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Benchmark Comparison of HyRAM and ALDEA Software for Hydrogen Release Behavior

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ABSTRACT

There are several different calculation approaches and tools that can be used to evaluate the risk of hydrogen energy applications. A comparative study of Air Liquide's ALDEA (Air Liquide Dispersion and Explosion Assessment) tools suite and Sandia's HyRAM (Hydrogen Risk Assessment Models) toolkit has been conducted. The purpose of this study was to understand and evaluate the differences between the two calculation approaches, and identify areas for model improvements. There were several scenarios examined in this effort regarding hydrogen release dynamics. These scenarios include free jet release cases at varying pressures, vessel blowdown, and hydrogen build-up scenarios with and without ventilation. For each scenario, the input and output of the HyRAM calculations are documented, along with a comparison to the ALDEA results. Generally, the results from the two different tools were reasonably aligned. However, there were fundamental differences in evaluation methodology and functional limitations in HyRAM that caused discrepancies in some calculations.

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ACRONYMS AND DEFINITIONS

Abbreviation	Definition
ALDEA	Air Liquide Dispersion and Explosion Assessment
HyRAM	Hydrogen Risk Assessment Models

1. INTRODUCTION

The Department of Energy and Sandia National Laboratories developed the Hydrogen Risk Assessment Models (HyRAM) toolkit that integrates data and methods relevant to assessing the safety of hydrogen fueling and storage infrastructure. The HyRAM toolkit integrates 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 overpressure effects from deflagration in enclosures. HyRAM incorporates generic probabilities for equipment failures for nine types of components, and probabilistic models for the effect of heat flux and overpressure on humans and structures. HyRAM also incorporates computationally and experimentally validated models of various aspects of hydrogen release and flame physics. HyRAM can be used to support multiple types of analysis, including code and standards development, safety basis development, and facility safety planning [1]. Further details and the software can be downloaded from hyram.sandia.gov. HyRAM version 3.1.0 was used for this analysis.

Air Liquide has an internal tool suite, titled the Air Liquide Dispersion and Explosion Assessment (ALDEA), which includes risk and consequence modeling for hydrogen and methane. The ALDEA tools suite includes models such as: high pressure and liquid releases and flammable cloud formation, delayed ignition and associate overpressure, hydrogen buildup in confined areas, jet fires and radiation, vented explosions and pressure vessel bursts. The models are based on Air Liquide research and development and open source publications. All models and scientific approaches implemented in ALDEA are published [2-18].

A comparative study of Air Liquide's ALDEA tools suite and Sandia's HyRAM toolkit has been performed to assess the risk of hydrogen energy applications and understand and evaluate the differences between the two calculation approaches. There were several scenarios examined in this effort regarding hydrogen release dynamics. These scenarios include free jet release cases at varying pressures, vessel blowdown, and hydrogen build-up scenarios with and without ventilation. For each scenario, the input and output of the HyRAM calculations are documented, along with a comparison to the ALDEA results.

The goal of the comparison is to improve both HyRAM and ALDEA toolkits if better models or calculations are identified in the study. This comparison will also serve as documentation for Air Liquide if, in the future, they wish to use HyRAM for future safety studies. Overall, the results and conclusions of this benchmark comparison exercise will improve future risk assessments performed by both toolkits and support the safe design of hydrogen fuel cell applications.

2. GASEOUS HYDROGEN RELEASE SCENARIOS

There are several different scenarios that were evaluated in HyRAM for the benchmarking effort, including cases related to high pressure free jet release, vessel behavior, and hydrogen accumulation in a room with and without ventilation. The specific inputs for each of the comparison cases are documented below.

2.1. Free Jet Release Scenarios

Table 2-1 shows the variables of interest for these scenarios. Note that the distance at a given percent is referring to the length of the plume, while the maximum jet radius at a given percent is referring to the width of the plume. The lower flammability limit for hydrogen is 4% (by volume), but it has been shown that in turbulent jets the concentration of more concern for ignition is around 10%. Concentrations between 4% and 10% may ignite locally but the flame kernel will extinguish. Concentrations above 10% have a much higher chance of forming a sustained jet flame after the local ignition. The different heat flux levels of 3, 5, and 8 kW/m^2 are a bit arbitrary (5 kW/m^2 is approximately the radiant heat flux to which a person can be exposed for 3 minutes); having the different levels enables comparison of the heat flux decay as a function of distance.

Table 2-1: Variables of Interest for Free Jet Release Scenarios

Variables of Interest
Release Mass Flow (g/sec)
Distance at 4% (m)
Distance at 10% (m)
Maximum Jet Radius (4%) (m)
Maximum Jet Radius (10%) (m)
Flame Length (m)
Distance (3 kW/m^2)
Distance (5 kW/m^2)
Distance (8 kW/m^2)

2.1.1. Low-pressure Free Jet Release Case

The low-pressure free jet release scenario models an important leak case in a H_2 production plant with the following relevant assumptions:

- Temperature: 15°C
- Release conditions
    - Gas released: H_2 at 40 bar
    - Orientation: Horizontal at 2 m from the floor
    - Circular breach (25 mm diameter)
    - Breach discharge coefficient C_d = 0.85
    - Continuous release, no decrease of the initial pressure

- Height of the observation for overpressure and radiation calculations: 1.5 m
- No wind
- The radiative fluxes are considered on the lateral sides on the flame
- The origin of the calculated distances is the release breach

Results Comparison with ALDEA

The results of the low-pressure free jet case from ALDEA and HyRAM are shown in Table 2-2. As shown, there is good agreement between the results of each evaluation method.

Table 2-2: Results Comparison of Low-pressure Free Jet Scenario

Variables of Interest	ALDEA Result	HyRAM Result
Release Mass Flow (g/sec)	1054	1047
Distance at 4% (m)	46	35
Distance at 10% (m)	18.5	13.5
Maximum Jet Radius (4%) (m)	2.6	4
Maximum Jet Radius (10%) (m)	1.1	1
Flame Length (m)	21	20
Distance (3 kW/m^2)	34	32
Distance (5 kW/m^2)	29	28
Distance (8 kW/m^2)	26	25

2.1.2. Medium-pressure Free Jet Release Case

The medium-pressure free jet release scenario models corrosion pinhole of 12 mm on the upper part of the pipeline with the following relevant assumptions:

- Temperature: 15°C
- Release conditions
  - Gas released: H_2 at 100 bar
  - Orientation: Vertical
  - Circular breach (12 mm diameter)
  - Breach discharge coefficient C_d = 0.85
  - Continuous release, no decrease of the initial pressure
- Height of the observation for overpressure and radiation calculations: 1.5 m
- No wind
- The origin of the calculated distances is the release breach

Results Comparison with ALDEA

The results of the medium-pressure free jet case from ALDEA and HyRAM are shown in Table 2-3. As shown, there is good agreement between the results of each evaluation method.

Table 2-3: Results Comparison of Medium-pressure Free Jet Scenario

Variables of Interest	ALDEA Result	HyRAM Result
Release Mass Flow (g/sec)	607	599
Distance at 4% (m)	35	25
Distance at 10% (m)	14	10
Maximum Jet Radius (4%) (m)	2	2
Maximum Jet Radius (10%) (m)	0.8	1
Flame Length (m)	15	15
Distance (3 kW/m^2)	10	11
Distance (5 kW/m^2)	8	8
Distance (8 kW/m^2)	6	5

2.1.3. High-pressure Free Jet Release Case

The high-pressure free jet release scenario models a leak in a hydrogen refueling station with the following relevant assumptions:

- Temperature: 15°C
- Release conditions
    - Gas released: H_2 at 700 bar
    - Orientation: Horizontal at 2 m from the floor
    - Circular breach (2 mm diameter)
    - Breach discharge coefficient C_d = 0.85
    - Continuous release, no decrease of the initial pressure
- Height of the observation for overpressure and radiation calculations: 1.5 m
- No wind
- The radiative fluxes are considered on the lateral sides of the flame
- The origin of the calculated distances is the release breach

Results Comparison with ALDEA

The results of the high-pressure free jet case from ALDEA and HyRAM are shown in Table 2-4. As shown, there is generally good agreement between the results of each evaluation method.

Table 2-4: Results Comparison of High-pressure Free Jet Scenario

Variables of Interest	ALDEA Result	HyRAM Result
Release Mass Flow (g/sec)	29.5	27
Distance at 4% (m)	8	5
Distance at 10% (m)	3	2
Maximum Jet Radius (4%) (m)	0.43	0.5
Maximum Jet Radius (10%) (m)	0.17	0.2
Flame Length (m)	3	3
Distance (3 kW/m^2)	4	4
Distance (5 kW/m^2)	3.5	3.6
Distance (8 kW/m^2)	3.2	3.25

2.2. Vessel Blowdown

The vessel blowdown scenarios model the blowdown of a pressurized vessel through different sized holes. The pressure drop considered is from an initial pressure of 700 bar down to a final pressure of 20 bar. The following relevant assumptions were used to evaluate these scenarios:

- Temperature: 15°C
- Composite type IV cylinder with an initial volume of 140 L

Table 2-5 shows the variables of interest for these scenarios.

Table 2-5: Variables of Interest for Free Jet Release Scenarios

Variables of Interest
Time for 1 mm release diameter
Time for 2.4 mm release diameter
Time for 4 mm release diameter

Results Comparison with ALDEA

The results of the vessel blowdown simulations from ALDEA and HyRAM are shown in Table 2-6. As shown, there are significant differences between the two methods of calculating blowdown. This is primarily due to the fact that currently, HyRAM assumes that the final pressure during a blowdown is ambient pressure (further assumed to be 101325 Pa). As described in Section A-2, this was approximated by calculating the blowdown time from the initial pressure (700 bar) and final pressure (20 bar) both to 101325 Pa and then subtracting the two times. However, this is likely not accurate. This is because HyRAM assumes an adiabatic tank, meaning that for the blowdown from 700 bar to ambient pressure, when the pressure is equal to 20 bar, the temperature of the gas in the tank will be much lower. By contrast, when a new blowdown simulation starts at 20 bar, the temperature is assumed to be at ambient temperature, resulting in different flowrates. This functionality could be added to a future release of HyRAM in order to improve the accuracy of this type of calculation.

Table 2-6: Results Comparison of Vessel Blowdown Scenarios

Variables of Interest	ALDEA Result	HyRAM Result
Time for 1 mm release diameter (s)	848	1016
Time for 2.4 mm release diameter (s)	147	176
Time for 4 mm release diameter (s)	53	63

2.3. Hydrogen Build-up in an Unventilated Room

Table 2-7 shows the variables of interest for this scenario.

Table 2-7: Variables of Interest for Hydrogen Build-up in an Unventilated Room Scenario

Variables of Interest
Max H_2% at 100 seconds
Max H_2% at 500 seconds
Max H_2% at 1,000 seconds
Max H_2% at 2,000 seconds
Max H_2% at 3,600 seconds

The scenario models the build-up of hydrogen inside a confined space like a garage or a room in the case of an accidental plume release. The following relevant assumptions were considered:

- Temperature: 15°C
- Closed unventilated empty room (4 m x 4 m x 2.5 m)
- Vertical upward release on the floor (60 NL/min)
- Release diameter of 100 mm
- Entrainment coefficient = 0.1

Results Comparison with ALDEA

The results of the hydrogen build-up in an unventilated room scenario from ALDEA and HyRAM are shown in Table 2-8. As shown, there is reasonable agreement between the results of each evaluation method. However, the HyRAM results are lower than the ALDEA results, which may be a result of the uniform concentration in the accumulation layer assumption made in HyRAM. Since HyRAM calculates the concentration values from the layer, which are near the ceiling, additional mixing may result in predictions of lower concentrations. Additionally, HyRAM does not assume a perfectly sealed enclosure; even with no ventilation, there is an escape to allow the hydrogen/air mixture to exit the enclosure. Therefore, if the hydrogen/air mixture is leaving the enclosure at the same volumetric rate that pure hydrogen is entering the enclosure, the resulting concentration will be lower than if all of the hydrogen was contained in the enclosure.

Table 2-8: Results Comparison of Hydrogen Build-up in an Unventilated Room Scenario

Variables of Interest	ALDEA Result	HyRAM Result
Max H_2% at 100 seconds	1	0.6
Max H_2% at 500 seconds	2.3	1.4
Max H_2% at 1,000 seconds	3.7	2.5
Max H_2% at 2,000 seconds	6.5	4.5
Max H_2% at 3,600 seconds	10.9	6.6

2.4. Hydrogen Build-up in a Naturally Ventilated Room

Table 2-9 shows the variables of interest for these scenarios.

Table 2-9: Variables of Interest for Hydrogen Build-up in a Naturally Ventilated Room Scenarios

Variables of Interest
Max H_2% at 50 NL/min
Max H_2% at 100 NL/min
Max H_2% at 250 NL/min
Max H_2% at 500 NL/min
Max H_2% at 1,000 NL/min
Max H_2% at 1,500 NL/min

2.4.1. Room with One Opening

This scenario evaluates the build-up of hydrogen inside a confined space as a result of an accidental release. The room is naturally ventilated due to the dedicated opening. This scenario was evaluated with the following relevant assumptions:

- Temperature: 15°C
- No external wind
- Empty room (5 m x 2.5 m x 2.5 m)
- Open vent on the upper part of the side wall (0.8 m x 0.3 m)
- No grids on vents
- Positive vertical release from the floor
- Release diameter of 200 mm

Results Comparison with ALDEA

The results of the hydrogen build-up in a naturally ventilated room with one opening scenario from ALDEA and HyRAM are shown in Table 2-10. As shown, there is significant disagreement between the results of each evaluation method. Moreover, the HyRAM results are much lower than the ALDEA results, which may be a result of the workarounds used to model the scenario in HyRAM. Similar to the previous scenario, this could be due to the uniform concentration assumption or the hydrogen/air mixture leaving the enclosure.

Table 2-10: Results Comparison of Hydrogen Build-up in a Naturally Ventilated Room (One Opening) Scenario

Variables of Interest	ALDEA Result	HyRAM Result
Max H_2% at 50 NL/min	4.2	1.0
Max H_2% at 100 NL/min	6.7	1.6
Max H_2% at 250 NL/min	12.4	2.8
Max H_2% at 500 NL/min	19.6	4.4
Max H_2% at 1,000 NL/min	31.2	6.7
Max H_2% at 1,500 NL/min	40.9	8.6

2.4.2. Room with Two Openings

This scenario evaluates the build-up of hydrogen inside a confined space as a result of an accidental release. The room is naturally ventilated due to the dedicated openings. This scenario was evaluated with the following relevant assumptions:

- Temperature: 15°C
- No external wind
- Empty room (5 m x 2.5 m x 2.5 m)
- Two open vents (0.8 m x 0.3 m) on opposite side walls, one at the top of the wall and the other at the bottom of the wall
- No grids on vents
- Positive vertical release from the floor
- Release diameter of 200 mm

Results Comparison with ALDEA

The results of the hydrogen build-up in a naturally ventilated room with two openings scenario from ALDEA and HyRAM are shown in Table 2-10. As shown, there is reasonable agreement between the results of each evaluation method. However, the HyRAM results are lower than the ALDEA results, which may be a result of the workarounds used to model the scenario in HyRAM. Similar to the previous scenarios, this could be due to the uniform concentration assumption or the hydrogen/air mixture leaving the enclosure. The HyRAM results do not appear to change from the scenario with one opening (Table 2-10). Without forced air (external wind), the natural ventilation rate calculated by HyRAM is likely the same, regardless of the number of openings while the ALDEA model seems to predict greater dilution with the addition of the secondary opening.

Table 2-11: Results Comparison of Hydrogen Build-up in a Naturally Ventilated Room (Two Openings) Scenario

Variables of Interest	ALDEA Result	HyRAM Result
Max H2% at 50 NL/min	1.6	1.0
Max H2% at 100 NL/min	2.5	1.6
Max H2% at 250 NL/min	4.5	2.8
Max H2% at 500 NL/min	7.2	4.4
Max H2% at 1,000 NL/min	11.4	6.7
Max H2% at 1,500 NL/min	15	8.6

3. LIQUID HYDROGEN RELEASE SCENARIOS

3.1. Pipe Full-Bore Rupture Before the Cryogenic Pump

Table 3-1 shows the variables of interest for this scenario.

Table 3-1: Variables of Interest for LH_2 Full Bore Rupture Case (Before Pump)

Variables of Interest
Release Mass Flow (g/sec)
Distance at 4% (m)
Distance at 10% (m)
Flame Length (m)
Distance (3 kW/m^2)
Distance (5 kW/m^2)
Distance (8 kW/m^2)

The scenario models the full-bore pipe rupture of liquid hydrogen before the pump. The following relevant assumptions were considered:

- Hydrogen mass: 1098 kg
- Saturated liquid at 8 bar
- Release diameter of 45 mm
- Orientation: horizontal
- Free field

Results Comparison with ALDEA

The results of the LH_2 full bore rupture case (before pump) from ALDEA and HyRAM are shown in Table 3-2. As shown, there is significant disagreement between the results of each evaluation method.

Table 3-2: Results Comparison of LH_2 Full Bore Rupture Case (Before Pump)

Variables of Interest	ALDEA Result Liquid H_2	ALDEA Result Cold gaseous H_2	HyRAM Result
Release Mass Flow (g/sec)	5730	2970	2683
Distance at 4% (m)	113	81	80
Distance at 10% (m)	45	32	35
Flame Length (m)	45	33	10
Distance (3 kW/m^2)	81	58	35.1
Distance (5 kW/m^2)	69	49	26.4
Distance (8 kW/m^2)	61	43	19.6

3.2. Pipe Partial Rupture Before the Cryogenic Pump

The Jet Flame/Radiative Heat Flux model and the Engineering Toolkit functions were used to calculate the liquid hydrogen pipe rupture results. Table 3-3 shows the variables of interest for this scenario.

Table 3-3: Variables of Interest for LH_2 Partial Bore Rupture Case (Before Pump)

Variables of Interest
Release Mass Flow (g/sec)
Distance at 4% (m)
Distance at 10% (m)
Flame Length (m)
Distance (3 kW/m^2)
Distance (5 kW/m^2)
Distance (8 kW/m^2)

The scenario models the full-bore pipe rupture of liquid hydrogen before the pump. The following relevant assumptions were considered:

- Hydrogen mass: 1098 kg
- Saturated liquid at 8 bar
- Release diameter of 8 mm
- Free field

Results Comparison with ALDEA

The results of the LH_2 partial bore rupture case (before pump) from ALDEA and HyRAM are shown in Table 3-4. As shown, there is significant disagreement between the results of each evaluation method. As these results were obtained, it was noted that the mass flow rate calculated by HyRAM for saturated liquid was more similar to the mass flow rate calculated by ALDEA for cold gaseous hydrogen (saturated vapor). Consequently, the HyRAM distances to different concentration levels and heat fluxes are also more in-line with the cold gaseous results from ALDEA. The mass flux for saturated liquid releases may be underpredicted by HyRAM; an aspect the development team for HyRAM is currently trying to resolve.

Table 3-4: Results Comparison of LH_2 Partial Bore Rupture Case (Before Pump)

Variables of Interest	ALDEA Result Liquid H_2	ALDEA Result Cold gaseous H_2	HyRAM Result
Release Mass Flow (g/sec)	181	94	85
Distance at 4% (m)	20	14	17
Distance at 10% (m)	8	6	6
Flame Length (m)	9	6.5	3
Distance (3 kW/m^2)	13.3	9.2	5.8
Distance (5 kW/m^2)	11.6	8.1	4.3
Distance (8 kW/m^2)	10.3	7.2	3.1

3.3. Pipe Full-Bore Rupture After the Cryogenic Pump

Table 3-5 shows the variables of interest for this scenario.

