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HyRAM V1.1 User Guide

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Abstract

Hydrogen Risk Assessment Models (HyRAM) is a software toolkit that provides a basis for quantitative risk assessment and consequence modeling for hydrogen infrastructure and transportation systems. HyRAM integrates validated, analytical models of hydrogen behavior, statistics, and a standardized QRA approach to generate useful, repeatable data for the safety analysis of various hydrogen systems. HyRAM is a software developed by Sandia National Laboratories for the U.S. Department of Energy. This document demonstrates how to use HyRAM to recreate a hydrogen system and obtain relevant data regarding potential risk. Specific examples are utilized throughout this document, providing detailed tutorials of HyRAM features with respect to hydrogen system safety analysis and risk assessment.

ACKNOWLEDGMENTS

This user guide is heavily based upon the work completed in the HyRAM V1.0 User Guide SAND2016-3385 by Katrina M. Groth, Hannah R. Zumwalt, and Andrew J. Clark of SNL. The current authors altered the document to correspond with revisions made to the HyRAM software over time.

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ACRONYMS

AIR Average Individual Risk

CFD Computational Fluid Dynamics

ESD Event Sequence Diagram

FAR Fatal Accident Rate

FCTO Fuel Cell Technologies Office

FT Fault Tree

HyRAM Hydrogen Risk Assessment ModelsNFPA National Fire Protection AssociationP&ID Piping and Instrumentation Diagram

PLL Potential Loss of Life

QRA Quantitative Risk Assessment

1. INTRODUCTION

1.1. What is HyRAM?

Hydrogen Risk Assessment Models (HyRAM) is a software toolkit that integrates data and methods relevant to assessing the safety of hydrogen fueling and storage infrastructure. The HyRAM toolkit uses deterministic and probabilistic models for quantifying accident scenarios, predicting physical effects, and characterizing the impact of hydrogen hazards, including thermal effects from jet fires and thermal pressure effects from deflagration. HyRAM version 1.1 incorporates generic probabilities for equipment failures for nine types of components, and probabilistic models for the impact of heat flux on humans and structures, with computationally and experimentally validated models of various aspects of gaseous hydrogen release and flame physics.

HyRAM is software developed by Sandia National Laboratories for the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy's Fuel Cell Technologies Office (FCTO).

1.2. Purpose of this Guide

This document provides examples of how to use HyRAM to conduct analysis of a fueling facility. This document will guide users through the software and how to enter and edit certain inputs that are specific to the user-defined facility. Descriptions of the methodology and models contained in HyRAM are provided in [1].

This User's Guide is intended to capture the main features of HyRAM version 1.1 (any HyRAM version numbered as 1.1.X.XXXX). This user guide was created with HyRAM version 1.1.1.174 and was based upon the HyRAM V1.0 User Guide [2]. Due to ongoing software development activities, newer versions of HyRAM may have differences from this guide.

1.3. Requirements

HyRAM is a research software tool under active development at Sandia National Laboratories for the U. S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy's Fuel Cell Technologies Office. HyRAM version 1.1 is available as a free executable download from http://hyram.sandia.gov. After downloading, users must also request a free product registration key via email.

HyRAM was designed to be installed on any 32-or-64-bit Intel-compatible computer with more than 4GB/RAM and 4GB free persistent storage (hard drive space), running Microsoft Windows.

The intended users are experienced safety professionals and researchers who are familiar with the modeling assumptions, limitations, and interpretation of Quantitative Risk Assessment (QRA) and consequence models.

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 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 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.

File Tools Help Debug QRA Mode Physics System Description The system description input window contains information a Input operational environment. This screen is part of the documen System Description Components System Parameters Facility Parameters Boundary Conditions Variable Value Unit Data / Probabilities # Compres 0 # Cylinders 0 Consequence Models # Valves 5 # Instruments 3 35 # Joints # Hoses Output Pipes (length) 20 Meter # Filters 0 Scenario Stats # Flanges 0

Note: Engineering Toolkit input will not be saved or loaded with workspaces.

Figure 1: Save/Load Workspace

2.2. Changing Units

Risk Metrics

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.

^{*} Colored text throughout this document corresponds to respectively colored indicators on associated figures to better illustrate HyRAM functionality and denote its features.

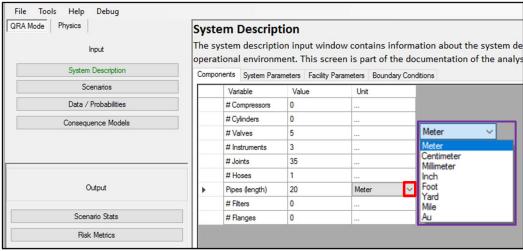


Figure 2: Changing Units

2.2.1. Engineering Toolkit

The user can also utilize the Engineering Toolkit under Tools, shown in Figure 3, to determine some parameters of a given system.

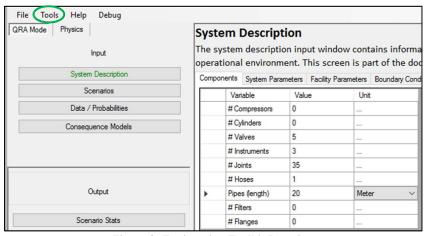


Figure 3: Engineering Toolkit Location

The Engineering Toolkit has four tabs to determine various quantities: Temperature, Pressure and Density; Tank Mass; Mass Flow Rate; and TNT Mass Equivalence. 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 4, 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 $0.0175 \, \text{g/cm}^3$.

