mass flow plot tab provides Mass, Pressure, and Temperature of gas present in the tank, as well as the mass flow rate as gas leaves the tank.
Figure 6-9. Mass flow rate plot

Figure 6-10 shows the Data tab output based on default inputs.
The units for Pressure and Time are kPa and seconds, respectively. The pressure data in the table represents the overpressure of the combined plot in Figure 6-5. The concentration data in the table represents the amounts given in the Layer Plot. In addition to the tabulated data, the Maximum Overpressure (Pa) and Time this Occurred (Seconds) are provided in the Data tab, as shown in Figure 6-10.

6.3. Jet Flame

There are two ways to use the Jet Flame model: Flame Temperature/Trajectory and Radiative Heat Flux.

6.3.1. Flame Temperature/Trajectory

The Flame Temperature/Trajectory window contains the variables that calculate behavior of a jet flame, including fuel temperature, direction, and leak size. An example hydrogen system has been modeled with flame and trajectory results based on the Notional Nozzle Model Yuceil/Otugen, and fluid phase Gas with Input parameters shown in Figure 6-11.
Figure 6-11. Flame Temperature/Trajectory Input

To generate the Output plot, the user must click the Calculate button located at the bottom right of the window. Based on the preceding example, the Flame Temperature/Trajectory output is shown by Figure 6-12.
If the user wishes to save the output, click the Save Plot button located at the bottom right of the window.

### 6.3.2. Radiative Heat Flux

The Radiative Heat Flux window contains the variables that calculate radiative heat flux values, the respective plot, and will also generate a temperature plot.

The user can specify both Notional Nozzle and Fluid Phase, provide Input Parameters, and determine the coordinates where the radiative heat flux is calculated by entering values in X Radiative Heat Flux Points (m), Y Radiative Heat Flux Points (m), and Z Radiative Heat Flux Points (m). For reference, a general sketch of the jet flame is provided to the right of the variable inputs to help the user visualize the coordinate system with respect to the flame and identify the variables related to the jet flame. The user also specifies the desired radiative heat flux Contour Levels (kW/m²) corresponding to desired harm criteria to be plotted. Based on the preceding example, with the default relative humidity of 0.89 and Radiative Heat Flux Points, the Radiative Heat Flux Input is displayed in Figure 6-13.

![Figure 6-13. Radiative Heat Flux Input](image-url)
Based on the preceding example, the Radiative Heat Flux output values are shown by Figure 6-14.

![Figure 6-14. Radiative Heat Flux Values Output](image)

The table provides the radiative heat flux calculated at the user specified positions (see Figure 6-13). By clicking the Copy to Clipboard button, the table is copied and can be pasted into another program, such as Microsoft Excel. The mass flow rate, total emitted radiative power, visible flame length (which is along the streamline), and radiant fraction are also reported.

The Radiative Heat Flux Plot output is depicted in Figure 6-15.

![Figure 6-15. Radiative Heat Flux Plot](image)
Presented in Figure 6-15 are three radiative heat flux 2-D plots that corresponds to the jet flame: a side view (top left), a front view (top right), a top view (bottom left), and a legend. The images show isosurfaces at which radiative heat flux is greater than or equal to the user specified contour levels (see Figure 6-13). To save the output, the user must click the Save Plot button located at the bottom right of the window.

The Radiative Heat Flux Temperature Plot output is shown by Figure 6-16. This is the same plot as described in Section 6.3.1.

![Figure 6-16. Radiative Heat Flux Temperature Plot](image)

### 6.4. Unconfined Overpressure

The unconfined overpressure model calculates the peak overpressure and impulse behavior for a pressure wave emanating from the delayed ignition of an unignited jet plume. In this context, overpressure is defined as the pressure above ambient, and impulse is the area under the curve for the pressure-time blast wave.

The user can specify a Calculation method, Notional Nozzle, Fluid phase and Mach flame speed (if using BST calculation method), and various fuel input parameters. In addition, the user can determine coordinates where the unconfined overpressure is calculated by entering values in X positions (m), Y positions (m), and Z positions (m). The user also specifies the overpressure and impulse contour levels corresponding to the desired harm criteria. The default value for Mach flame speed is 0.35 as seen in Figure 6-17.
Based on the preceding example the unconfined overpressure and impulse values are shown below in Figure 6-18.

The table provides the unconfined overpressure calculated at the user specified positions, along with the mass flow rate of the leak. Similar to the radiative heat flux output values, the user can copy the table and paste it into another program (see Figure 6-14). The Overpressure plot is depicted below in Figure 6-19.
Presented in Figure 6-19 are three unconfined overpressure 2-D plots that correspond to an unignited jet: a side view (Top Left), front view (Top Right), and top view (Bottom Left), and a legend. The images show contours at which overpressure and impulse are greater than or equal to the user specified contour levels. To save the output the user must click the Save Plot button located at the bottom right of the window.

The relative Unconfined Overpressure Impulse plot is shown by Figure 6-20. Similar to the overpressure plot, it shows side, front, and top views for impulse values.
In the Temperature, Pressure and Density tab, the user enters two known quantities to determine an unknown quantity. When the user selects which parameter to calculate, the parameter will be “grayed-out” and no value can be entered in the corresponding box. In Figure 6-21, the density is chosen under Calculate. The Temperature is 300 K and the Pressure is 250 bar. With these two values entered, the Calculate Density button can be clicked to determine the density; in this case, the Calculated Density is 0.0175 g/cm$^3$. 

Figure 6-20. Unconfined Overpressure Impulse plot
6.6. **Tank Mass Parameter**

The Tank Mass tab determines the relationships for fuel inside the tank. The user supplies 3 inputs, in this case for the **Temperature**, **Pressure**, and **Volume**. In Figure 6.22, the temperature is 300 K, the pressure is 250 bar and the volume is 50 L. Once all the inputs are provided, the user can click **Calculate**; in this example, the **Calculated Mass** is 0.874 kg.
Alternatively, another parameter (temperature, pressure, or volume) could be selected as the calculation output, and inputs can be provided for the other 3 parameters (including tank mass). If a saturated phase (saturated liquid or saturated vapor) is selected, then the temperature will be calculated by the program, and so is not needed as an input.

6.7. Mass Flow Rate

The Mass Flow Rate tab is used to determine mass flow rates for either a steady or blowdown type of release. In addition to inputting the parameters Temperature, Pressure, Volume, and Orifice Diameter (i.e., the release diameter) as shown in Figure 6-23, the user also inputs the Discharge Coefficient. The user may select a fluid phase for the fluid in use; if a saturated phase is selected, then the temperature will be calculated by the program, and so is not needed as an input. The user must also select the Release Type before clicking the Calculate Mass button. Figure 6-23 illustrates a blowdown example for a 1 mm orifice diameter release.

![Figure 6-23. Example Input for Mass Flow Rate Tab](image)

Once all inputs are provided the user can click the Calculate Mass Flow Rate button with the Time to Empty (seconds) equal to 480.7 seconds. The Output plots are shown in Figure 6-24, the user may also save an image of the generated plots by clicking Save Plot.

Note: Selecting a Steady Release Type will not produce a plot for the output or the time to empty, just a mass flow rate value.
6.8. **TNT Mass Equivalence**

The amount of energy released by combusting a specific mass of hydrogen can be compared to the amount of energy released in an explosion of TNT. In Figure 6-25, the Flammable Vapor Release Mass is 1 kg, and Explosive Energy Yield is 100%. These input values yield an Equivalent TNT Mass of 25.64 kg. After the user inputs the required values, the Equivalent TNT Mass will automatically be calculated and displayed in a “grayed-out” box.
REFERENCES


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