Table 3-5: Variables of Interest for LH_2 Full Bore Rupture Case (After Pump)

Variables of Interest
Distance at 4% (m)
Distance at 10% (m)
Flame Length (m)
Distance (3 kW/m^2)
Distance (5 kW/m^2)
Distance (8 kW/m^2)

The scenario models the full-bore pipe rupture of liquid hydrogen after the pump. The following relevant assumptions were considered:

- Leak flow rate imposed by the pump: 50 kg/hr
- Release diameter of 30.1 mm

- Supercritical state at 1000 bar
- Free field

Results Comparison with ALDEA

The results of the LH_2 full bore rupture case (after pump) from ALDEA and HyRAM are shown in Table 3-6. As shown, there is a slight disagreement between the results of each evaluation method. In this case, because the mass flow rate was specified and the fluid was supercritical, the differences are not as great as the previous case of rupture before the pump.

Table 3-6: Results Comparison of LH_2 Full Bore Rupture Case (After Pump)

Variables of Interest	ALDEA Result	HyRAM Result
Distance at 4% (m)	5	7
Distance at 10% (m)	2	5
Flame Length (m)	2	1.5
Distance (3 kW/m^2)	3	2.3
Distance (5 kW/m^2)	2	1.7
Distance (8 kW/m^2)	2	1.2

3.4. Pipe Partial Rupture After the Cryogenic Pump

The Jet Flame/Radiative Heat Flux model and the Engineering Toolkit functions were used to calculate the liquid hydrogen pipe rupture results. Table 3-7 shows the variables of interest for this scenario.

Table 3-7: Variables of Interest for LH_2 Partial Bore Rupture Case (After Pump)

Variables of Interest
Distance at 4% (m)
Distance at 10% (m)
Flame Length (m)
Distance (3 kW/m^2)
Distance (5 kW/m^2)
Distance (8 kW/m^2)

The scenario models the partial-bore pipe rupture of liquid hydrogen after the pump. The following relevant assumptions were considered:

- Leak flow rate imposed by the pump: 50 kg/hr
- Release diameter of 5.2 mm

- Supercritical state at 1000 bar
- Free field

Results Comparison with ALDEA

The results of the LH_2 partial-bore rupture case (after pump) from ALDEA and HyRAM are shown in Table 3-8. As shown, there is a slight disagreement between the results of each evaluation method. When comparing Table 3-8 to Table 3-7, the ALDEA results do not seem to be sensitive to the release diameter for a given flow rate, while the HyRAM model does predict some differences.

Table 3-8: Results Comparison of LH_2 Partial Bore Rupture Case (After Pump)

Variables of Interest	ALDEA Result	HyRAM Result
Distance at 4% (m)	5	7
Distance at 10% (m)	2	3
Flame Length (m)	2	3
Distance (3 kW/m^2)	3	3.7
Distance (5 kW/m^2)	2	3.3
Distance (8 kW/m^2)	2	2.9

4. SUMMARY AND CONCLUSIONS

A comparative study of Air Liquide's ALDEA tools suite and Sandia's HyRAM toolkit has been conducted. There were several scenarios examined in this effort regarding hydrogen release dynamics. Three free jet release scenarios were evaluated, including low-pressure, medium-pressure, and high-pressure cases. Generally, good agreement was seen between the results of the two toolkits. Both predicted similar distances to 4 and 10% concentrations, flame lengths, and distances to 3, 5, and 8 kW/m^2. A vessel blowdown case was evaluated in which the vessel was depressurized from 700 bar to 20 bar. The blowdown times for HyRAM in these scenarios were about 20% longer than those predicted by ALDEA. Longer HyRAM blowdown times are attributed to the fact that the engineering toolkit in HyRAM does not enable specification of the final pressure, and the workaround to 'stop' the blowdown at 20 bar did not account for all of the physics. Enabling specification of the final blowdown pressure within HyRAM is a feature request for future versions of HyRAM.

Three hydrogen build-up scenarios were evaluated. For each scenario, limitations in the HyRAM software required a workaround to be used to perform the evaluation. The first scenario evaluated build-up of hydrogen inside a confined space without ventilation, such as in the case of an accidental plume release. The results were aligned; however, HyRAM consistently predicted a lower maximum H_2% at each of the evaluated times. Next, two hydrogen build-up scenarios were evaluated with varying levels of natural ventilation. HyRAM predicted the same H_2% at each specified flowrate for both ventilation conditions. The results from HyRAM were consistent with the ALDEA results from the natural ventilation case with two openings. However, HyRAM underpredicted the H_2% when compared to the ALDEA results with a single opening.

In addition to the gaseous hydrogen scenarios, four liquid hydrogen release cases were evaluated. Pipe ruptures were modeled in the liquid hydrogen system for partial-bore and full-bore scenarios, before and after the cryogenic pump. Generally, for the liquid hydrogen modeling cases, the results between HyRAM and ALDEA were significantly different. Because of the differences, ALDEA calculations were performed for both liquid and cold gaseous hydrogen releases. The HyRAM results are similar to the ALDEA cold gaseous hydrogen results, especially the mass flow rate calculations. However, the large difference between the ALDEA liquid hydrogen mass flow rate and that of HyRAM leads to the large differences in the distances to concentration levels, flame length, and distance to heat flux values. The calculation of liquid hydrogen flowrates within HyRAM will be reviewed and updated in a future release, as the ALDEA calculations of liquid hydrogen flows are believed to be more accurate.

Generally, the results from the two different tools were well aligned for the gaseous hydrogen simulations. However, there were fundamental differences in evaluation methodology and functional limitations that caused discrepancies in some calculations. Several assumptions and workarounds implemented in HyRAM to match the prescriptive conditions led to many of the differences between the two modeling software packages. Improvements to the HyRAM toolkit have been identified by this work and will be implemented in a future release.

5. REFERENCES

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APPENDIX A. HYRAM CALCULATIONS

This appendix documents the inputs and outputs from the HyRAM version 3.1.0 software for each of the scenarios in this report.

A-1. Free Jet Release Scenarios

The Gas Plume Dispersion model, Jet Flame/Radiative Heat Flux model, and the Engineering Toolkit functions were used to evaluate the free jet release scenarios.

A-1.1. Low-pressure Free Jet Release Case

Engineering Toolkit

The engineering toolkit was used to calculate the release mass flow of the low-pressure free jet case. Figure A-1 shows the input parameters used in the calculation.

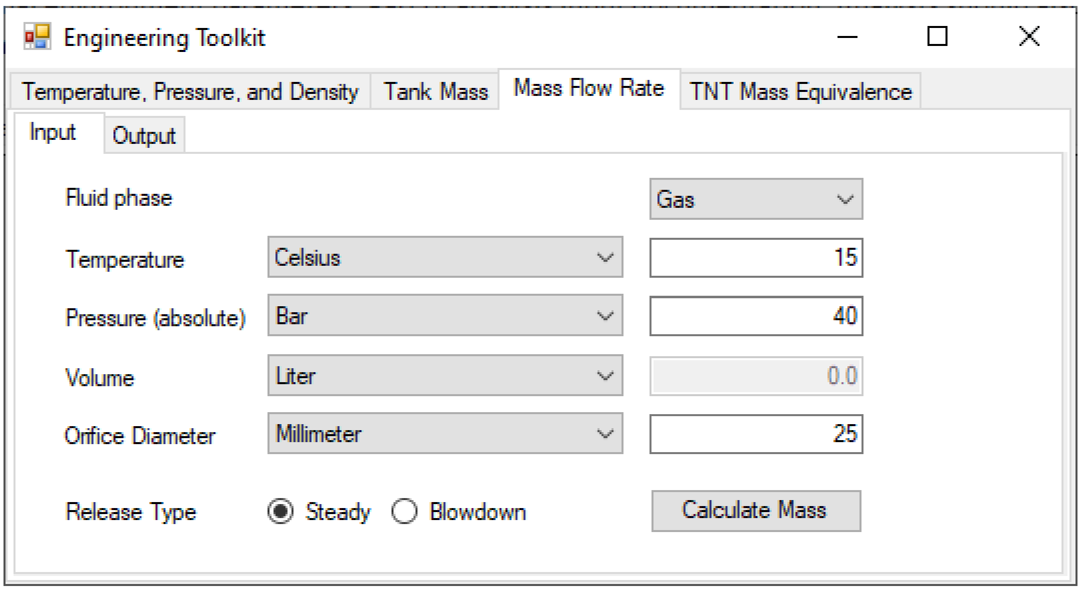


Figure A-1 : Input to Engineering Toolkit for Low-pressure Jet Release Case

Using these inputs, the mass flow rate was calculated (as shown in Figure A-2). Note, the calculated mass flow rate of 1,232 g/s does not account for the discharge coefficient of 0.85. When correcting the HyRAM output for the discharge coefficient, the mass flow rate would be 1,047 g/s.

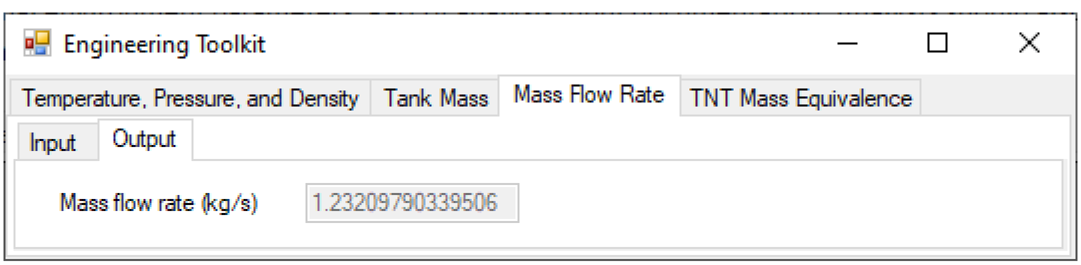


Figure A-2 : Output of Engineering Toolkit Calculation for Low-pressure Jet Release Case

Gas Plume Dispersion Model

The gas plume dispersion model was used to calculate the horizontal distance of the hydrogen at different mole fractions, as well as the maximum width of the cloud for different mole fractions. Figure A-3 and Figure A-4 show the inputs to the gas plume dispersion model for the 4% and 10% mole fraction calculations, respectively.

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	45	Meter
Y lower limit	-3	Meter
Y upper limit	3	Meter
Contours (mole fraction)	0.04	...
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Orifice diameter	25	Millimeter
Orifice discharge coefficient	0.85	...
Angle of jet	0	Radians
Fluid pressure (absolute)	40	Bar
Fluid temperature	15	Celsius

Figure A-3 : Input for 4% Mole Fraction Calculation for Low-pressure Jet Release Case

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	20	Meter
Y lower limit	-3	Meter
Y upper limit	3	Meter
Contours (mole fraction)	0.1	...
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Orifice diameter	25	Millimeter
Orifice discharge coefficient	0.85	...
Angle of jet	0	Radians
Fluid pressure (absolute)	40	Bar
Fluid temperature	15	Celsius

Figure A-4 : Input for 10% Mole Fraction Calculation for Low-pressure Jet Release Case

Figure A-5 and Figure A-6 show the results of the 4% and 10% mole fraction calculations, respectively. From these figures, the variables of interest were visually determined. For the 4% mole fraction case, the horizontal distance was determined to be approximately 35 meters, while the maximum width of the cloud was determined to be approximately 4 meters. For the 10% mole fraction case, the horizontal distance was determined to be approximately 13.5 meters, while the maximum width of the cloud is approximately 1 meter.

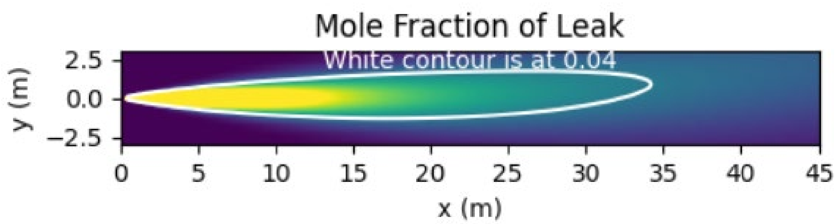


Figure A-5 : Contour at 4% Mole Fraction for Low-pressure Jet Release Case

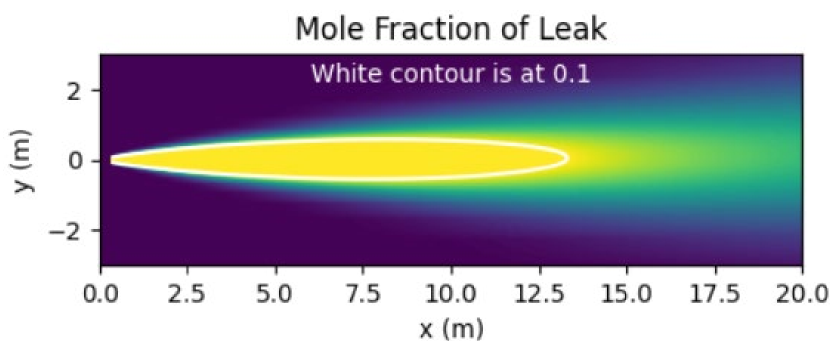


Figure A-6 : Contour at 10% Mole Fraction for Low-pressure Jet Release Case

Jet Flame/Radiative Heat Flux Model

The jet flame/radiative heat flux model was used to calculate the flame length, as well as the horizontal distance at which certain heat flux values were reached. Figure A-7 shows the input used in the jet flame/radiative heat flux model calculations.

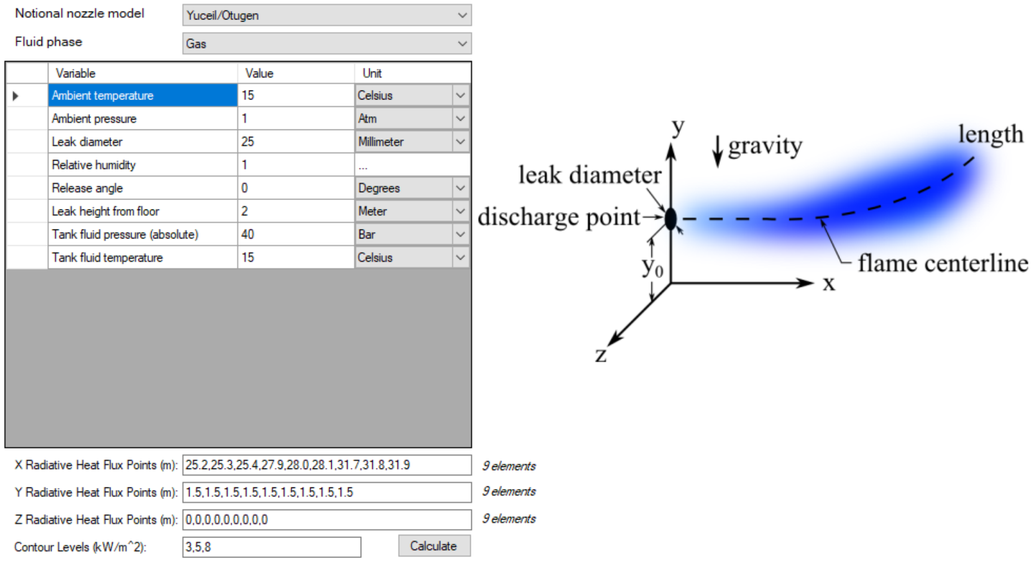


Figure A-7 : Input for the Jet Flame Model Calculation for Low-pressure Jet Release Case

Table A-1 shows the radiative heat flux results for the low-pressure jet release case. As shown, the horizontal distances at which heat flux of 3, 5, and 8 kW/m2 are seen are approximately 31.8 meters, 28.0 meters, and 25.2 meters, respectively.

Table A-1 : Radiative Heat Flux Results for Low-pressure Jet Release Case

X(m)	Y(m)	Z(m)	Flux (kW/m^2)
25.2	1.5	0	8.0750
25.3	1.5	0	7.9202
25.4	1.5	0	7.7698
27.9	1.5	0	5.0704
28.0	1.5	0	4.9935
28.1	1.5	0	4.9185
31.7	1.5	0	3.0468
31.8	1.5	0	3.0112
31.9	1.5	0	2.9762

Figure A-8 shows the flame length for the low-pressure jet release case. From this figure, the variable of interest was visually determined to be approximately 20 meters.

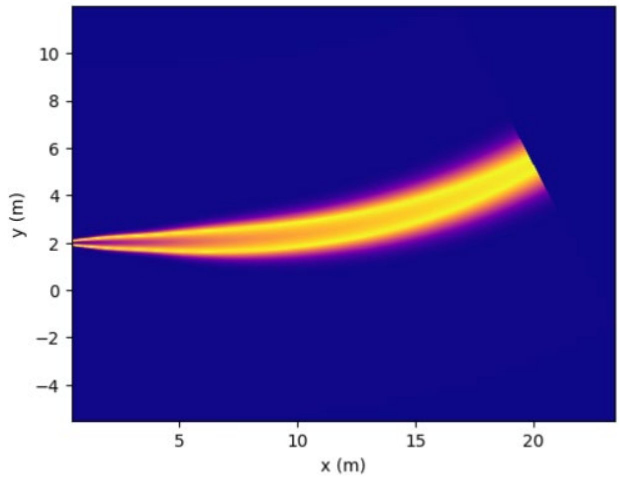


Figure A-8 : Flame Length for Low-pressure Jet Release Case

A-1.2. Medium-pressure Free Jet Release Case

Engineering Toolkit

The engineering toolkit was used to calculate the release mass flow of the medium-pressure free jet case. Figure A-9 shows the input parameters used in the calculation.

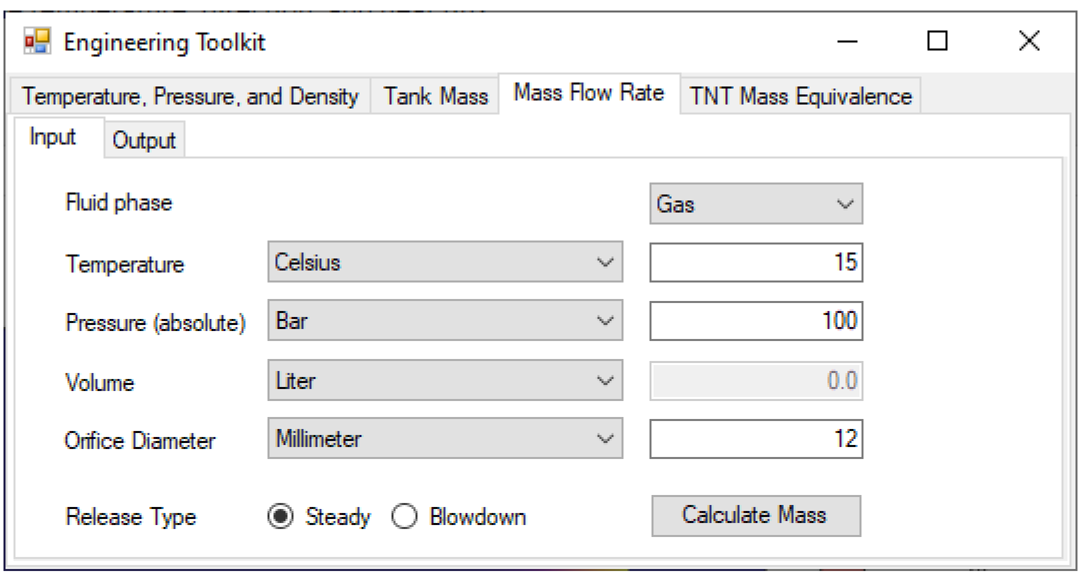


Figure A-9 : Input to Engineering Toolkit for Medium-pressure Jet Release Case

Using these inputs, the mass flow rate was calculated (as shown in Figure A-10). Note, the calculated mass flow rate of 705 g/s does not account for the discharge coefficient of 0.85. When correcting the HyRAM output for the discharge coefficient, the mass flow rate would be 599 g/s.