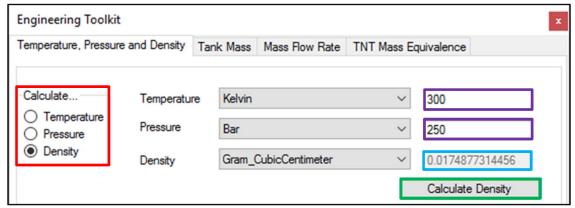


Figure 4: Example Calculation for Temperature, Pressure and Density Tab

The Tank Mass tab determines the mass of hydrogen inside a given tank. The user supplies inputs for the Temperature, Pressure, and Volume. In Figure 5, 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 Mass; in this example, the Calculated Mass is 0.874 kg.

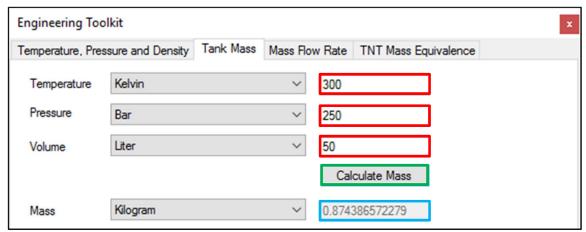


Figure 5: Example Calculation for Hydrogen Mass in Tank Mass Tab

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 Temperature, Pressure and Volume as shown in Figure 6, the user also inputs the Orifice Diameter (i.e., the release diameter). The user must also select the Release Type before clicking the Calculate Mass Flow Rate button. Figure 6 illustrates a blowdown example for a 1 mm orifice diameter release.

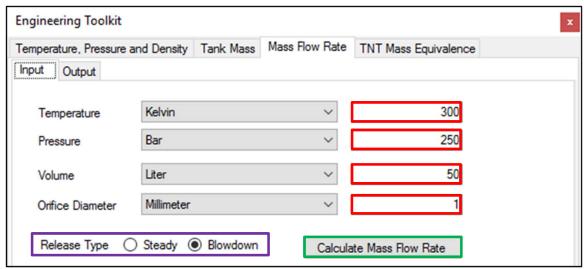


Figure 6: Example Input for Mass Flow Rate Tab

After the user clicks the Calculate Mass Flow Rate button, as shown in Figure 6, the screen will change to the Output tab. The Output tab is shown in Figure 7, with the Time to Empty (seconds) equal to 480.8 seconds. The user may also save an image of the generated plot by clicking Save Plot.

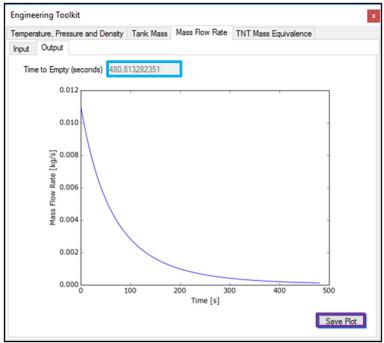


Figure 7: Mass Flow Rate Output Tab

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. The mass of TNT required to release the same amount of energy as a mass of hydrogen can be calculated using the TNT Mass Equivalence Tab in the Engineering Toolkit. In Figure 8, the Flammable Vapor Release Mass is 1 kg, Explosive Energy Yield is 100%, and Net Heat of Combustion is 118,830 kJ/kg. These input values yield an Equivalent TNT Mass of 26.41 kg. After the user inputs the required values, the Equivalent TNT Mass will automatically be calculated and displayed in a "grayed-out" box.

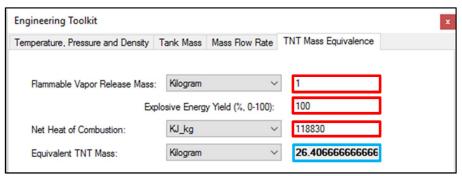


Figure 8: Example Calculation for TNT Mass Equivalence Tab

2.2.2. QRA Master Input Editor

The Quantitative Risk Assessment (QRA) Master Input Editor tab provides the user with a quick view of the System Description inputs. The user can edit any of the values in this window and the changes will be reflected in the System Description tabs. Refer to Section 4.1 for further information on these tabs and variables.

Note: Because the System Description tab is a "loaded" window, the user will have to move away from this tab for the changes to be visible. For example, after changing inputs in the QRA Master Input Editor, close the window, click on the Scenarios tab, and then go back to System Description tab to see the changes made in the QRA Master Input Editor.

2.3. Sorting

All inputs are pre-organized. To change the rank or sorting of a column, click on the Title Box of the column, as in Figure 9. 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.

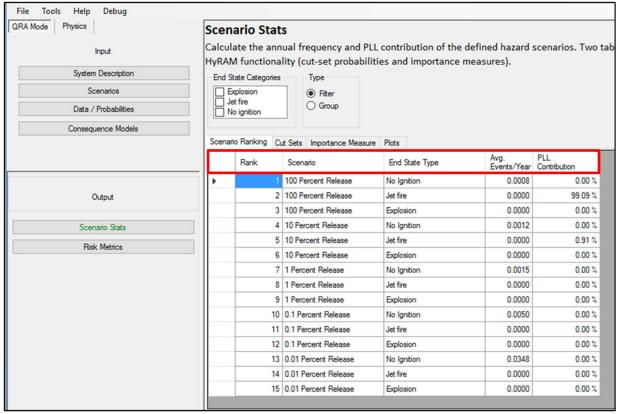


Figure 9: Sorting of Scenario Stats

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 fueling system and The National Fire Protection Association's (NFPA) Hydrogen Technologies Code (NFPA 2) requirements and industry practices. The example installation is based off the generic indoor fueling system further documented in [1] and [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). There are 50 employees in the warehouse at any time. 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 orifice diameter within the piping is 3.25 mm. The facility temperature is 15°C and pressure is atmospheric (0.101325 MPa). Figure 10 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): two cylinders, two valves, two instruments, eight joints, 10 m of piping, and three filters. In total, the system has two cylinders, seven valves, five instruments, 43 joints, one hose, 30 m of piping, and three filters.

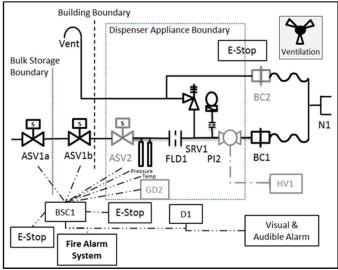


Figure 10: P&ID for the generic dispenser used in this example [3]

4. QRA MODE—INPUT

4.1. System Description

The System Description window, depicted in Figure 11, contains four tabs (Components, System Parameters, Facility Parameters, and Boundary Conditions) which enable the user to input design specifications for the system.

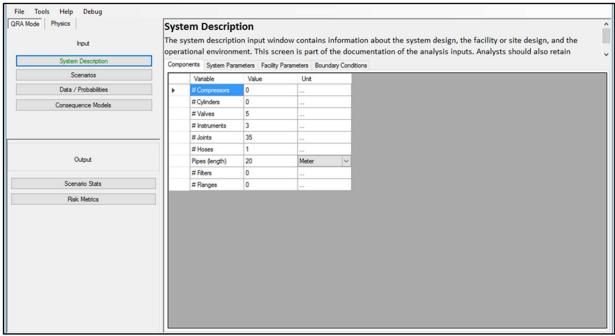


Figure 11: QRA Mode System Description Window

4.1.1. Components

The Components tab contains user input for nine types of components commonly seen in hydrogen applications. The user should refer to a P&ID for the proper number of components. The Components Input, based on the preceding example, is portrayed in Figure 12.

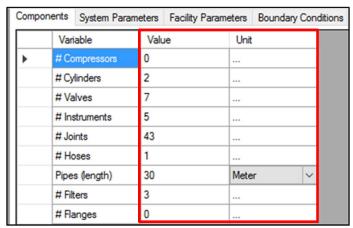


Figure 12: Components Input Window

4.1.2. 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.

4.1.2.1. Piping

The Piping tab contains inputs for pipe dimensions of the system and the operating conditions (both internal to the system and in the surrounding external environment). This information is used in calculations for release sizes and characteristics. Based on the preceding example, the Piping tab Input is shown by Figure 13.

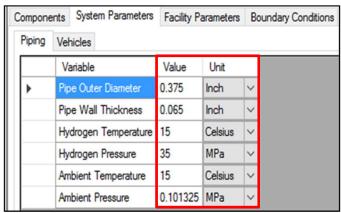


Figure 13: Piping Input

4.1.2.2. Vehicles

The Vehicles tab contains inputs that establish the use conditions of the station. Users input the number of vehicles (# Vehicles), the number of times a vehicle is fueled per day (nFuelingsPerVehicleDay), and the number of operating days of the vehicles (nVehicleOperatingDays). HyRAM calculates the annual demands as the product of those three inputs. Based on the preceding example, Vehicles Input is depicted by Figure 14.

Note: The annual number of demands is used in the calculation of the frequency of releases from elements contained in the Fault Tree (FT). If a FT is not used, the user should input 0 for one of the inputs.

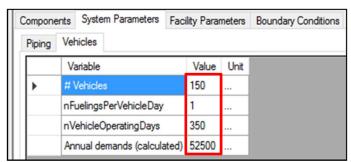


Figure 14: Vehicles Input

4.1.3. Facility Parameters

The Facility Parameters tab contains the Facility and Occupants tabs.

4.1.3.1. Facility

The Facility tab contains measurements for the entire facility, as shown in Figure 15. Based on the preceding example, Facility Input would be:

Note: Only the input values for Width and Length are used in plotting generated positions (in HyRAM version 1.1).

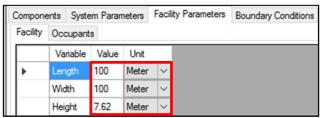


Figure 15: Facility Input

4.1.3.2. 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 define a specific location using the deterministic distribution. 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 Targets (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 coordinate 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 16) 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 in a new value in the last row for Number of Targets and press Enter on the keyboard, then a new row will be created.

When selecting the Normal Location Distribution Type, Location Distribution Parameter A corresponds to the mean (μ) and Location Distribution Parameter B corresponds to the standard deviation (σ) . For the 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 hydrogen system; that is, the hydrogen system is at the origin of the coordinate space (0,0,0), which effectively occurs at the lower left corner of 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 ($\mu = 0$ m) and a standard deviation of 50/3 = 16.67 m ($\mu = 0$ m, $\sigma = 16.67$ 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 16.