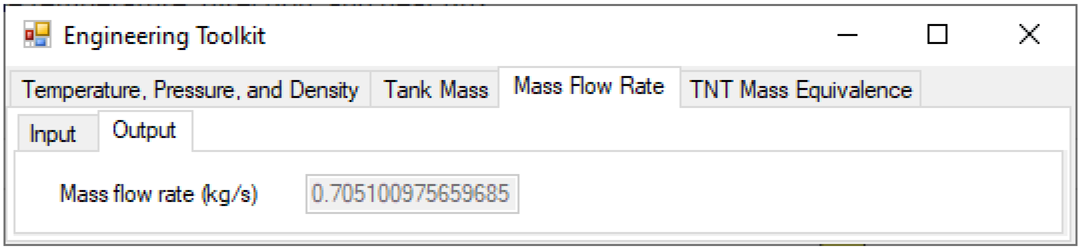


Figure A-10 : Output of Engineering Toolkit Calculation for Medium-pressure Jet Release Case

Gas Plume Dispersion Model

The gas plume dispersion model was used to calculate the vertical distance of the hydrogen at different mole fractions, as well as the maximum width of the cloud for different mole fractions. Figure A-11 and Figure A-12 show the input to the gas plume dispersion model for the 4% and 10% mole fraction calculations, respectively.

Variable	Value	Unit
X lower limit	-2	Meter
X upper limit	2	Meter
Y lower limit	0	Meter
Y upper limit	35	Meter
Contours (mole fraction)	0.04	...
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Orifice diameter	12	Millimeter
Orifice discharge coefficient	0.85	...
Angle of jet	90	Degrees
Fluid pressure (absolute)	100	Bar
Fluid temperature	15	Celsius

Figure A-11 : Input for 4% Mole Fraction Calculation for Medium-pressure Jet Release Case

	Variable	Value	Unit
▸	X lower limit	-2	Meter
	X upper limit	2	Meter
	Y lower limit	0	Meter
	Y upper limit	15	Meter
	Contours (mole fraction)	0.1	...
	Ambient pressure	1	Atm
	Ambient temperature	15	Celsius
	Orifice diameter	12	Millimeter
	Orifice discharge coefficient	0.85	...
	Angle of jet	90	Degrees
	Fluid pressure (absolute)	100	Bar
	Fluid temperature	15	Celsius

Figure A-12 : Input for 10% Mole Fraction Calculation for Medium-pressure Jet Release Case

Figure A-13 and Figure A-14 show the results of the 4% and 10% mole fraction calculations, respectively. From these figures, the variables of interest were visually determined. For the 4% mole fraction case, the vertical distance was determined to be approximately 25 meters, while the maximum width of the cloud was determined to be approximately 2 meters. For the 10% mole fraction case, the vertical distance was determined to be approximately 10 meters, while the maximum width of the cloud is approximately 1 meter.

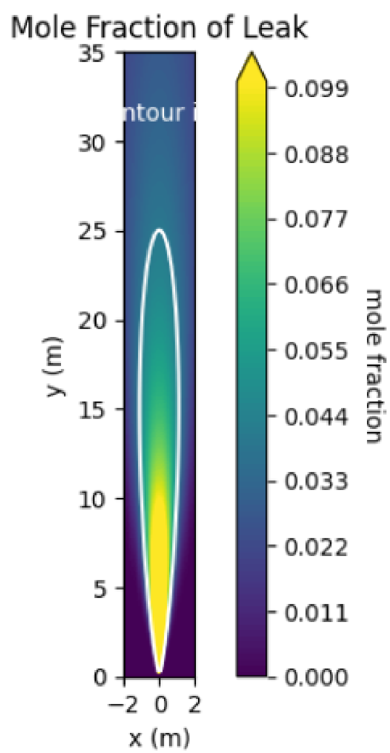


Figure A-13 : Contour at 4% Mole Fraction for Medium-pressure Jet Release Case

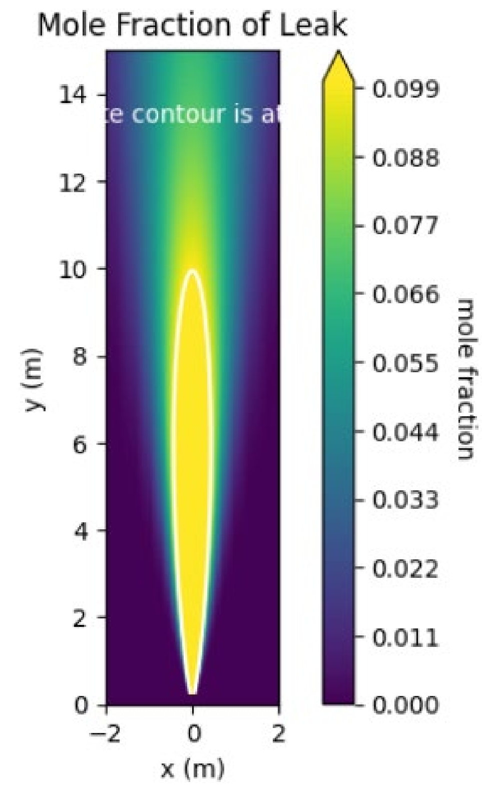


Figure A-14 : Contour at 10% Mole Fraction for Medium-pressure Jet Release Case

Jet Flame/Radiative Heat Flux Model

The jet flame/radiative heat flux model was used to calculate the flame length, as well as the horizontal distance at which certain heat flux values were reached. Figure A-15 shows the input used in the jet flame/radiative heat flux model calculations.

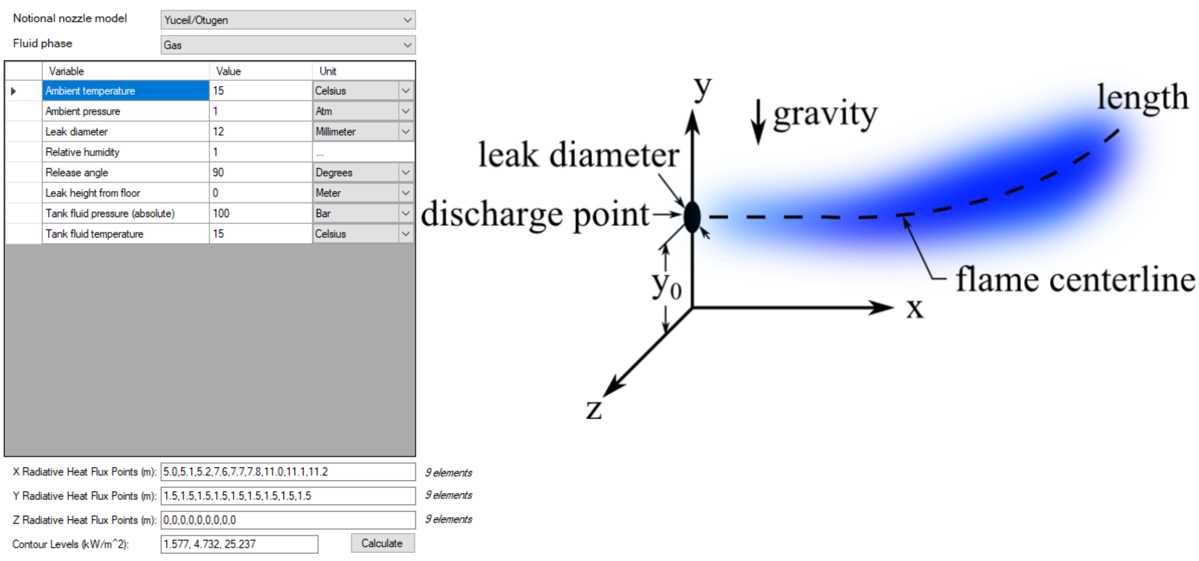


Figure A-15 : Input for the Jet Flame Model Calculation for Medium-pressure Jet Release Case

Table A-2 shows the radiative heat flux results for the medium-pressure jet release case. As shown, the horizontal distances at which heat flux of 3, 5, and 8 kW/m2 are seen are approximately 11.1 meters, 7.7 meters, and 5.2 meters, respectively.

Table A-2 : Radiative Heat Flux Results for Medium-pressure Jet Release Case

X(m)	Y(m)	Z(m)	Flux (kW/m^2)
5.0	1.5	0.0	8.3276
5.1	1.5	0.0	8.1493
5.2	1.5	0.0	7.9769
7.6	1.5	0.0	5.0694
7.7	1.5	0.0	4.9842
7.8	1.5	0.0	4.9010
11.0	1.5	0.0	3.0209
11.1	1.5	0.0	2.9798
11.2	1.5	0.0	2.9395

Figure A-16 shows the flame length for the medium-pressure jet release case. From this figure, the variable of interest was visually determined to be approximately 15 meters.

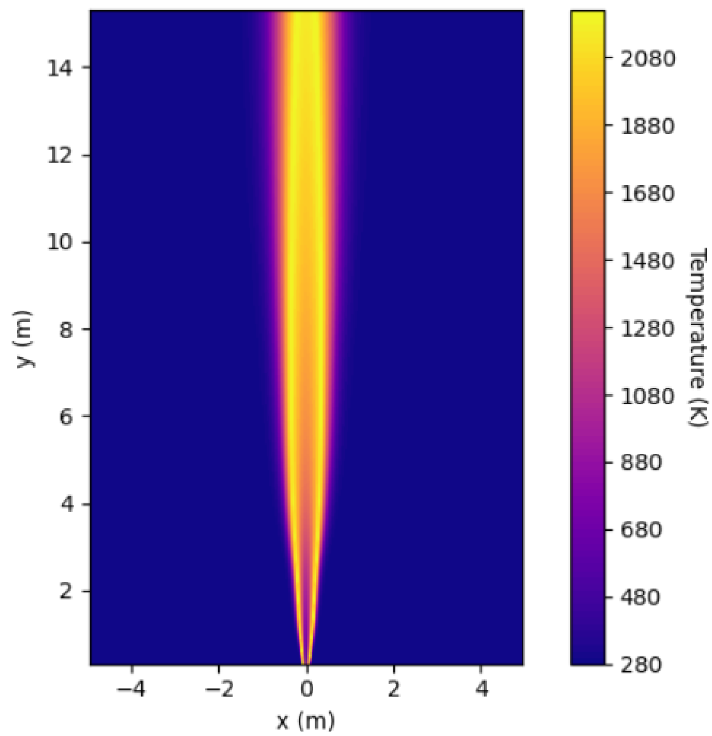


Figure A-16 : Flame Length for Medium-pressure Jet Release Case

A-1.3. High-pressure Free Jet Release Case

Engineering Toolkit

The engineering toolkit was used to calculate the release mass flow of the high-pressure free jet case. Figure A-17 shows the input parameters used in the calculation.

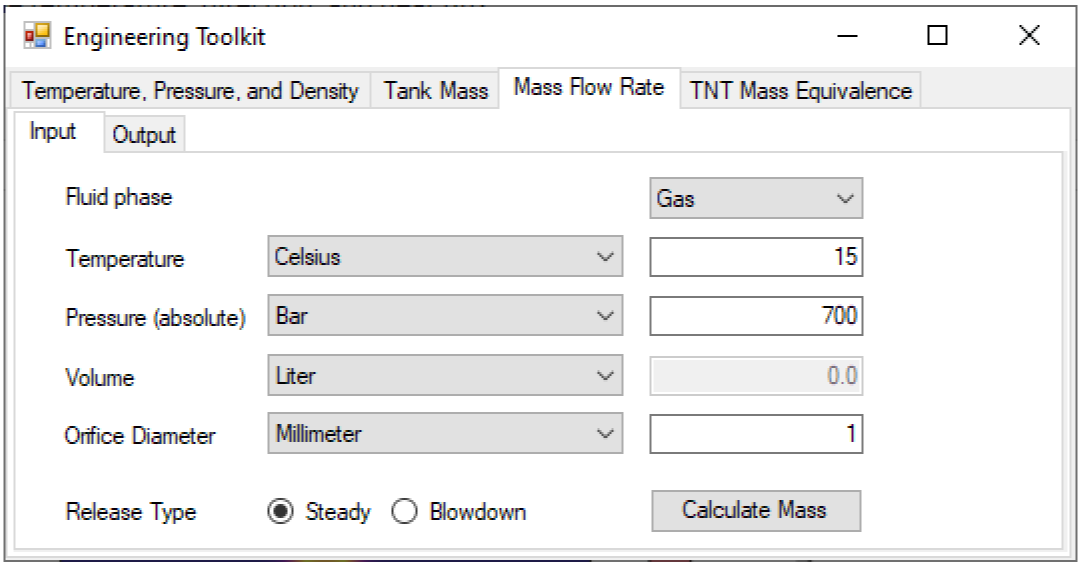


Figure A-17 : Input to Engineering Toolkit for High-pressure Jet Release Case

Using these inputs, the mass flow rate was calculated (as shown in Figure A-18). Note, the calculated mass flow rate of 32 g/s does not account for the discharge coefficient of 0.85. When correcting the HyRAM output for the discharge coefficient, the mass flow rate would be 27 g/s.

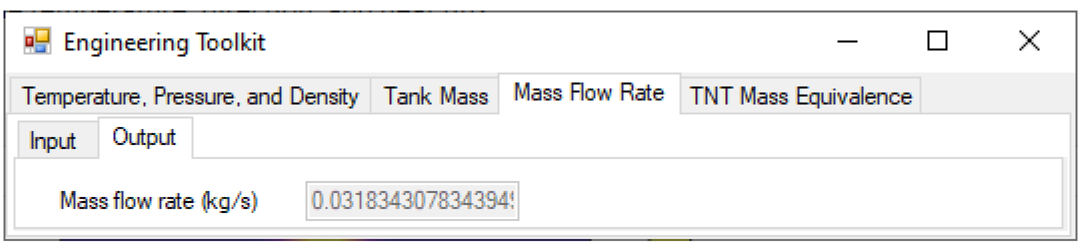


Figure A-18 : Output of Engineering Toolkit Calculation for High-pressure Jet Release Case

Gas Plume Dispersion Model

The gas plume dispersion model was used to calculate the vertical distance of the hydrogen at different mole fractions, as well as the maximum width of the cloud for different mole fractions. Figure A-19 and Figure A-20 show the input to the gas plume dispersion model for the 4% and 10% mole fraction calculations, respectively.

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	8	Meter
Y lower limit	-0.5	Meter
Y upper limit	0.5	Meter
Contours (mole fraction)	0.04	...
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Orifice diameter	1	Millimeter
Orifice discharge coefficient	0.85	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	700	Bar
Fluid temperature	15	Celsius

Figure A-19 : Input for 4% Mole Fraction Calculation for High-pressure Jet Release Case

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	4	Meter
Y lower limit	-0.2	Meter
Y upper limit	0.2	Meter
Contours (mole fraction)	0.1	...
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Orifice diameter	1	Millimeter
Orifice discharge coefficient	0.85	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	700	Bar
Fluid temperature	15	Celsius

Figure A-20 : Input for 10% Mole Fraction Calculation for High-pressure Jet Release Case

Figure A-21 and Figure A-22 show the results of the 4% and 10% mole fraction calculations, respectively. From these figures, the variables of interest were visually determined. For the 4% mole fraction case, the horizontal distance was determined to be approximately 5 meters, while the maximum width of the cloud was determined to be approximately 0.5 meters. For the 10% mole fraction case, the horizontal distance was determined to be approximately 2 meters, while the maximum width of the cloud is approximately 0.2 meters.

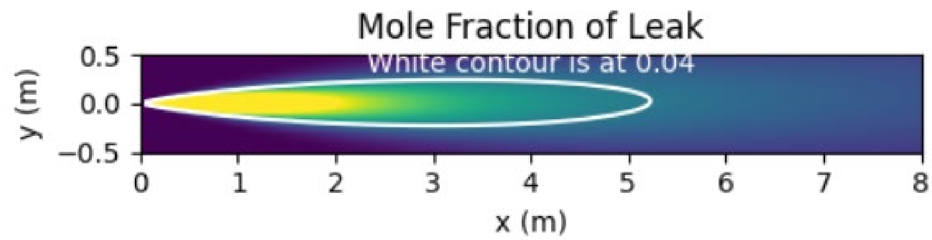


Figure A-21 : Contour at 4% Mole Fraction for High-pressure Jet Release Case

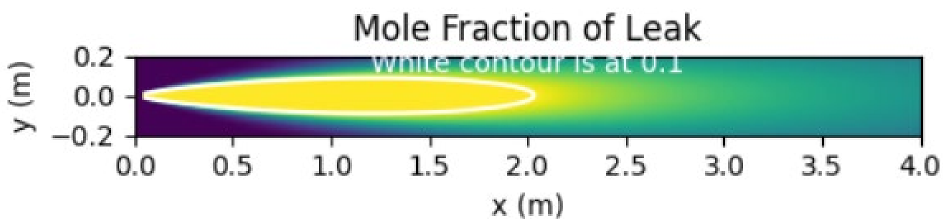


Figure A-22 : Contour at 10% Mole Fraction for High-pressure Jet Release Case

Jet Flame/Radiative Heat Flux Model

The jet flame/radiative heat flux model was used to calculate the flame length, as well as the horizontal distance at which certain heat flux values were reached. Figure A-23 shows the input used in the jet flame/radiative heat flux model calculations.

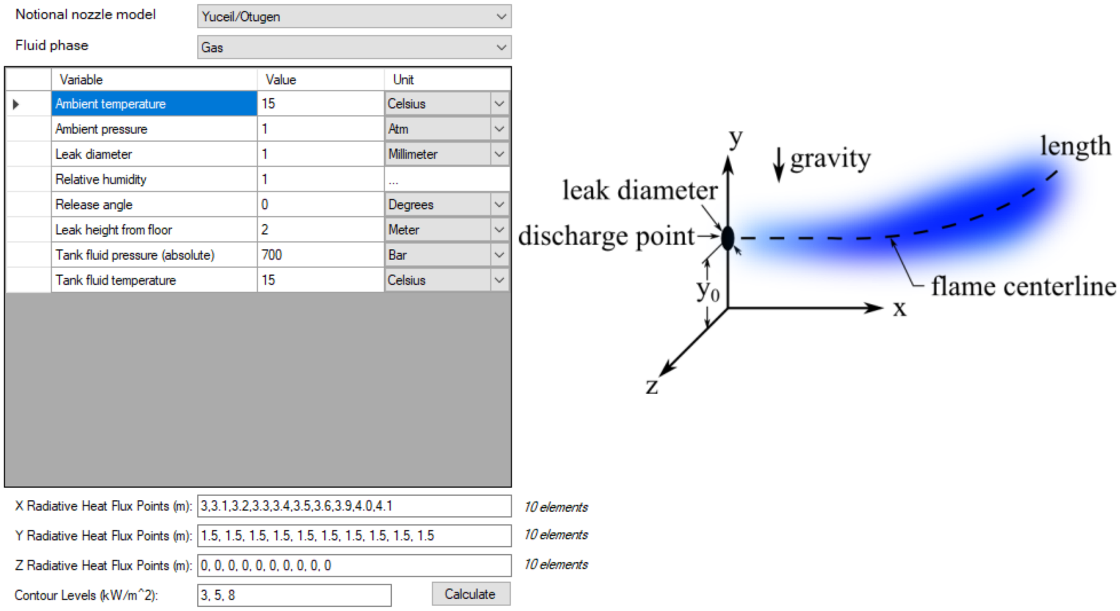


Figure A-23 : Input for the Jet Flame Model Calculation for High-pressure Jet Release Case

Table A-3 shows the radiative heat flux results for the High-pressure jet release case. As shown, the horizontal distances at which heat flux of 3, 5, and 8 kW/m2 are seen are approximately 4 meters, 3.6 meters, and 3.25 meters, respectively.

Table A-3 : Radiative Heat Flux Results for High-pressure Jet Release Case

X(m)	Y(m)	Z(m)	Flux (kW/m^2)
3.0	1.5	0.0	11.8228
3.1	1.5	0.0	10.1254
3.2	1.5	0.0	8.6538
3.3	1.5	0.0	7.4087
3.4	1.5	0.0	6.3717
3.5	1.5	0.0	5.5146
3.6	1.5	0.0	4.8067
3.9	1.5	0.0	3.3215
4.0	1.5	0.0	2.9746
4.1	1.5	0.0	2.6791

Figure A-24 shows the flame length for the high-pressure jet release case. From this figure, the variable of interest was visually determined to be approximately 3 meters.

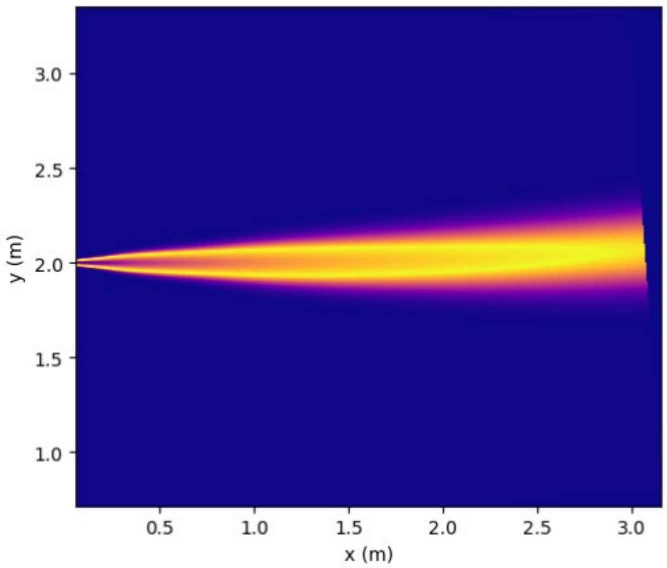


Figure A-24 : Flame Length for High-pressure Jet Release Case

A-2. Vessel Blowdown

The Engineering Toolkit function was used to evaluate the vessel blowdown scenarios.

The engineering toolkit was used to calculate the (adiabatic) blowdown times for the different orifice sizes. To consider the blowdown time from 700 bar to 20 bar, the blowdown time of 700 bar to 0 bar was calculated first. Subsequently, the blowdown time from 20 bar to 0 bar was calculated and subtracted from the 700 bar blowdown time.

A-2.1. 1 mm Orifice Diameter

Figure A-25 and Figure A-26 show the input parameters used to calculate the blowdown times for 700 bar and 20 bar, respectively.

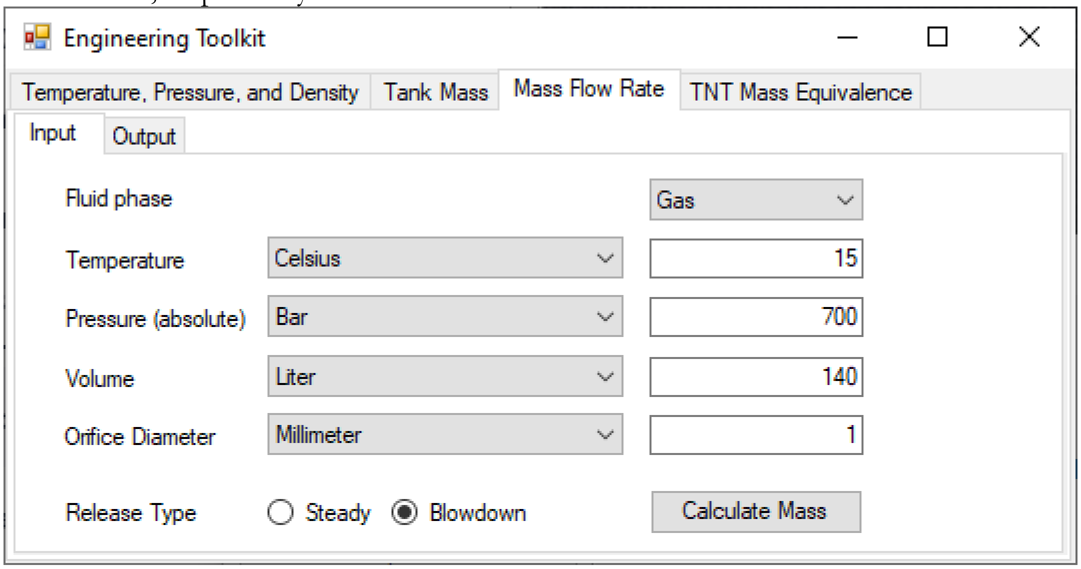


Figure A-25 : Input to Engineering Toolkit for 1 mm Blowdown Case (700 bar)

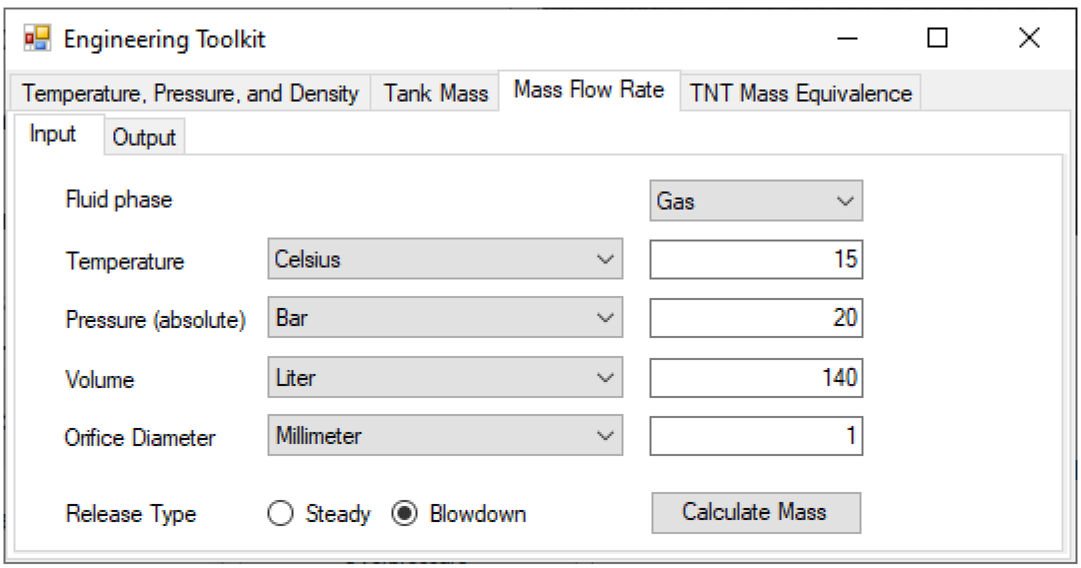


Figure A-26 : Input to Engineering Toolkit for 1 mm Blowdown Case (20 bar)

Figure A-27 and Figure A-28 show the time to empty for the 700 bar and 20 bar cases, respectively. The blowdown time from 700 bar to 20 bar is calculated 1684 seconds – 668 seconds = 1,016 seconds.

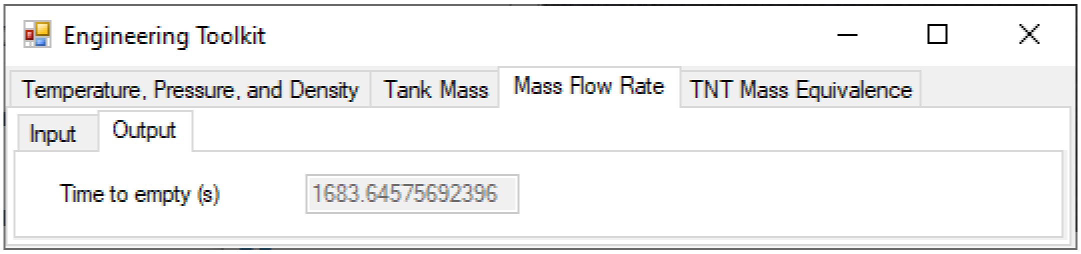


Figure A-27 : Blowdown time for 1 mm Case (700 bar)

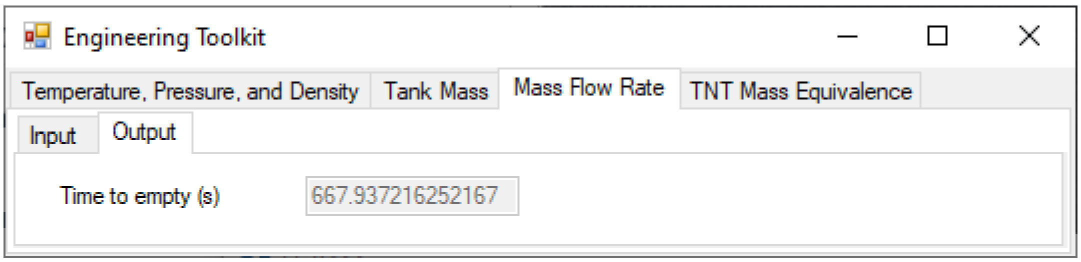


Figure A-28 : Blowdown time for 1 mm Case (20 bar)

A-2.2. 2.4 mm Orifice Diameter

Figure A-29 and Figure A-30 show the input parameters used to calculate the blowdown times for 700 bar and 20 bar, respectively.

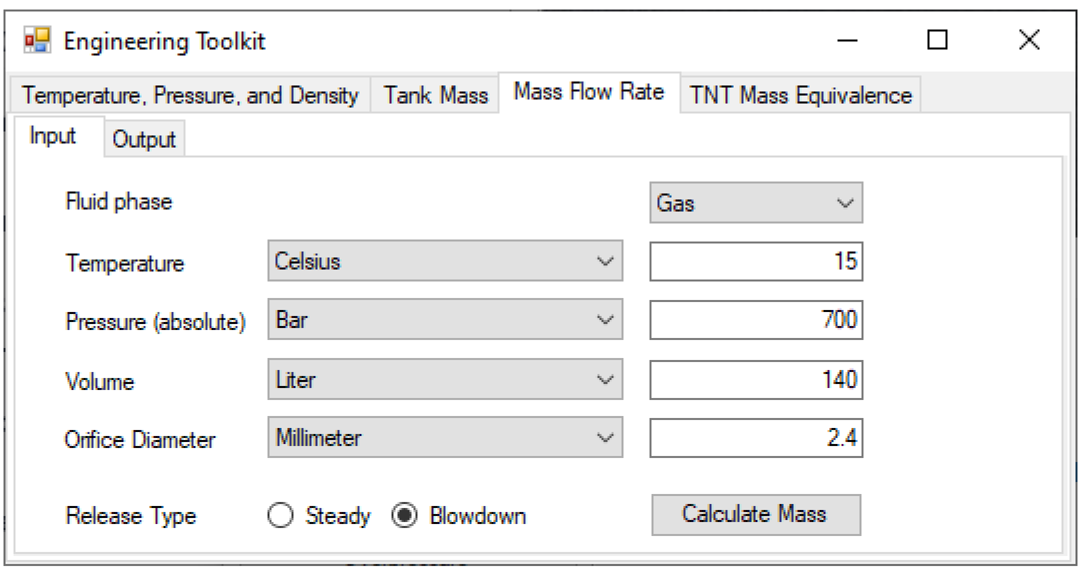


Figure A-29 : Input to Engineering Toolkit for 2.4 mm Blowdown Case (700 bar)

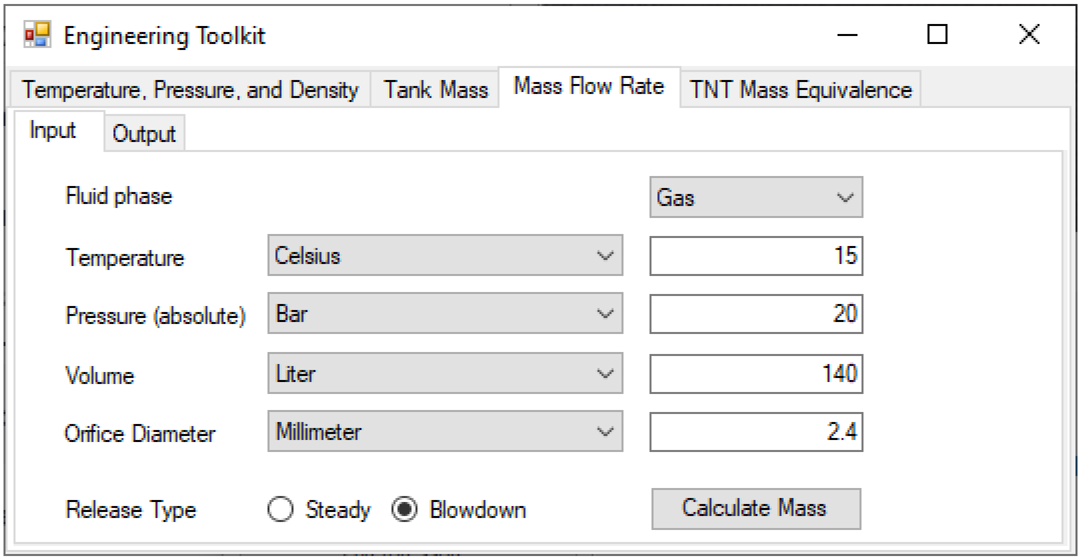


Figure A-30 : Input to Engineering Toolkit for 2.4 mm Blowdown Case (20 bar)

Figure A-31 and Figure A-32 show the time to empty for the 700 bar and 20 bar cases, respectively. The blowdown time from 700 bar to 20 bar is calculated 292 seconds – 116 seconds = 176 seconds.

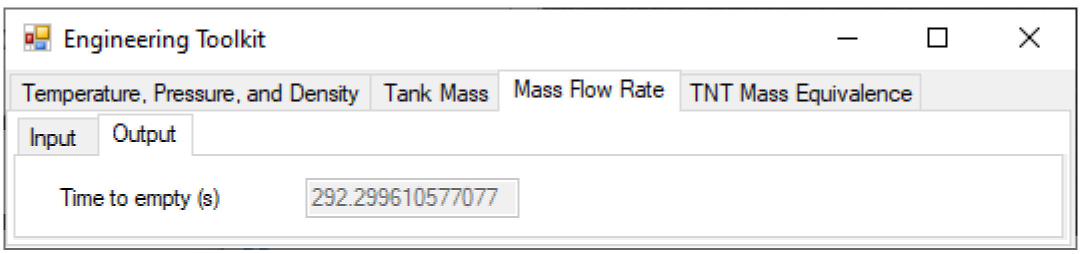


Figure A-31 : Blowdown time for 2.4 mm Case (700 bar)

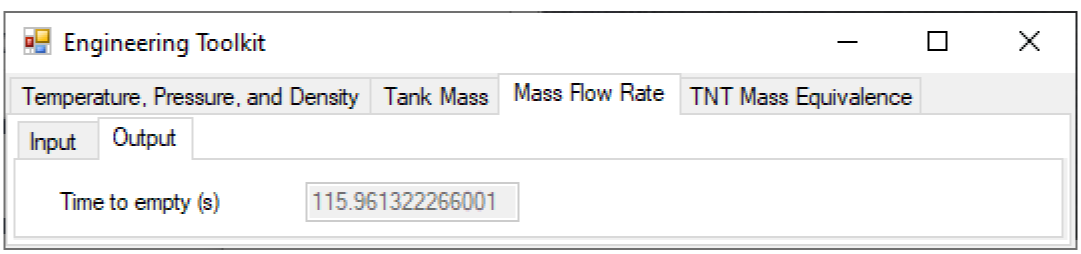


Figure A-32 : Blowdown time for 2.4 mm Case (20 bar)

A-2.3. 4 mm Orifice Diameter

Figure A-33 and Figure A-34 show the input parameters used to calculate the blowdown times for 700 bar and 20 bar, respectively.

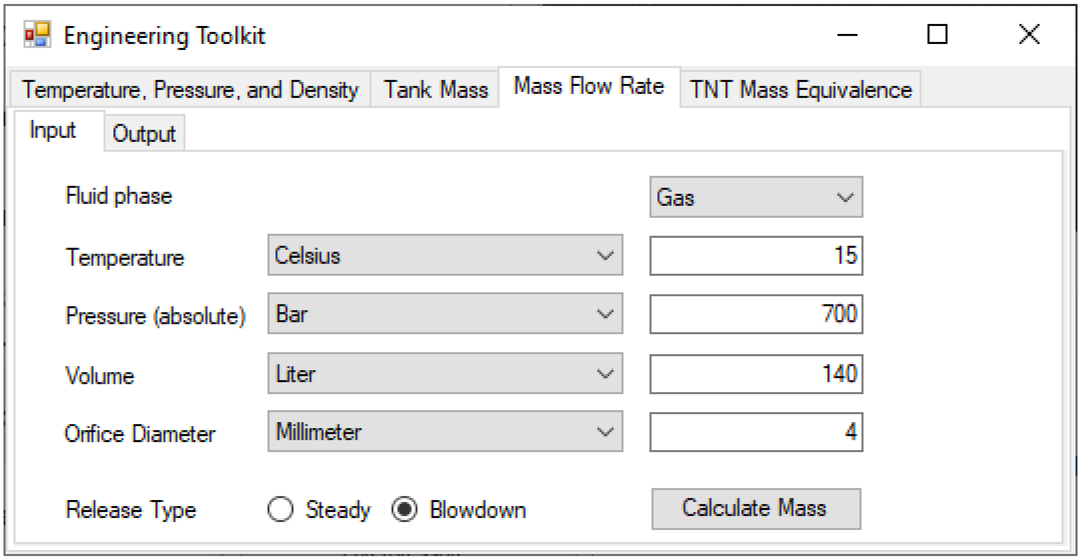


Figure A-33 : Input to Engineering Toolkit for 4 mm Blowdown Case (700 bar)

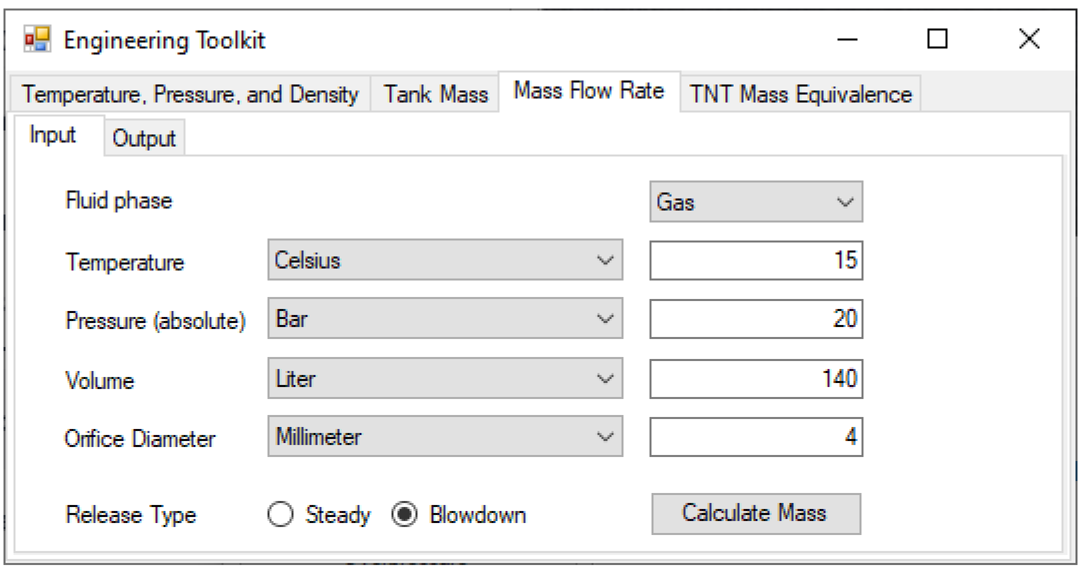


Figure A-34 : Input to Engineering Toolkit for 4 mm Blowdown Case (20 bar)

Figure A-35 and Figure A-36 show the time to empty for the 700 bar and 20 bar cases, respectively. The blowdown time from 700 bar to 20 bar is calculated 105 seconds – 42 seconds = 63 seconds.