Figure 16: Example Input for Occupants Tab

4.1.4. Boundary Conditions

The Boundary Conditions tab inputs are used to generate positions of targets. Likewise, the location distributions (from the System Description, Facility Parameters, Occupants tab) are used to generate 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. Figure 17 shows the default Boundary Conditions input used for this example.

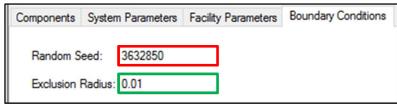


Figure 17: Boundary Conditions Input

4.2. Scenarios

The Scenarios window contains Event Sequence Diagrams (ESDs), which model the hydrogen release scenarios, and Fault Trees (FTs), which model causes of hydrogen releases.

Note: The ESDs and FTs cannot be modified in HyRAM 1.1 – modifiable ESDs and FTs will be introduced in a later version of HyRAM.

4.2.1. Event Sequence Diagrams

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

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

The Event Sequence Diagram coded in HyRAM models these scenarios. The user may Input a value (between 0.0 and 1.0) for gas and flame detection credit (the probability of successful release detection and isolation before ignition), as shown in Figure 18. This value is the

probabilistically associated with the ESD event *yes/true* (upper branch) for a single node "Leak detected and isolated" (illustrated as two nodes in Figure 18, but treated as a single node in the HyRAM logic). 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.

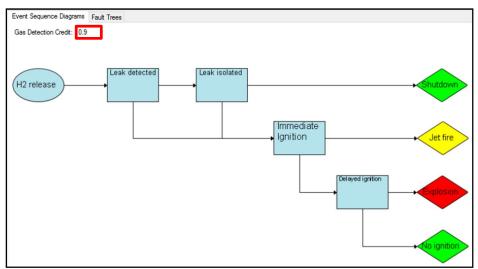


Figure 18: Event Sequence Diagram showing the scenarios coded in HyRAM

4.2.2. Fault Trees

The top event probability from the FTs (5.5e-9 failures/demand) is hard-coded into HyRAM: this value is multiplied by the annual number of demands from Section 4.1.2.2, and the resulting product is added to the frequency of 100% releases. To remove the FT from the calculation, the user should enter 0 in one of the inputs in Section 4.1.2.2. The model images contained on this tab are used only to illustrate the concept of the FT feature for future versions of HyRAM.

4.3. Data/Probabilities

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

4.3.1. Component Leaks

The Component Leaks tab contains assumptions about the frequency of leaks of five size categories for nine types of components used in hydrogen 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 4.1.2.1.

HyRAM contains default values for the leak frequency from each type of component. These frequencies were assembled from generic data from offshore oil, process chemical, and nuclear power industries and documented in [4]. 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. Figure 19 portrays the default Component Leaks values for Compressors.

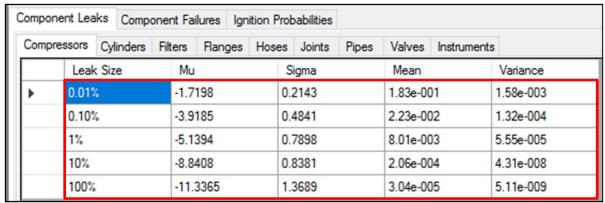


Figure 19: Component Leaks Frequencies Input for Compressors

4.3.2. Component Failures

The Component Failures tab, depicted by Figure 20, contains generic hydrogen data about the likelihood of (non-leak) failure mechanisms of specific components, and about the likelihood of different accident-related events such as drive-offs.

Note: The user cannot edit the Component Failures input values, however, these values are used in the calculation of the frequency of releases along with the vehicle demands as described in Section 4.1.2.2.

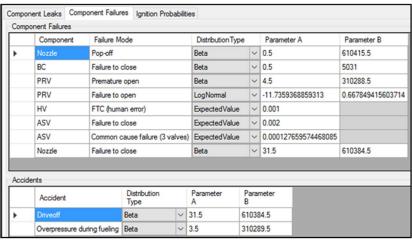


Figure 20: Component Failures Input Window concept

4.3.3. Ignition Probabilities

The Ignition Probabilities tab is portrayed by Figure 21 and contains ignition probabilities associated with different release flow rate thresholds. The probabilities are associated with two ignition event classes: either that the gas ignites immediately (leading to a jet fire) or ignites with a delay (leading to an explosion).

The default input is based on published values for probabilities of hydrogen ignition cited in [4]. 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 Selected button.

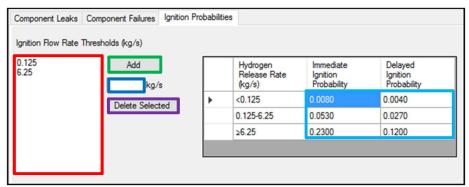


Figure 21: Ignition Probabilities Input

4.4. 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.

4.4.1. Physical Consequence Models

The Physical Consequence Models tab contains input parameters for the Notional Nozzle Model, Deflagration Model, and Radiative Source Model as shown in Figure 22.

The default selections for physical effect models are the Birch2 notional nozzle model, Bauwens/Ekoto deflagration model, and Multiple radiation sources, integrated radiative source model. The default options can be changed by selecting another option from the dropdown menus. Description of the different physical consequence models can be found in [1].