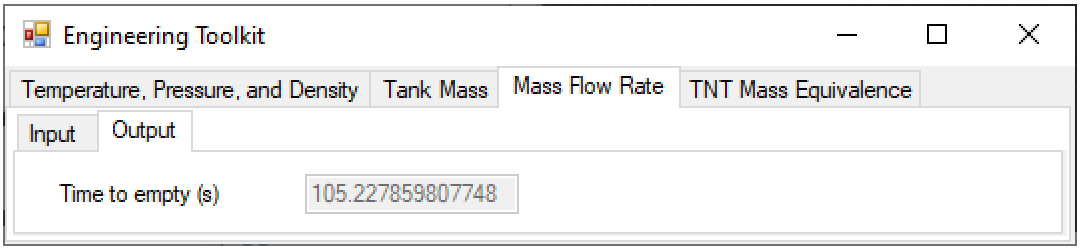


Figure A-35 : Blowdown time for 4 mm Case (700 bar)

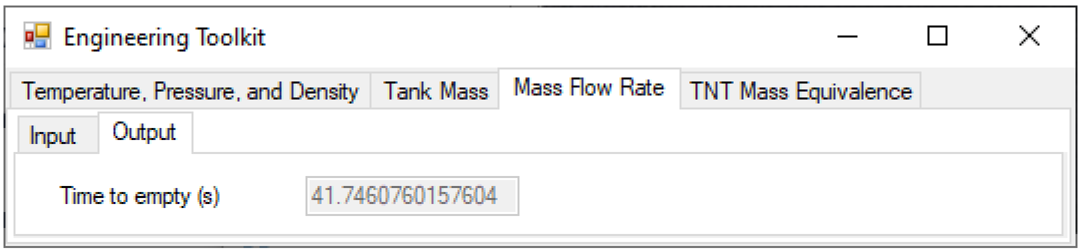


Figure A-36 : Blowdown time for 4 mm Case (20 bar)

A-3. Hydrogen Build-up in an Unventilated Room

The Engineering Toolkit and Accumulation functions were used to evaluate the hydrogen build-up in an unventilated room scenario.

HyRAM cannot directly model the case as prescribed due to the following limits in functionality:

1. HyRAM does not allow the user to prescribe a steady-flow of hydrogen into an enclosed area (see workaround below).
2. The HyRAM accumulation model cannot model a hermetically sealed confined space. The calculations include natural ventilation. To minimize the effect of natural ventilation on these results, the vent area was minimized and the vent height was maximized. The vent parameters used in these cases are shown in Figure A-39. The vent height was maximized due to the process that HyRAM uses to calculate the hydrogen concentration. The initial layer in which the hydrogen accumulates and mixes with air is the volume between the top of the vent and the total height of the enclosure. As hydrogen continues to accumulate, the mixing layer grows. This will give a better time-resolved hydrogen concentration then assuming the vent is lower in the enclosure.

Note that originally, a comparison of a jet release case was supposed to be evaluated in addition to the plume release in an unventilated room case. However, due to these limitations, the results of each case would be identical in HyRAM. Therefore, only the plume case was modeled for comparison.

Engineering Toolkit

To approximate a steady-flow of hydrogen, a large H_2 tank was modeled with low pressure. Note that in order to match the prescribed rate of 60 L/min, an orifice diameter of 100 mm could not be used. Instead, an orifice diameter of 0.95 mm was input into HyRAM. Figure A-37 and Figure A-38 show the H_2 tank input parameters and resulting mass flow rate, respectively. As shown, a theoretical tank with 100 ML volume, 2 bar pressure, and a 0.95 mm orifice diameter results in a 0.00009 kg/s flow rate over the time range of interest. This flow rate is converted to NL/min using a hydrogen density of 0.09 kg/m^3 (H_2 @ 0 °C, 1 atm) as follows:

$$Q = \frac{0.00009\frac{kg}{s}}{0.09\frac{kg}{m^3}} * \frac{1000\ L}{1\ m^3} * \frac{60\ s}{1\ min} = \sim 60\,\frac{NL}{min}$$

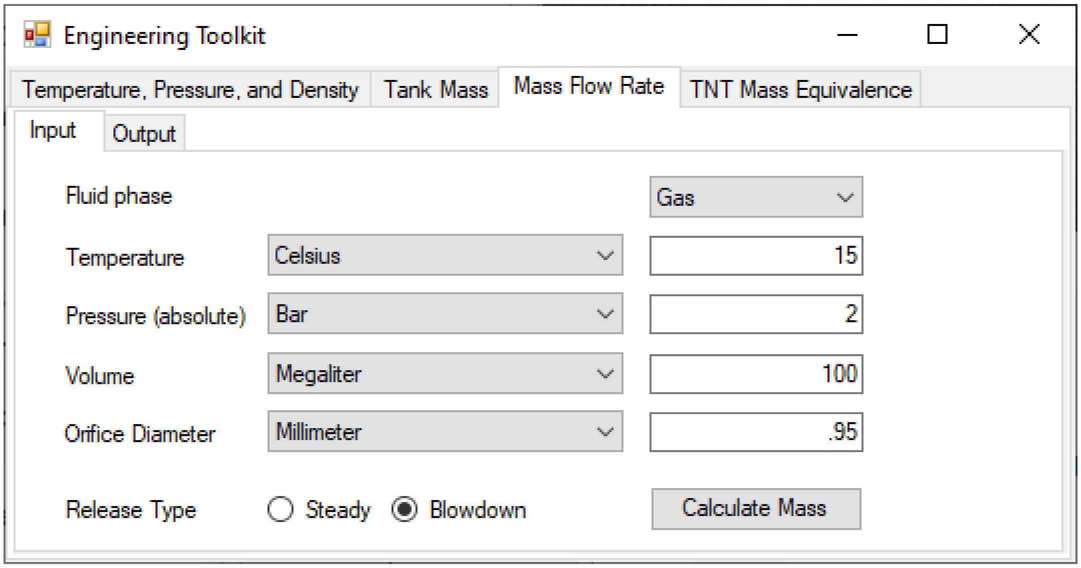


Figure A-37 : Steady Flow H2 Tank Inputs for Plume Case

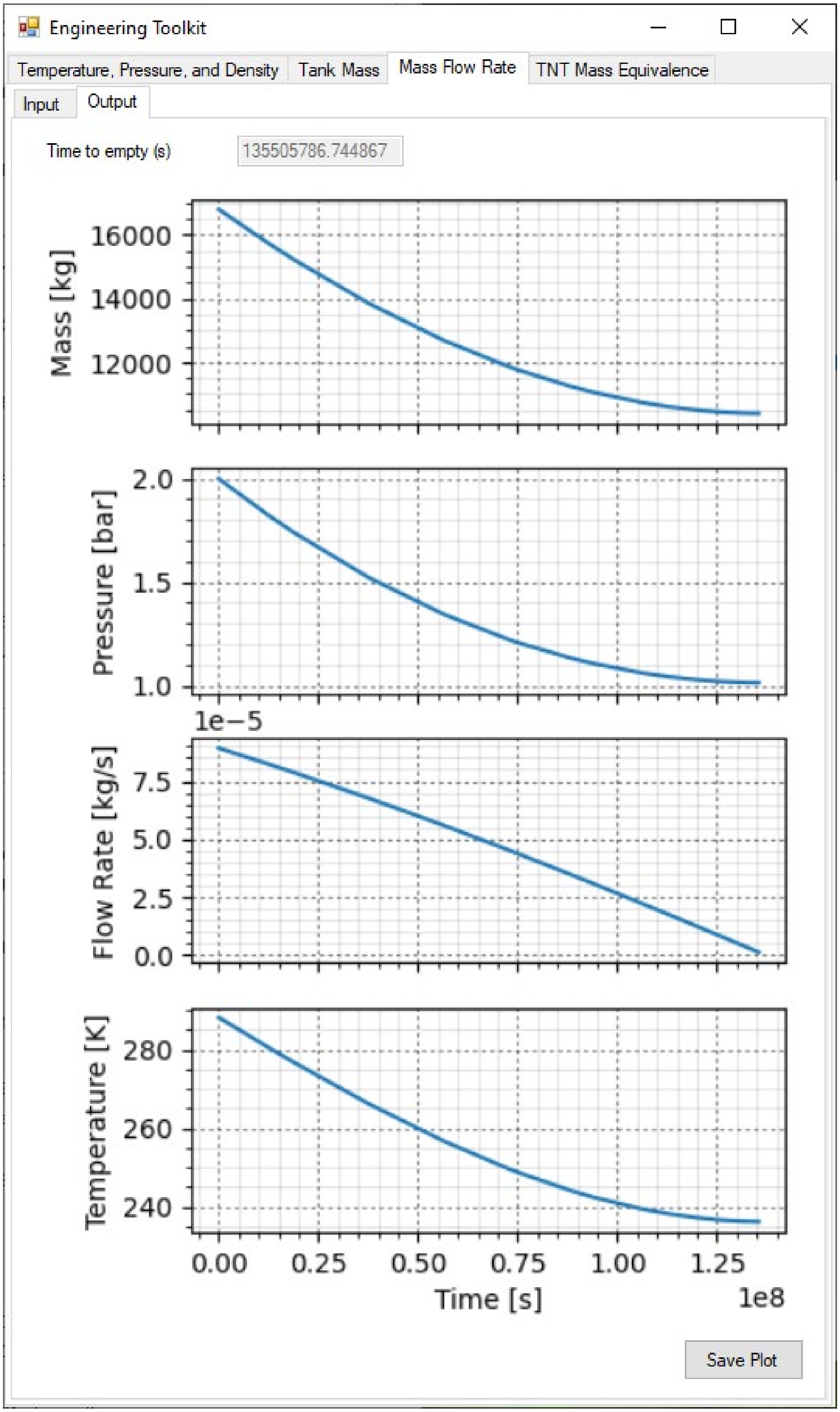


Figure A-38 : Steady Flow H2 Tank Mass Flow Rate for Plume Case

Accumulation Model

With the tank parameters set, the Accumulation model in HyRAM can be used to calculate the hydrogen build-up as a function of time. Figure A-39 shows the inputs into the accumulation model. Note, the release area of the leak (0.7085 mm^2) was calculated from the orifice leak diameter of 0.95 mm and the discharge coefficient of 1.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	0.95	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	7.085E-07	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	16	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.008	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0.008	SqMeters
Vent 2 (floor vent) height from floor	2.4	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-39 : Accumulation model Inputs for HyRAM Plume Calculations

Figure A-40 shows the resulting plot of H2 concentration as a function of time. Note that HyRAM calculates the concentration values from the layer, which are near the ceiling. As shown, the hydrogen concentration is approximately 0.6% at 100 seconds, 1.4% at 500 seconds, 2.5% at 1000 seconds, 4.5% at 2000 seconds, and 6.6% at 3600 seconds.

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 323,927.03

Time this Occurred (Seconds): 1.237E+04

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	6.128E-001	1.079	0.598
500	4.236E-001	2.269	1.385
1000	1.723E-001	2.423	2.501
2000	1.462E+005	2.409	4.483
3600	2.286E+005	2.388	6.588

Figure A-40 : Results of Accumulation model Calculations from HyRAM for Plume Case

A-4. Hydrogen Build-up in a Naturally Ventilated Room

The Engineering Toolkit and Accumulation functions were used to evaluate the hydrogen build-up in a naturally ventilated room scenarios.

A-4.1. Room with One Opening

The accumulation model was used to calculate the hydrogen percentage values as a function of volumetric flowrate. The steady-flow workaround documented in Section 2.3 was employed in this section as well. Table A-4 shows the equivalent mass flow rate, and orifice inputs used to achieve the steady-flow rates. As in the hydrogen build up in a closed room, the temperature (15 °C), pressure (2 bar), and volume (100 ML) were kept constant.

Table A-4 : Steady-Flow Inputs for HyRAM for One Opening Scenario

Flow Rate (NL/min)	Mass Flow Rate (kg/s)	Orifice Diameter (mm)	Orifice Area (mm^2)
50	0.000075	0.866	0.5887
100	0.00015	1.226	1.1799
250	0.000375	1.935	2.9392
500	0.00075	2.74	5.8935
1000	0.0015	3.875	11.7873
1500	0.00225	4.75	17.7116

50 NL/min Case

Figure A-41 and Figure A-42 show the input parameters and the mass flow rate for the 50 NL/min steady flow case, respectively.

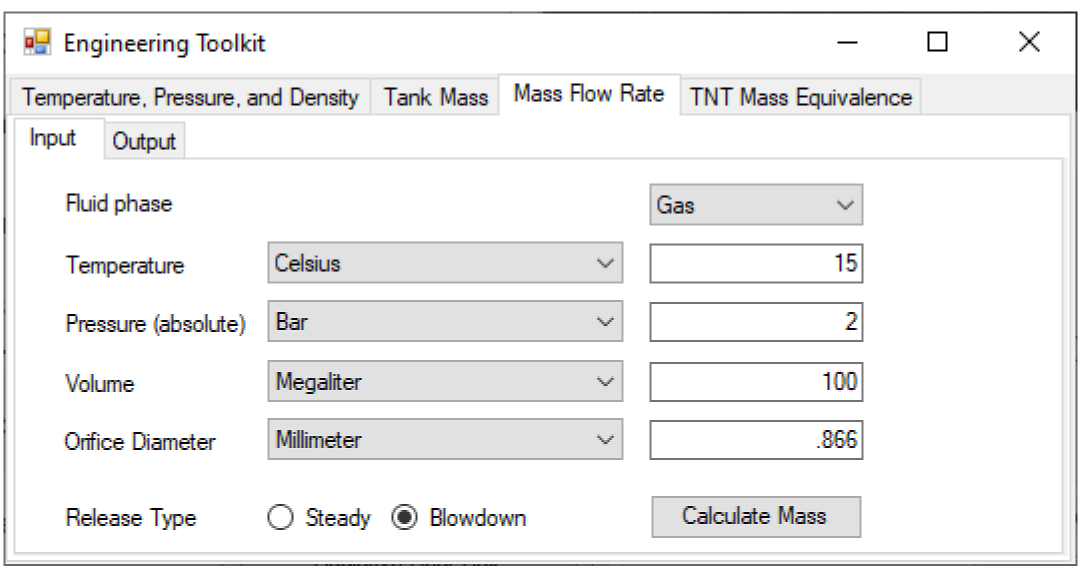


Figure A-41 : Steady Flow H2 Tank Inputs for 50 NL/min Case (One Opening)

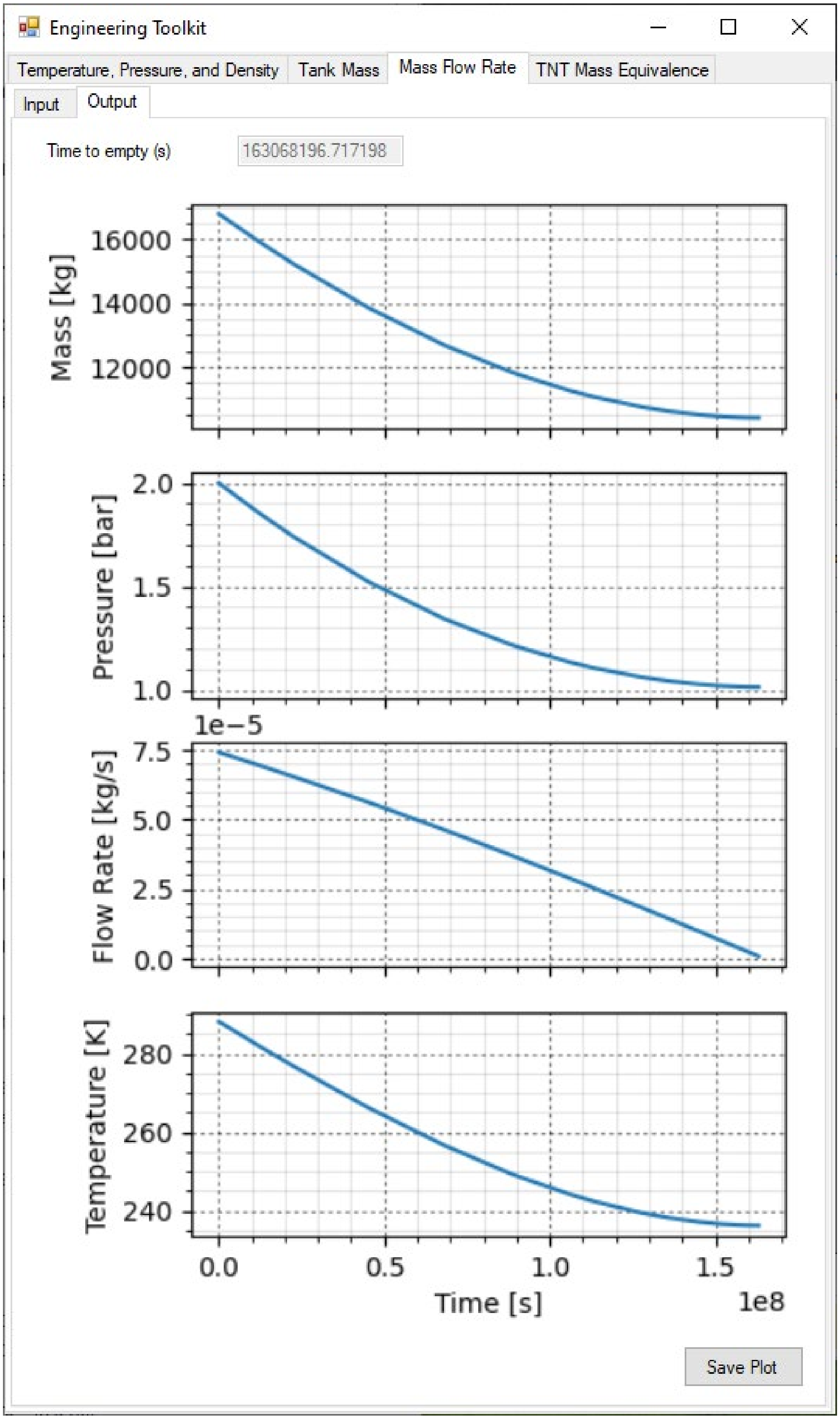


Figure A-42 : Steady Flow H2 Tank Mass Flow Rate for 50 NL/min Case (One Opening)

Figure A-43 shows the inputs used in HyRAM to model this case. Figure A-44 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 1.0%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	0.866	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	5.887E-07	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0	SqMeters
Vent 2 (floor vent) height from floor	2.4	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-43 : Input to Blowdown for 50 NL/min Case (One Opening)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 0.59

Time this Occurred (Seconds): 1.284E+04

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	5.943E-001	0.987	0.566
500	5.943E-001	1.439	0.968
1000	5.943E-001	1.409	1.027
2000	5.944E-001	1.407	1.026
3600	5.944E-001	1.407	1.026
5000	5.944E-001	1.407	1.026

Figure A-44 : Hydrogen Mole Fraction Results for 50 NL/min Case (One Opening)

100 NL/min Case

Figure A-45 and Figure A-46 show the input parameters and the mass flow rate for the 100 NL/min steady flow case, respectively.

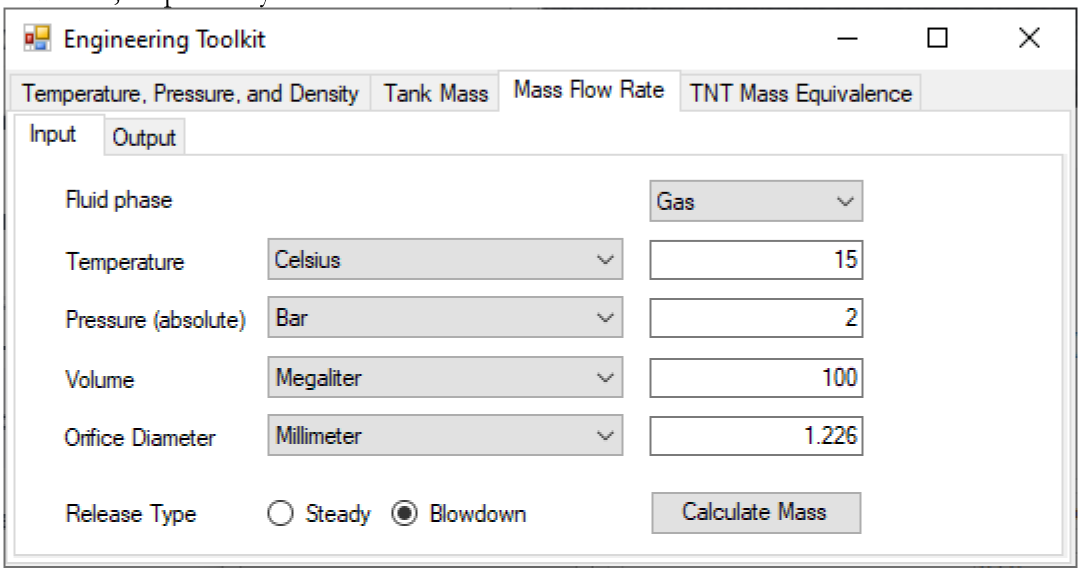


Figure A-45 : Steady Flow H2 Tank Inputs for 100 NL/min Case (One Opening)

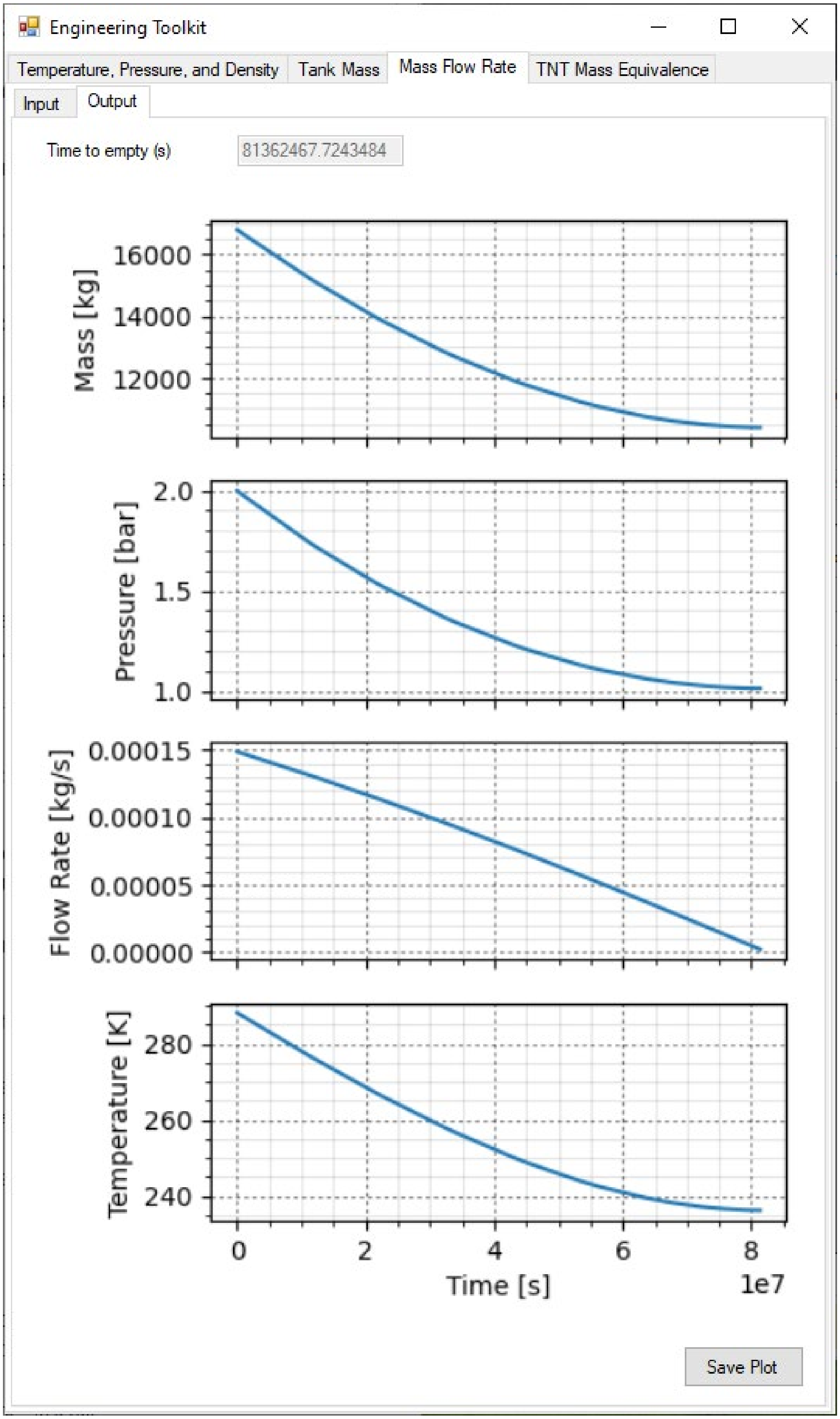


Figure A-46 : Steady Flow H2 Tank Mass Flow Rate for 100 NL/min Case (One Opening)

Figure A-47 shows the inputs used in HyRAM to model this case. Figure A-48 shows the resulting plot of H2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 1.6%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	1.226	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	1.18E-06	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0	SqMeters
Vent 2 (floor vent) height from floor	2.4	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-47 : Input to Blowdown for 100 NL/min Case (One Opening)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 1.67

Time this Occurred (Seconds): 1117

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.673E+000	1.201	0.898
500	1.673E+000	1.526	1.549
1000	1.673E+000	1.506	1.587
2000	1.671E+000	1.506	1.587
3600	1.667E+000	1.506	1.586
5000	1.664E+000	1.506	1.587

Figure A-48 : Hydrogen Mole Fraction Results for 100 NL/min Case (One Opening)

250 NL/min Case

Figure A-49 and Figure A-50 show the input parameters and the mass flow rate for the 250 NL/min steady flow case, respectively.

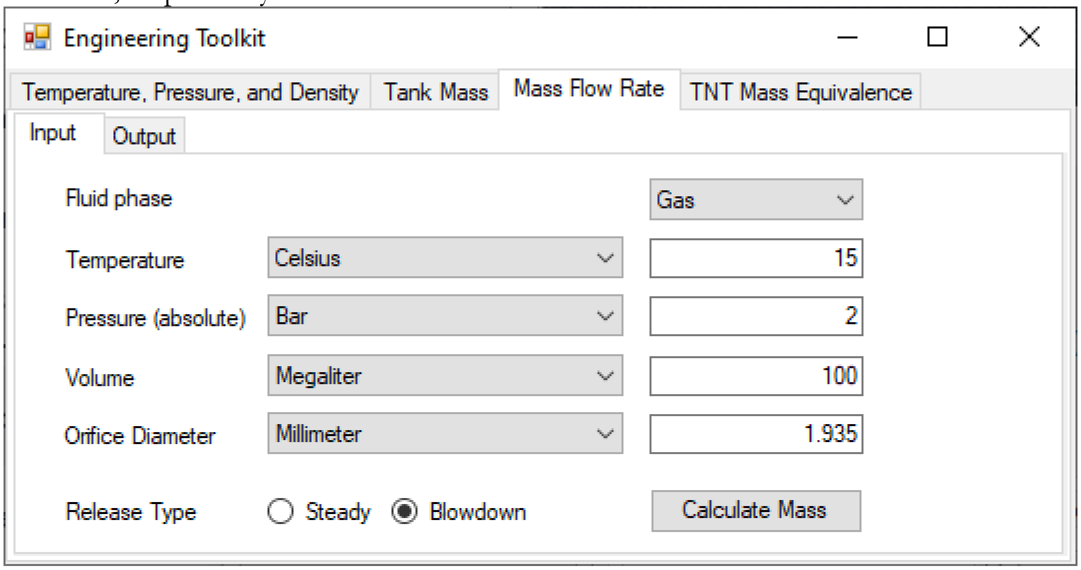


Figure A-49 : Steady Flow H2 Tank Inputs for 250 NL/min Case (One Opening)

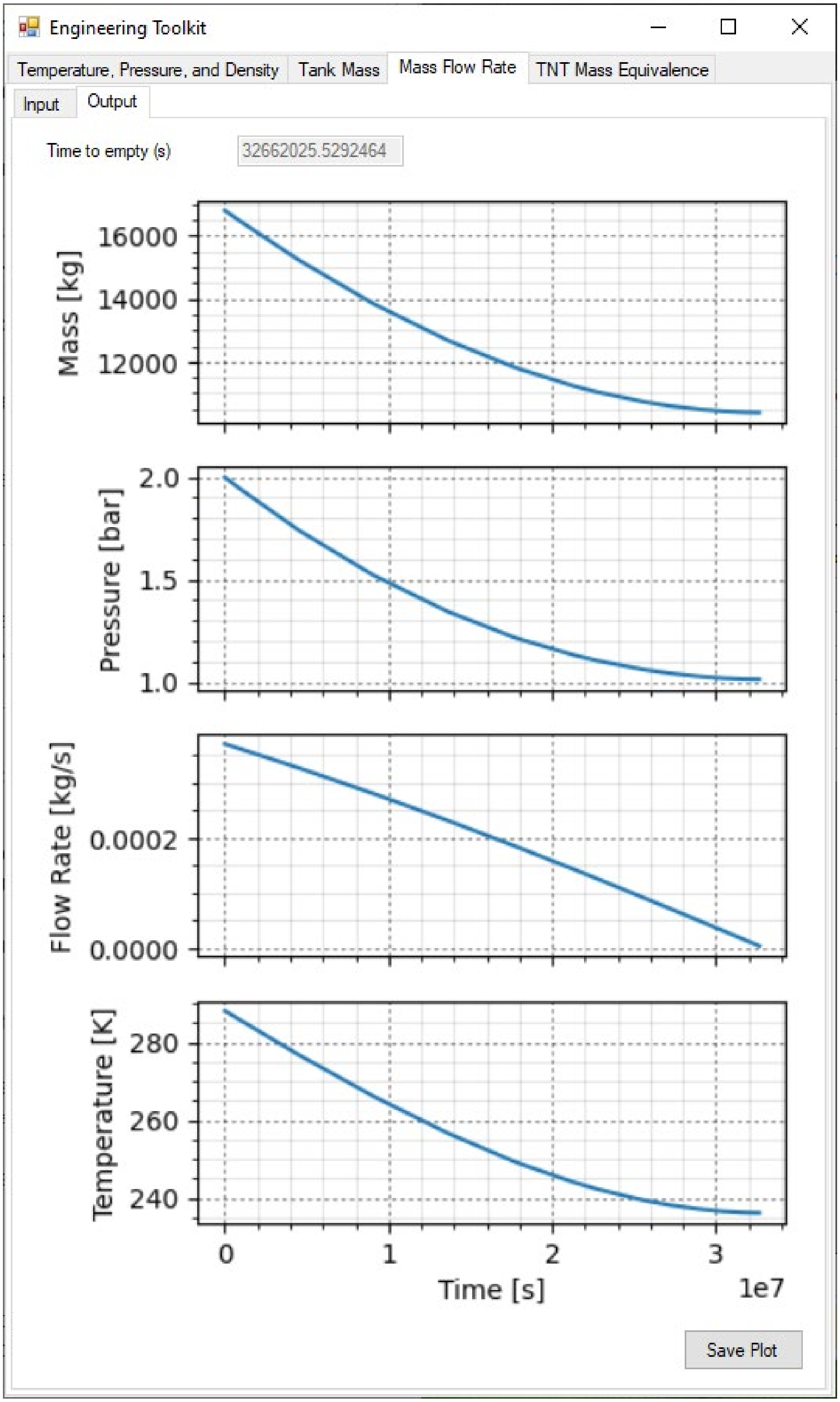


Figure A-50 : Steady Flow H2 Tank Mass Flow Rate for 250 NL/min Case (One Opening)

Figure A-51 shows the inputs used in HyRAM to model this case. Figure A-52 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 2.8%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	1.935	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	2.939E-06	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0	SqMeters
Vent 2 (floor vent) height from floor	2.4	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-51 : Input to Blowdown for 250 NL/min Case (One Opening)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 6.59

Time this Occurred (Seconds): 0.08847

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	6.586E+000	1.507	1.707
500	6.568E+000	1.624	2.809
1000	6.549E+000	1.617	2.819
2000	6.549E+000	1.617	2.820
3600	6.549E+000	1.617	2.818
5000	6.549E+000	1.617	2.819

Figure A-52 : Hydrogen Mole Fraction Results for 250 NL/min Case (One Opening)

500 NL/min Case

Figure A-53 and Figure A-54 show the input parameters and the mass flow rate for the 500 NL/min steady flow case, respectively.

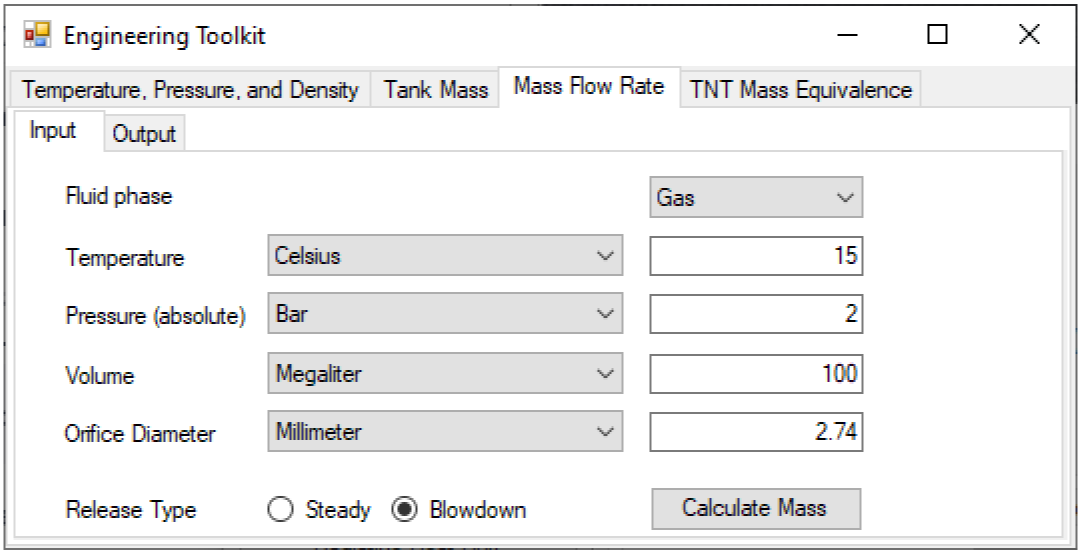


Figure A-53 : Steady Flow H2 Tank Inputs for 500 NL/min Case (One Opening)

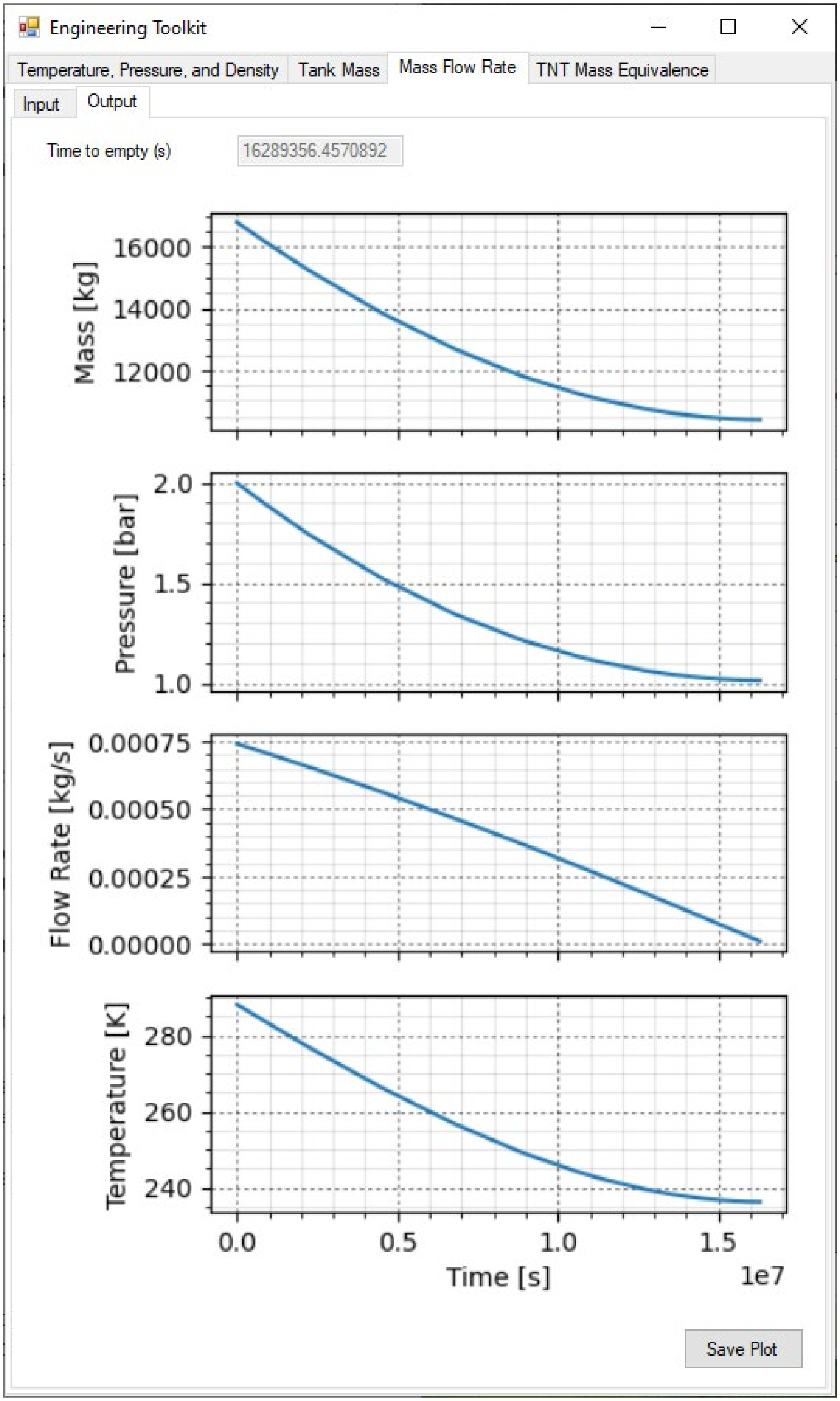


Figure A-54 : Steady Flow H2 Tank Mass Flow Rate for 500 NL/min Case (One Opening)

Figure A-55 shows the inputs used in HyRAM to model this case. Figure A-56 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 4.4%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	2.74	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	5.893E-06	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0	SqMeters
Vent 2 (floor vent) height from floor	2.4	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-55 : Input to Blowdown for 500 NL/min Case (One Opening)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 95,047.33

Time this Occurred (Seconds): 6337

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.531E+001	1.704	2.865
500	9.502E+004	1.702	4.355
1000	9.502E+004	1.701	4.356
2000	9.501E+004	1.701	4.355
3600	9.501E+004	1.701	4.355
5000	9.501E+004	1.701	4.355

Figure A-56 : Hydrogen Mole Fraction Results for 500 NL/min Case (One Opening)

1000 NL/min Case

Figure A-57 and Figure A-58 show the input parameters and the mass flow rate for the 1000 NL/min steady flow case, respectively.