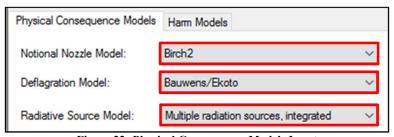


Figure 22: Physical Consequence Models Input

The Deflagration Model has two options: Bauwens/Ekoto and Computational Fluid Dynamics (CFD). The CFD model requires an Input of Peak Overpressure (the default units are Pa) and Impulse (always in units of pressure seconds: Pa sec for the default pressure units) for the five release (leak) size categories, depicted in Figure 23.

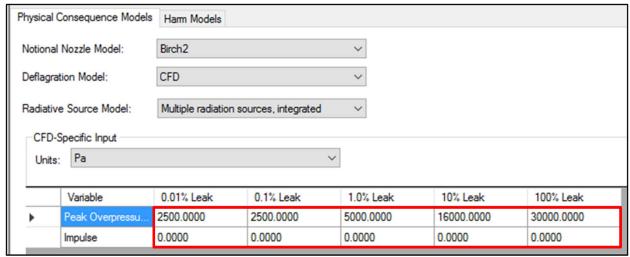


Figure 23: Physical Consequence CFD Model Input

4.4.2. Harm Models

The Harm Models tab, shown by Figure 24, 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.

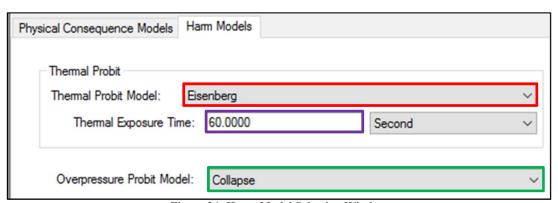


Figure 24: Harm Model Selection Window

5. QRA MODE—OUTPUT

5.1. Scenario Stats

The Scenario Stats window is divided into three sections: Scenario Ranking, Cut Sets, and Importance Measures.

5.1.1. Scenario Ranking

The Scenario Ranking tab contains the end state types, frequencies, and potential loss of life (PLL) contribution 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 (it is recommended to sort by Avg. Events/Year or by PLL Contribution). Based on the preceding example, Figure 25 shows the Scenario Ranking output tab.

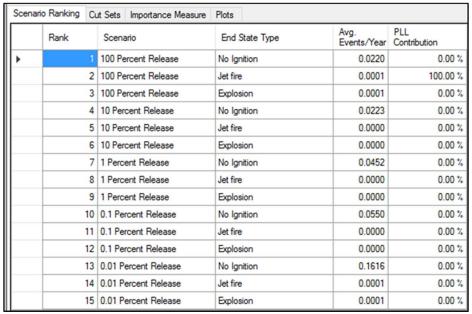


Figure 25: Scenario Ranking Output

The filter option allows users to view the Scenario results tab for an individual end state type, shown in Figure 26. To filter the results, click which end state type(s) you would like to have isolated in the End State Categories box. The grouping option is not currently enabled.

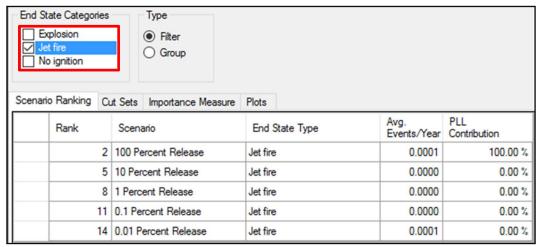


Figure 26: Scenario Results filtered to show only Jet Fire End States

5.1.2. Cut Sets

The Cut Sets tab is currently inactive and no results are generated in version 1.1. The same output is displayed regardless of user-defined inputs or the system being modeled by the user.

5.1.3. Importance Measure

The Importance Measure tab is currently inactive and no results are generated in version 1.1. The same output is displayed regardless of user-defined inputs or the system being modeled by the user.

5.1.4. Plots

The Plots tab generates visual representations of the Radiative Heat Flux that system occupants may experience while in the presence of varying hydrogen leak sizes. The Radiative Heat Flux sustained by the occupants may serve as an indication of potential harm associated with the scenario. The parameters of the generated plots can be altered through the HyRAM QRA mode inputs. The facility in the following example 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 plot locations of facility occupants relative to a hydrogen leak.

In Figure 27, there are 20 occupants in the facility with Uniform X Location Distribution A and B Parameters set to 1 and 99 meters, respectively, to represent the length at which the occupants may be in the plot. The width that the facility occupants may be located is represented by the Uniform Z Location Distribution A and B Parameters set to 1 and 99 meters. The height from the ground at which the facility occupants would experience heat flux, relative to the hydrogen leak, was set at a Deterministic Y Location Distribution A Parameter of 1 meter. The time that occupants are exposed to a potential hydrogen leak per year was set to 2000 hours. After the user clicks on Scenario Stats to generate data, they have the option to choose plots with varying hydrogen leak diameter sizes. In this example, the leak size is 7.874 mm:

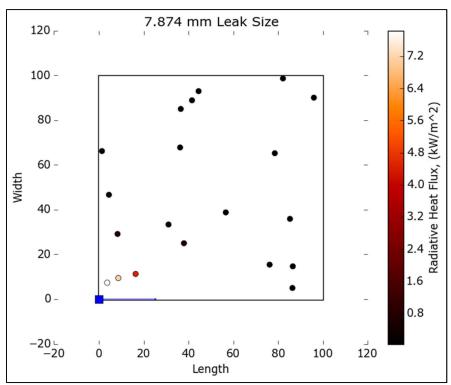


Figure 27: Plots Tab Output

The blue square in the corner of the generated facility plot represents the 7.874 mm hydrogen leak while the blue line on the bottom, x-axis, is the jet centerline of the hydrogen leak. The dots represent locations of the 20 facility occupants and respective dot colors indicate the radiative heat flux (in kW/m^2) that those facility occupants would experience relative to their locations to the hydrogen leak.