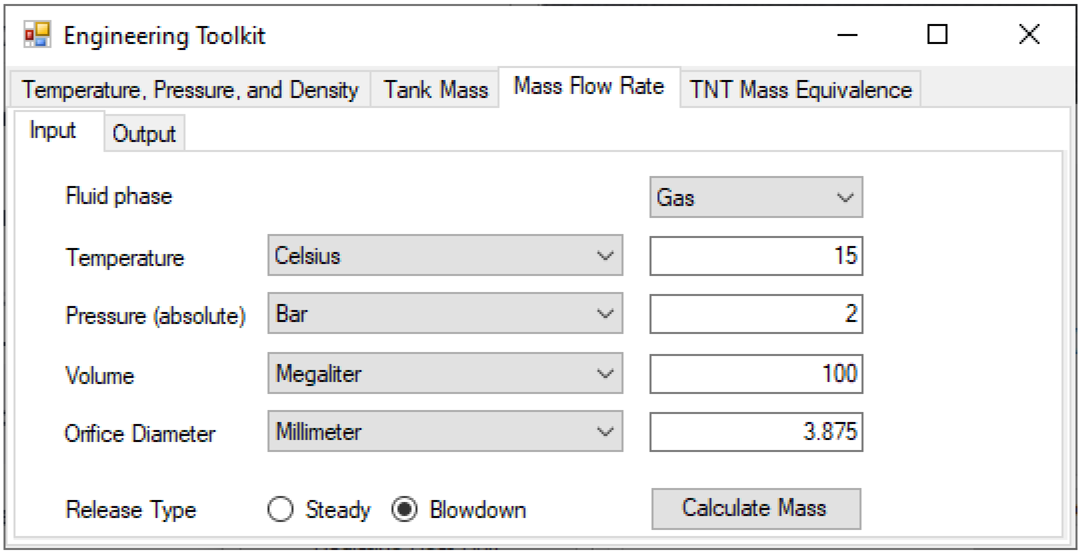


Figure A-57 : Steady Flow H2 Tank Inputs for 1000 NL/min Case (One Opening)

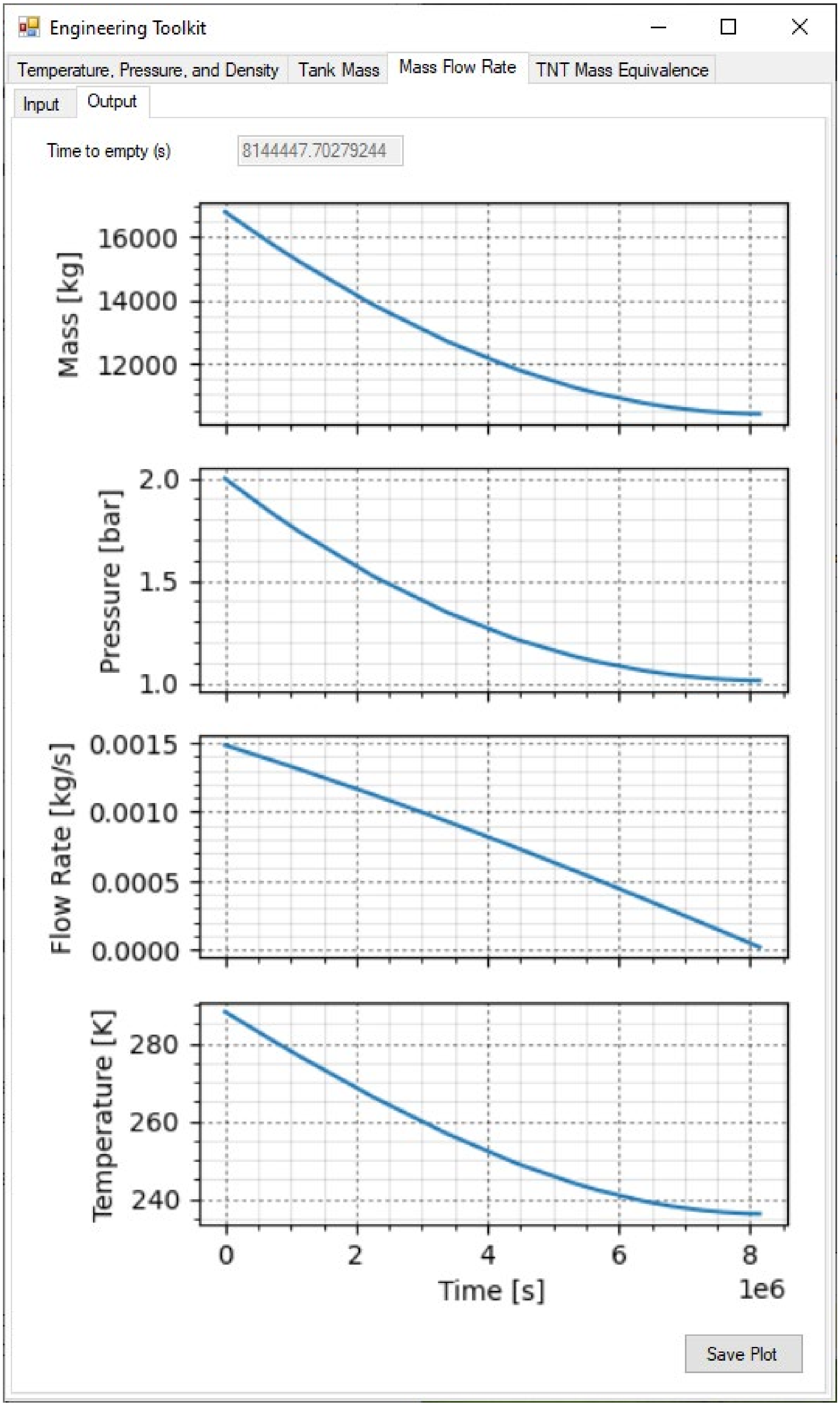


Figure A-58 : Steady Flow H2 Tank Mass Flow Rate for 1000 NL/min Case (One Opening)

Figure A-59 shows the inputs used in HyRAM to model this case. Figure A-60 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 6.7%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	3.875	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	1.179E-05	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0	SqMeters
Vent 2 (floor vent) height from floor	2.4	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-59 : Input to Blowdown for 1000 NL/min Case (One Opening)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 163,849.83

Time this Occurred (Seconds): 4490

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.179E+005	1.838	4.876
500	1.638E+005	1.780	6.693
1000	1.638E+005	1.780	6.693
2000	1.638E+005	1.780	6.691
3600	1.638E+005	1.780	6.693
5000	1.638E+005	1.780	6.694

Figure A-60 : Hydrogen Mole Fraction Results for 1000 NL/min Case (One Opening)

1500 NL/min Case

Figure A-61 and Figure A-62 show the input parameters and the mass flow rate for the 1500 NL/min steady flow case, respectively.

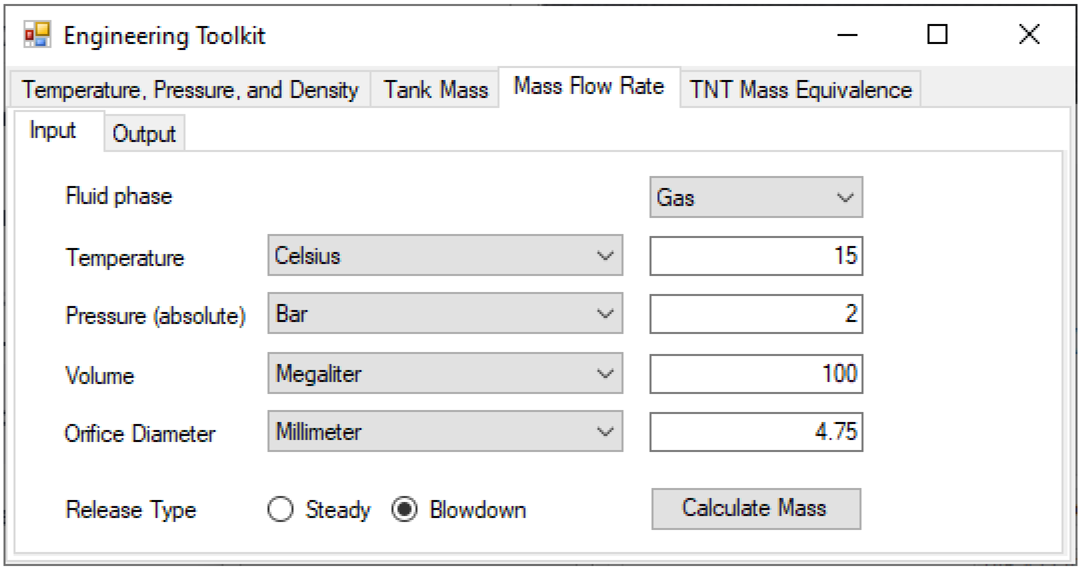


Figure A-61 : Steady Flow H2 Tank Inputs for 1500 NL/min Case (One Opening)

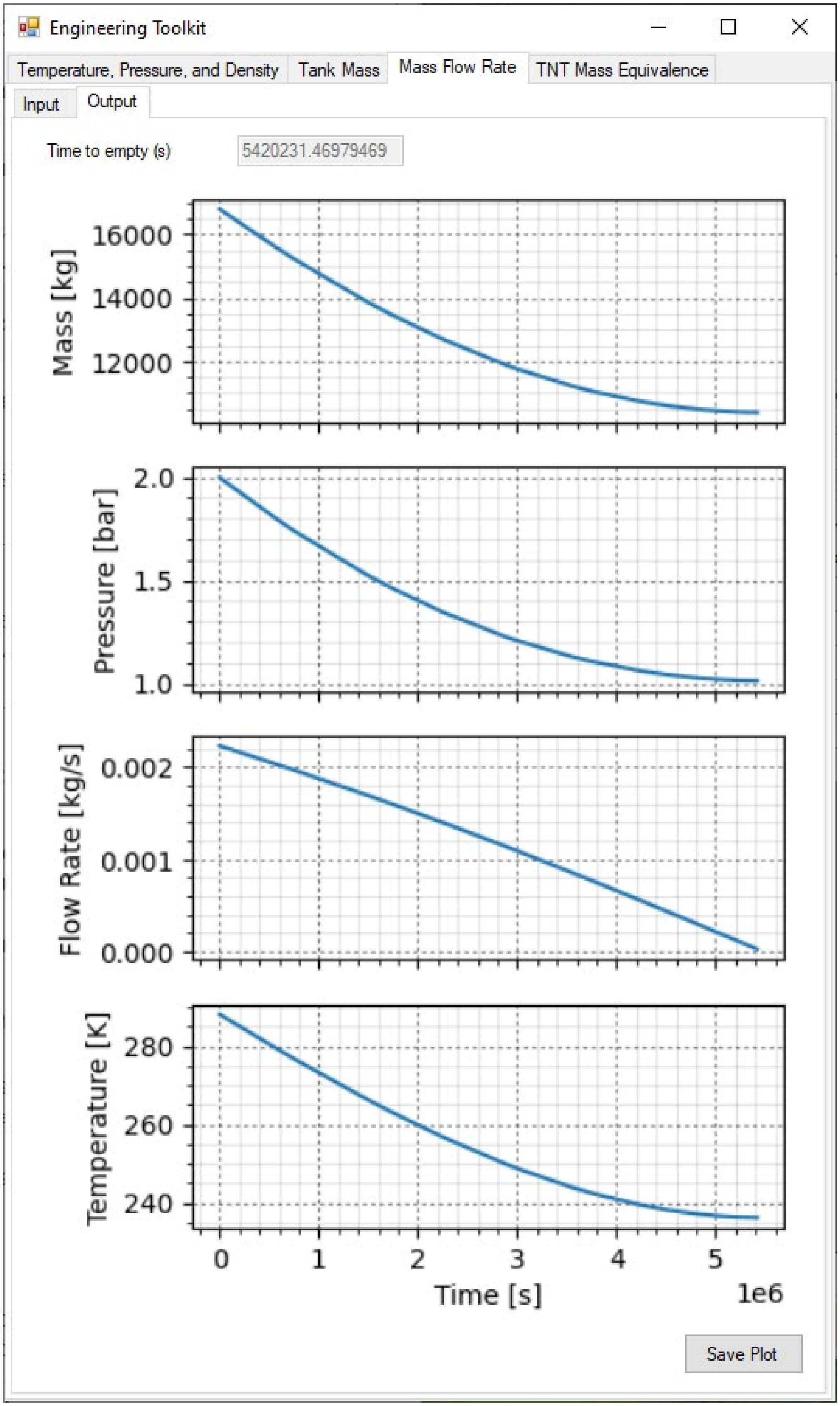


Figure A-62 : Steady Flow H2 Tank Mass Flow Rate for 1500 NL/min Case (One Opening)

Figure A-63 shows the inputs used in HyRAM to model this case. Figure A-64 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 8.6%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	4.75	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	1.771E-05	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0	SqMeters
Vent 2 (floor vent) height from floor	2.4	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-63 : Input to Blowdown for 1500 NL/min Case (One Opening)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 227,569.59

Time this Occurred (Seconds): 6186

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.760E+005	1.895	6.680
500	2.275E+005	1.826	8.583
1000	2.275E+005	1.826	8.583
2000	2.275E+005	1.826	8.584
3600	2.275E+005	1.826	8.584
5000	2.275E+005	1.826	8.584

Figure A-64 : Hydrogen Mole Fraction Results for 1500 NL/min Case (One Opening)

A-4.2. Room with Two Openings

The accumulation model was used to calculate the hydrogen percentage values as a function of volumetric flowrate. The steady-flow workaround documented in Section 2.3 was employed in this section as well. Table A-4 shows the equivalent mass flow rate, and orifice inputs used to achieve the steady-flow rates. As in the hydrogen build up in a closed room, the temperature (15 °C), pressure (2 bar), and volume (100 ML) were kept constant.

50 NL/min Case

Figure A-65 shows the inputs used in HyRAM to model this case. Figure A-66 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 1.0%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	0.866	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	5.887E-07	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0.24	SqMeters
Vent 2 (floor vent) height from floor	0.1	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-65 : Input to Blowdown for 50 NL/min Case (Two Openings)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 0.59

Time this Occurred (Seconds): 1.284E+04

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	5.943E-001	0.987	0.566
500	5.943E-001	1.439	0.968
1000	5.943E-001	1.409	1.027
2000	5.944E-001	1.407	1.026
3600	5.944E-001	1.407	1.026
5000	5.944E-001	1.407	1.026

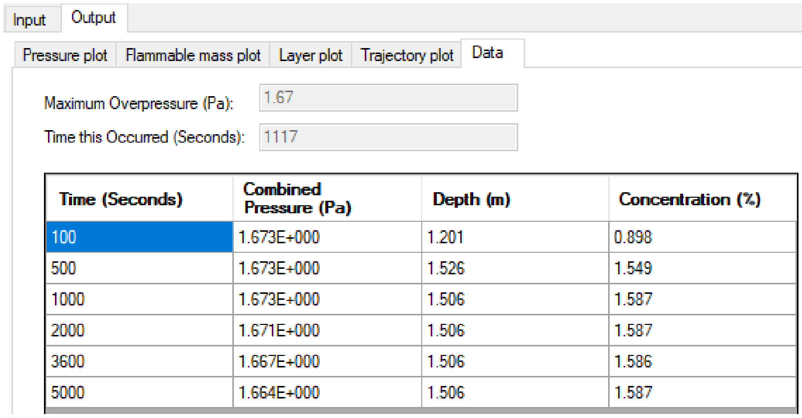
Figure A-66 : Hydrogen Mole Fraction Results for 50 NL/min Case (Two Openings)

100 NL/min Case

Figure A-67 shows the inputs used in HyRAM to model this case. Figure A-68 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 1.6%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	1.226	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	1.18E-06	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0.24	SqMeters
Vent 2 (floor vent) height from floor	0.1	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-67 : Input to Blowdown for 100 NL/min Case (Two Openings)



Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.673E+000	1.201	0.898
500	1.673E+000	1.526	1.549
1000	1.673E+000	1.506	1.587
2000	1.671E+000	1.506	1.587
3600	1.667E+000	1.506	1.586
5000	1.664E+000	1.506	1.587

Figure A-68 : Hydrogen Mole Fraction Results for 100 NL/min Case (Two Openings)

250 NL/min Case

Figure A-69 shows the inputs used in HyRAM to model this case. Figure A-70 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 2.8%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	1.935	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	2.939E-06	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0.24	SqMeters
Vent 2 (floor vent) height from floor	0.1	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-69 : Input to Blowdown for 250 NL/min Case (Two Openings)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 6.59

Time this Occurred (Seconds): 0.08847

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	6.586E+000	1.507	1.707
500	6.568E+000	1.624	2.809
1000	6.549E+000	1.617	2.819
2000	6.549E+000	1.617	2.820
3600	6.549E+000	1.617	2.818
5000	6.549E+000	1.617	2.819

Figure A-70 : Hydrogen Mole Fraction Results for 250 NL/min Case (Two Openings)

500 NL/min Case

Figure A-71 shows the inputs used in HyRAM to model this case. Figure A-72 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 4.4%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	2.74	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	5.893E-06	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0.24	SqMeters
Vent 2 (floor vent) height from floor	0.1	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-71 : Input to Blowdown for 500 NL/min Case (Two Openings)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 95,047.33

Time this Occurred (Seconds): 6337

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.531E+001	1.704	2.865
500	9.502E+004	1.702	4.355
1000	9.502E+004	1.701	4.356
2000	9.501E+004	1.701	4.355
3600	9.501E+004	1.701	4.355
5000	9.501E+004	1.701	4.355

Figure A-72 : Hydrogen Mole Fraction Results for 500 NL/min Case (Two Openings)

1000 NL/min Case

Figure A-73 shows the inputs used in HyRAM to model this case. Figure A-74 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 6.7%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	3.875	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	1.179E-05	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0.24	SqMeters
Vent 2 (floor vent) height from floor	0.1	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-73 : Input to Blowdown for 1000 NL/min Case (Two Openings)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 163,849.83

Time this Occurred (Seconds): 4490

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.179E+005	1.838	4.876
500	1.638E+005	1.780	6.693
1000	1.638E+005	1.780	6.693
2000	1.638E+005	1.780	6.691
3600	1.638E+005	1.780	6.693
5000	1.638E+005	1.780	6.694

Figure A-74 : Hydrogen Mole Fraction Results for 1000 NL/min Case (Two Openings)

1500 NL/min Case

Figure A-75 shows the inputs used in HyRAM to model this case. Figure A-76 shows the resulting plot of H_2 concentration as a function of time. As shown, the maximum hydrogen concentration is approximately 8.6%.

Variable	Value	Unit
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Leak diameter	4.75	Millimeter
Discharge coefficient-orifice	1	...
Discharge coefficient-release	1	...
Release area	1.771E-05	SqMeters
Release height	0	Meter
Enclosure height	2.5	Meter
Floor/ceiling area	12.5	SqMeters
Distance from release to wall	2	Meter
Vent 1 (ceiling vent) cross-sectional area	0.24	SqMeters
Vent 1 (ceiling vent) height from floor	2.4	Meter
Vent 2 (floor vent) cross-sectional area	0.24	SqMeters
Vent 2 (floor vent) height from floor	0.1	Meter
Angle of release (0=horz.)	90	Degrees
Tank fluid pressure (absolute)	2	Bar
Tank fluid temperature	15	Celsius
Tank volume	100	Megaliter
Vent volumetric flow rate	0	CubicMetersPerSe...

Figure A-75 : Input to Blowdown for 1500 NL/min Case (Two Openings)

Input | Output

Pressure plot | Flammable mass plot | Layer plot | Trajectory plot | Data

Maximum Overpressure (Pa): 227,569.59

Time this Occurred (Seconds): 6186

Time (Seconds)	Combined Pressure (Pa)	Depth (m)	Concentration (%)
100	1.760E+005	1.895	6.680
500	2.275E+005	1.826	8.583
1000	2.275E+005	1.826	8.583
2000	2.275E+005	1.826	8.584
3600	2.275E+005	1.826	8.584
5000	2.275E+005	1.826	8.584

Figure A-76 : Hydrogen Mole Fraction Results for 1500 NL/min Case (Two Openings)

A-5. Liquid Hydrogen Accident Scenarios

The Jet Flame/Radiative Heat Flux model, Gas Plume Dispersion model, and the Engineering Toolkit functions were used to calculate the liquid hydrogen pipe rupture results. Note, in order to perform these calculations, it was assumed that the release of the plume is horizontal and the vertical height at which the heat flux was calculated is 0 meters. Also, the release is assumed to occur at a vertical height of 0 meters and the orifice discharge coefficient is assumed to be 1.

A-5.1. Pipe Full Bore Rupture before the Pump

Engineering Toolkit

The engineering toolkit was used to calculate the release mass flow of the liquid hydrogen full bore pipe rupture case. Figure A-77 shows the input parameters used in the calculation.