5.2. 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 [1]. Based on preceding example, the Risk Metric output is portrayed by Figure 28:

	Risk Metric	Value	Unit
•	Potential Loss of Life (PLL)	1.511e-12	Fatalities/system-year
	Fatal Accident Rate (FAR)	0.0000	Fatalities in 10^8 person-ho
	Average individual risk (AIR)	3.451e-13	Fatalities/year

Figure 28: Risk Metrics Output

6. PHYSICS MODE

6.1. Gas Plume Dispersion

The Gas Plume Dispersion window contains variables that calculate the characteristics of a gaseous hydrogen plume. Before clicking the Calculate button located at the bottom right of the window, the user should input values in the Plot Properties, Standard, and Advanced tabs.

6.1.1. Plot Properties

The Plot Properties tab, depicted by Figure 29, contains the characteristics of the output plot for the gaseous hydrogen plume. The user can alter the Plot Title, Lower/Upper Limit, and Contour Inputs to generate the appropriate plume characteristics.

Note: Saving a workspace will not save the Plot Properties input values, so the user will have to re-enter these values after loading a saved workspace. Saving a workspace will, however, save the entered Standard and Advanced values.

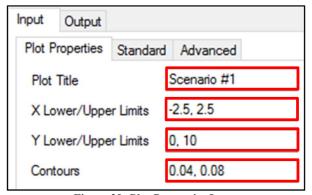


Figure 29: Plot Properties Input

6.1.2. Standard

The Standard input tab contains the standard physical variables that will affect the gaseous hydrogen plume. The orifice diameter (diameter of the release) is 3.25 mm. Figure 30 displays the Standard Input based on the preceding example.

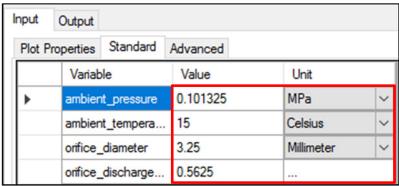


Figure 30: Standard Input

6.1.3. Advanced

The Advanced tab, shown in Figure 31, contains the advanced physical variables that will affect the gaseous hydrogen plume. Based on the preceding example, the Advanced Input would be:

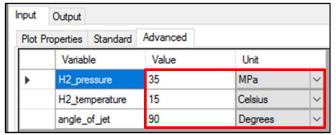


Figure 31: Advanced Tab Input

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

6.1.4. Gas Plume Dispersion Output

Figure 32 shows the Gas Plume Dispersion Output based on the preceding example.

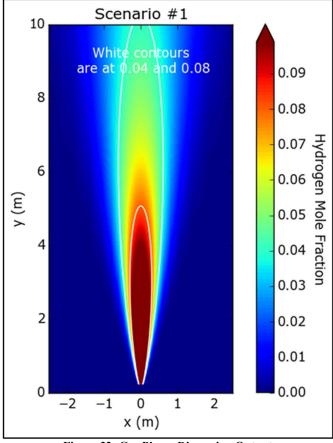


Figure 32: Gas Plume Dispersion Output

If the user wishes to save the output, click the Save Plot button located at the bottom right of the window.

6.2. Overpressure

6.2.1. Indoor Release Parameters

The Indoor Release Parameters tab contains measurements to calculate the overpressure 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 33.

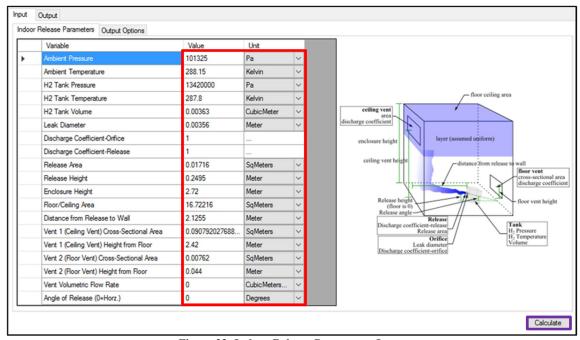


Figure 33: Indoor Release Parameters Input

6.2.2. Output Options

The Output Options tab, portrayed by Figure 34, 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 33) in the bottom right corner of the input window to produce the output.

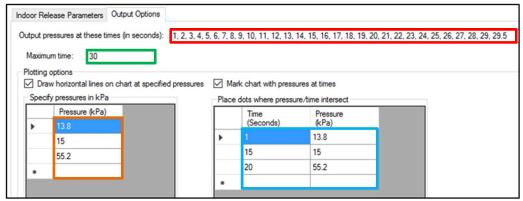


Figure 34: Output Options Input

6.2.3. Overpressure Output

The Output tab contains a Pressure plot, Flammable Mass plot, Layer plot, and Data table for those plots. Based on the default inputs, the Pressure plot is shown by Figure 35.

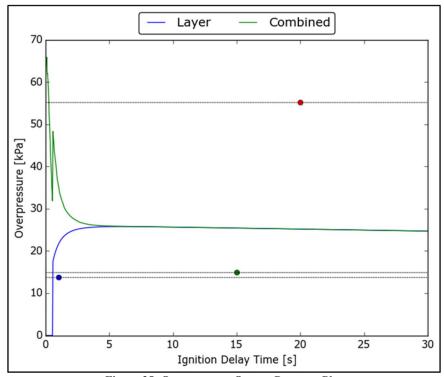


Figure 35: Overpressure Output Pressure Plot

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 36 shows the Flammable mass plot based on default inputs.

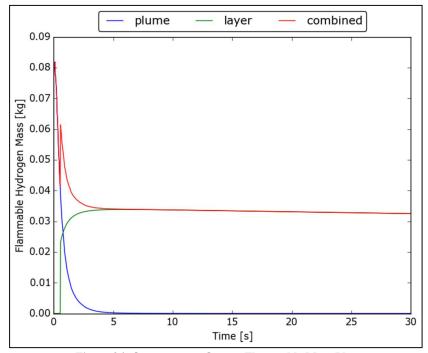


Figure 36: Overpressure Output Flammable Mass Plot

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 37 shows the Layer plot based on the default inputs.

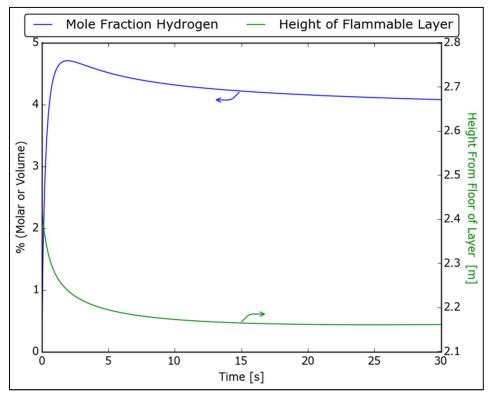
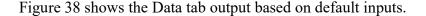


Figure 37: Overpressure Output Layer Plot

The Height of Flammable Layer represents the height of the hydrogen layer that develops above the floor. At 30 seconds, the hydrogen layer height is about 2.175 m above the floor and extends to the top of the enclosure. The hydrogen mole fraction of this layer is represented by the left vertical axis % (Molar or Volume). At 30 seconds, the hydrogen mole fraction is about 4%. It is assumed that at any point in space within the hydrogen layer, the hydrogen mole fraction is represented by % (Molar or Volume); i.e., the hydrogen mole fraction from 2.175 m to 2.72 m (height of enclosure) is 4% at 30 seconds.

Furthermore, in the Pressure plot (Figure 35), overpressure is non-zero from 0 seconds to 30 seconds. Comparing this 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 (χ_{H_2} = 0.04) in this timeframe. To save the output, the user must click the Save Plot button located at the bottom right of the window.

Note: HyRAM (version 1.1) incorrectly lists the hydrogen layer as the Height from Floor of Layer. The hydrogen layer can only be regarded as the flammable layer when the mole fraction is between 0.04 and 0.75. This label will be corrected in subsequent versions.



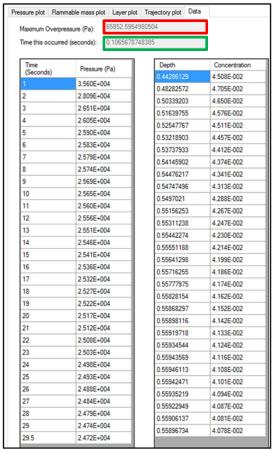


Figure 38: Overpressure Output Data

The units for Pressure and Time are Pa and seconds, respectively. The pressure data in the first table represents the overpressure of the combined plot in Figure 35. The concentration data in the second table represents the % (Molar or Volume) amounts given in the Layer Plot. In addition to the tabulated data, the Maximum Pressure (Pa) and Time this occurred (seconds) are provided in the Data tab, as shown in Figure 38.

6.3. Jet Flame

Jet Flame contains two windows: 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 flame temperature, direction, and heat flux. A hydrogen system in a warehouse has been modeled with flame and trajectory results based on the Notional Nozzle Model Birch2 with Input parameters shown in Figure 39.

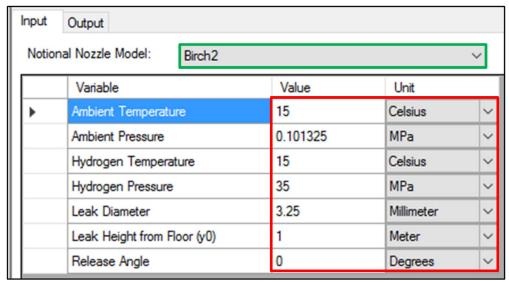


Figure 39: Flame Temperature/Trajectory Input

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 40.

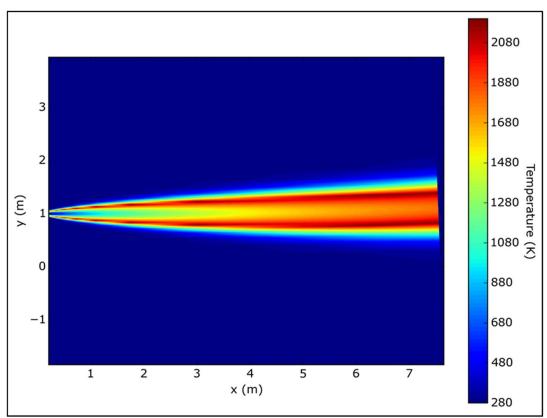


Figure 40: Flame Temperature/Trajectory Output

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 the temperature plot.

The user can specify both Notional Nozzle and Radiative Source Models, 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/m^2) 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 41.

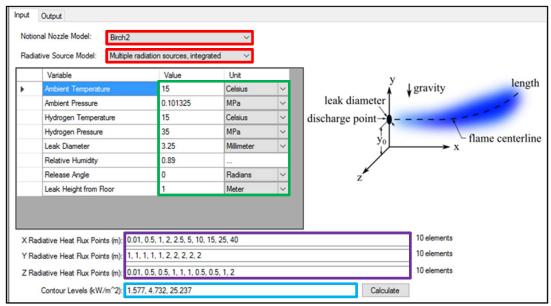


Figure 41: Radiative Heat Flux Input

Based on the preceding example, the Radiative Heat Flux output values are shown by Figure 42.

alues	s ISO plot Tem	perature Plot		
Radia	ative heat flux cald	culated (kW/m^2):		
	X (m)	Y (m)	Z (m)	Flux (kW/m^2)
•	0.0100	1.0000	0.0100	16.4435
	0.5000	1.0000	0.5000	19.2371
	1.0000	1.0000	0.5000	30.3459
	2.0000	1.0000	1.0000	25.3463
	2.5000	1.0000	1.0000	30.3498
	5.0000	2.0000	1.0000	29.9838
	10.0000	2.0000	0.5000	3.5119
	15.0000	2.0000	0.5000	0.8147
	25.0000	2.0000	1.0000	0.1961
	40.0000	2.0000	2.0000	0.0618

Figure 42: Radiative Heat Flux Values Output

The table provides the radiative heat flux calculated at the user specified positions (see Figure 41). By clicking the Copy to Clipboard button, the table is copied and can be pasted into another program, such as Microsoft Excel. The Radiative Heat Flux ISO Plot output is depicted in Figure 43.

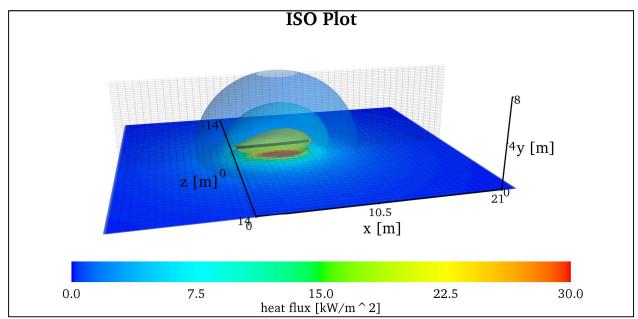


Figure 43: Radiative Heat Flux ISO Plot

The ISO plot output is a visual representation of the radiative heat flux. The image shows a plot of the 3-D isometric surfaces at which radiative heat flux is greater than or equal to the user specified contour levels (see Figure 41). 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 44.

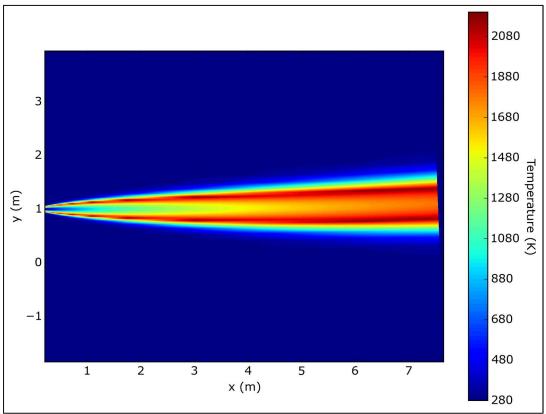


Figure 44: Radiative Heat Flux Temperature Plot

7. REFERENCES

- 1. Groth KM, Hecht ES, Reynolds JT, Blaylock ML, Carrier EE. Methodology for assessing the safety of Hydrogen Systems: HyRAM 1.1 Technical Reference Manual. Albuquerque, NM: Sandia National Laboratories, 2017 March. Report No.: SAND2017-2998.
- 2. Groth KM, Zumwalt HR, Clark AJ. HyRAM V1.0 User Guide. Albuquerque, NM: Sandia National Laboratories, 2016 March. Report No.: SAND2016-3385.
- 3. Groth KM, LaChance JL, Harris AP. Early-Stage Quantitative Risk Assessment to Support Development of Codes and Standard Requirements for Indoor Fueling of Hydrogen Vehicles. Albuquerque, NM: Sandia National Laboratories, 2012 November. Report No.: SAND2012-10150.
- 4. LaChance J, Houf W, Middleton B, Fluer L. Analyses to Support Development of Risk-Informed Separation Distances for Hydrogen Codes and Standards. Albuquerque, NM: Sandia National Laboratories, 2009 March. Report No.: SAND2009-0874.

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