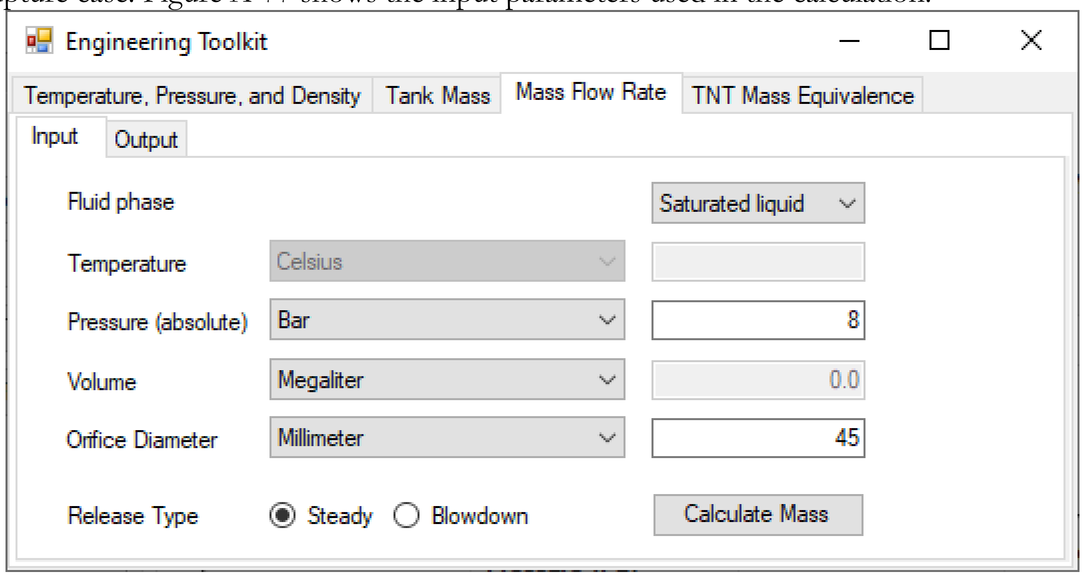


Figure A-77 : Input to Engineering Toolkit for LH_2 Full Bore Rupture Case (Before Pump)

Using these inputs, the mass flow rate was calculated (as shown in Figure A-78).

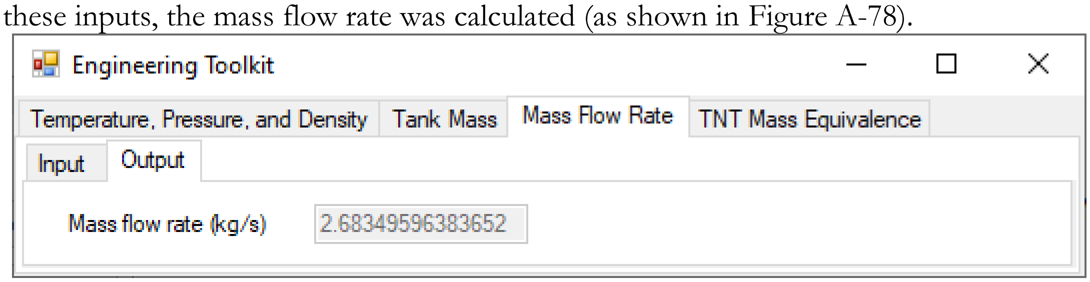


Figure A-78 : Output of Engineering Toolkit Calculation for LH2 Full Bore Rupture Case (Before Pump)

Gas Plume Dispersion Model

The gas plume dispersion model was used to calculate the horizontal distance of the hydrogen at different mole fractions. Figure A-79 and Figure A-80 show the input to the gas plume dispersion model for the 4% and 10% mole fraction calculations, respectively.

	Variable	Value	Unit
▶	X lower limit	0	Meter
	X upper limit	80	Meter
	Y lower limit	-10	Meter
	Y upper limit	30	Meter
	Contours (mole fraction)	0.04	...
	Ambient pressure	1	Atm
	Ambient temperature	288	Kelvin
	Orifice diameter	45	Millimeter
	Orifice discharge coefficient	1	...
	Angle of jet	0	Degrees
	Fluid pressure (absolute)	8	Bar

Figure A-79 : Input for 4% Mole Fraction Calculation for LH2 Full Bore Rupture Case (Before Pump)

	Variable	Value	Unit
▶	X lower limit	0	Meter
	X upper limit	40	Meter
	Y lower limit	-5	Meter
	Y upper limit	5	Meter
	Contours (mole fraction)	0.1	...
	Ambient pressure	1	Atm
	Ambient temperature	288	Kelvin
	Orifice diameter	45	Millimeter
	Orifice discharge coefficient	1	...
	Angle of jet	0	Degrees
	Fluid pressure (absolute)	8	Bar

Figure A-80 : Input for 10% Mole Fraction Calculation for LH_2 Full Bore Rupture Case (Before Pump)

Figure A-81 and Figure A-82 show the results of the 4% and 10% mole fraction calculations, respectively. From these figures, the variables of interest were visually determined. For the 4% mole fraction case, the horizontal distance was determined to be approximately 80 meters. For the 10% mole fraction case, the horizontal distance was determined to be approximately 35 meters.

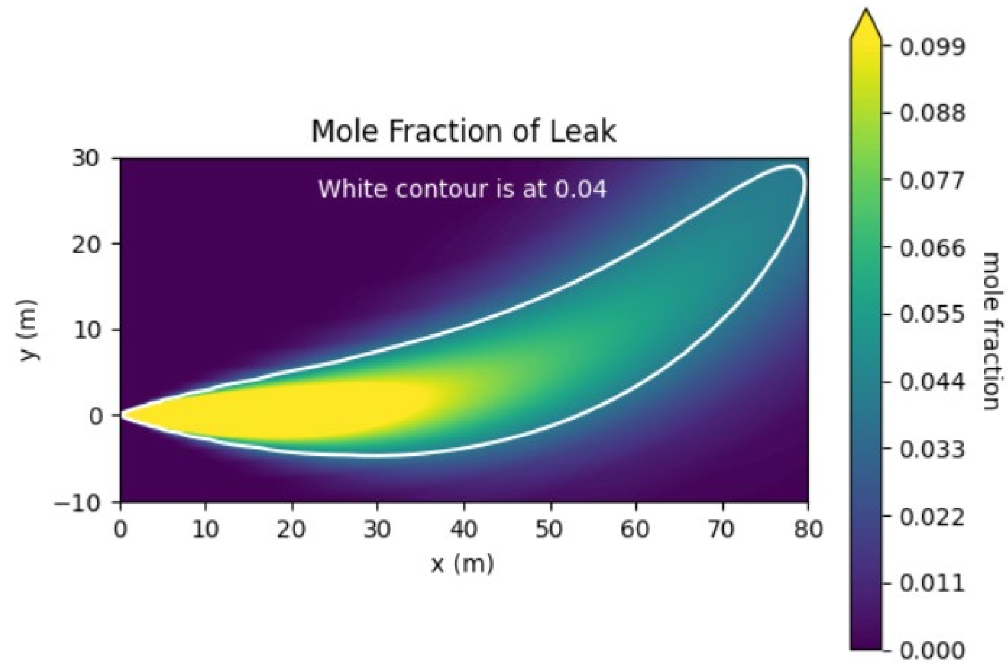


Figure A-81 : Contour at 4% Mole Fraction for LH_2 Full Bore Rupture Case (Before Pump)

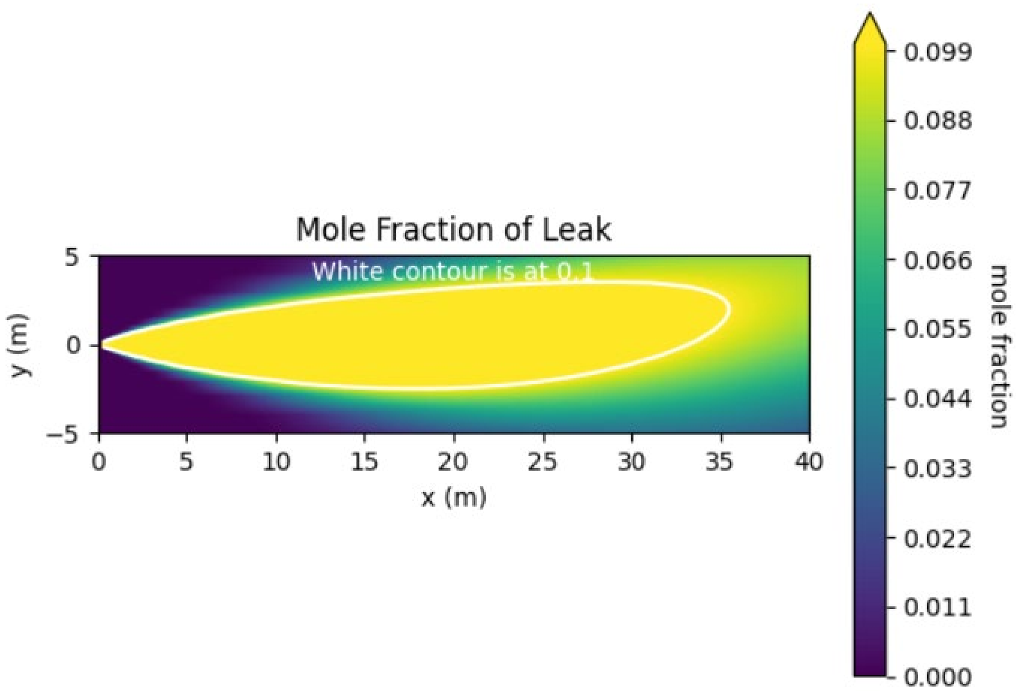


Figure A-82 : Contour at 10% Mole Fraction for LH_2 Full Bore Rupture Case (Before Pump)

Jet Flame/Radiative Heat Flux Model

The jet flame/radiative heat flux model was used to calculate the horizontal distance at which certain heat flux values were reached. Figure A-83 shows the input used in the jet flame/radiative heat flux model calculations.

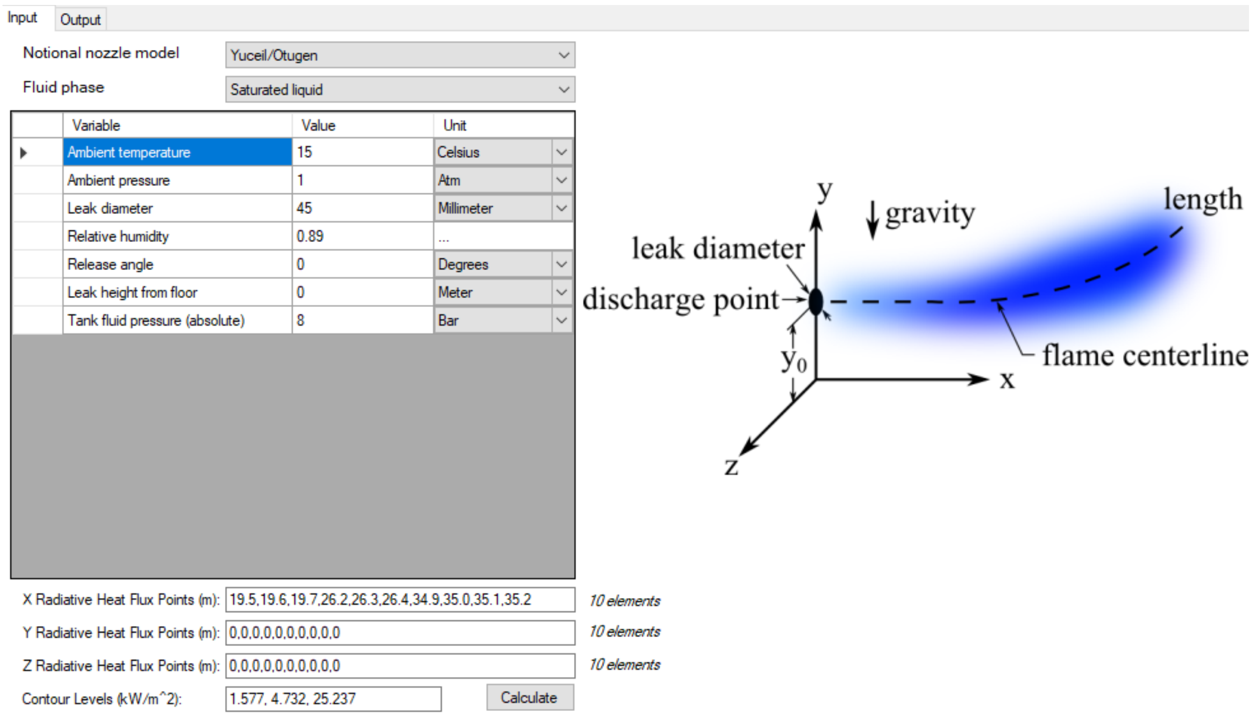


Figure A-83 : Input for the Jet Flame Model Calculation for LH_2 Full Bore Rupture Case (Before Pump)

Table A-5 shows the radiative heat flux results for the full bore rupture case (before pump). As shown, the horizontal distances at which heat flux of 3, 5, and 8 kW/m^2 are seen are approximately 35.1 meters, 26.4 meters, and 19.6 meters, respectively.

Table A-5: Radiative Heat Flux Results for LH_2 Full Bore Rupture Case (Before Pump)

X(m)	Y(m)	Z(m)	Flux (kW/m^2)
19.5000	0.0000	0.0000	8.0662
19.6000	0.0000	0.0000	8.0048
19.7000	0.0000	0.0000	7.9440
26.2000	0.0000	0.0000	5.0469
26.3000	0.0000	0.0000	5.0146
26.4000	0.0000	0.0000	4.9825
34.9000	0.0000	0.0000	3.0285
35.0000	0.0000	0.0000	3.0123
35.1000	0.0000	0.0000	2.9962

Figure A-84 shows the flame length for the full bore rupture case (before pump). From this figure, the variable of interest was visually determined to be approximately 10 meters.

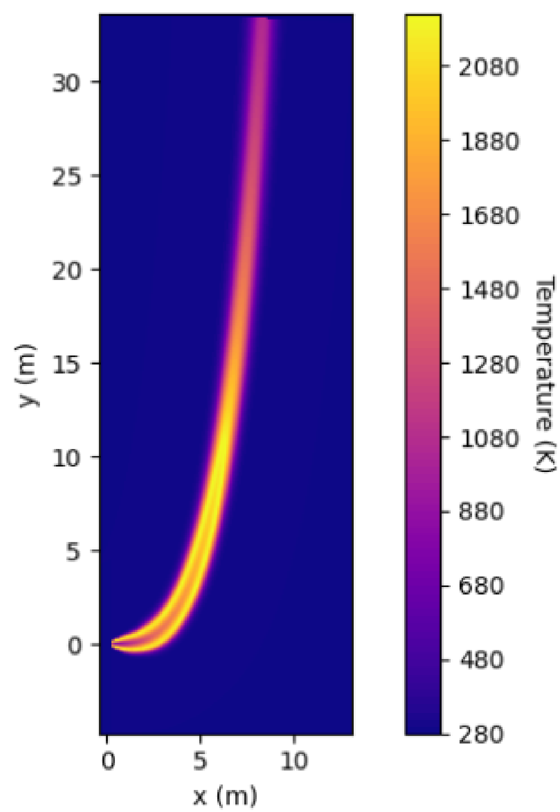


Figure A-84 : Flame Length for LH_2 Full Bore Rupture Case (Before Pump)

A-5.2. Pipe Partial Rupture before the Pump

Engineering Toolkit

The engineering toolkit was used to calculate the release mass flow of the liquid hydrogen partial bore pipe rupture case. Figure A-85 shows the input parameters used in the calculation.

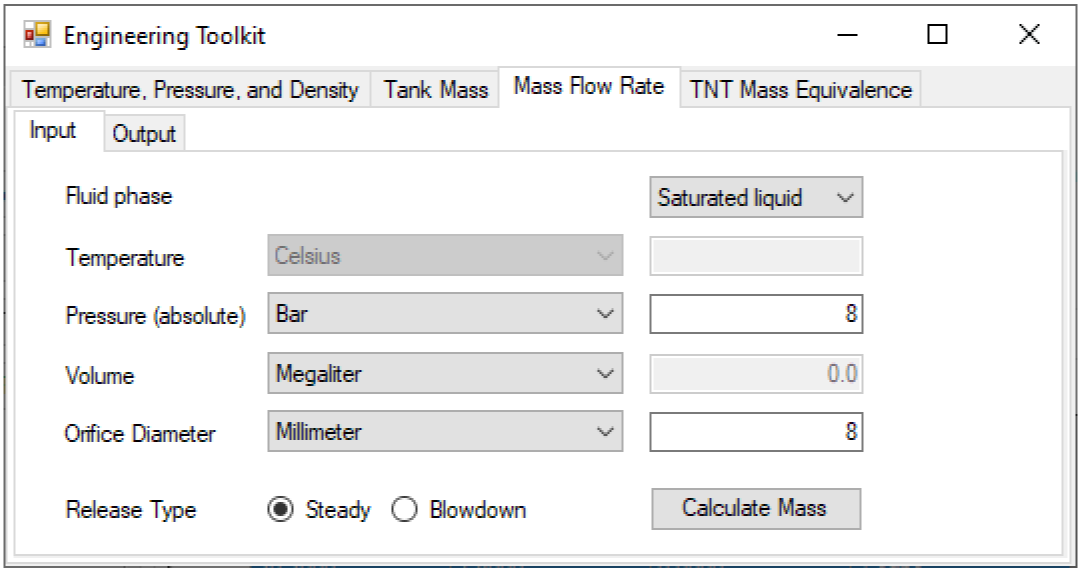


Figure A-85 : Input to Engineering Toolkit LH_2 for Partial Bore Rupture Case (Before Pump)

Using these inputs, the mass flow rate was calculated (as shown in Figure A-86).

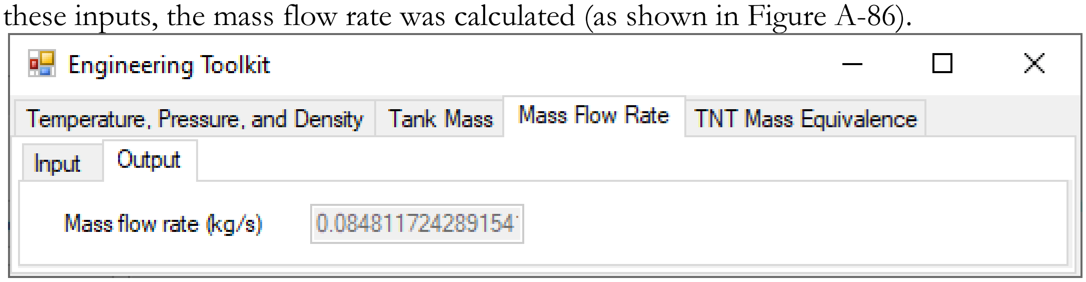


Figure A-86 : Output of Engineering Toolkit Calculation for LH2 Partial Bore Rupture Case (Before Pump)

Gas Plume Dispersion Model

The gas plume dispersion model was used to calculate the horizontal distance of the hydrogen at different mole fractions. Figure A-87 and Figure A-88 show the input to the gas plume dispersion model for the 4% and 10% mole fraction calculations, respectively.

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	20	Meter
Y lower limit	-2	Meter
Y upper limit	2	Meter
Contours (mole fraction)	0.04	...
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Orifice diameter	8	Millimeter
Orifice discharge coefficient	1	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	8	Bar

Figure A-87 : Input for 4% Mole Fraction Calculation for LH2 Partial Bore Rupture Case (Before Pump)

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	10	Meter
Y lower limit	-2	Meter
Y upper limit	2	Meter
Contours (mole fraction)	0.1	...
Ambient pressure	1	Atm
Ambient temperature	15	Celsius
Orifice diameter	8	Millimeter
Orifice discharge coefficient	1	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	8	Bar

Figure A-88 : Input for 10% Mole Fraction Calculation for LH2 Partial Bore Rupture Case (Before Pump)

Figure A-89 and Figure A-90 show the results of the 4% and 10% mole fraction calculations, respectively. From these figures, the variables of interest were visually determined. For the 4% mole fraction case, the horizontal distance was determined to be approximately 17 meters. For the 10% mole fraction case, the horizontal distance was determined to be approximately 6 meters.

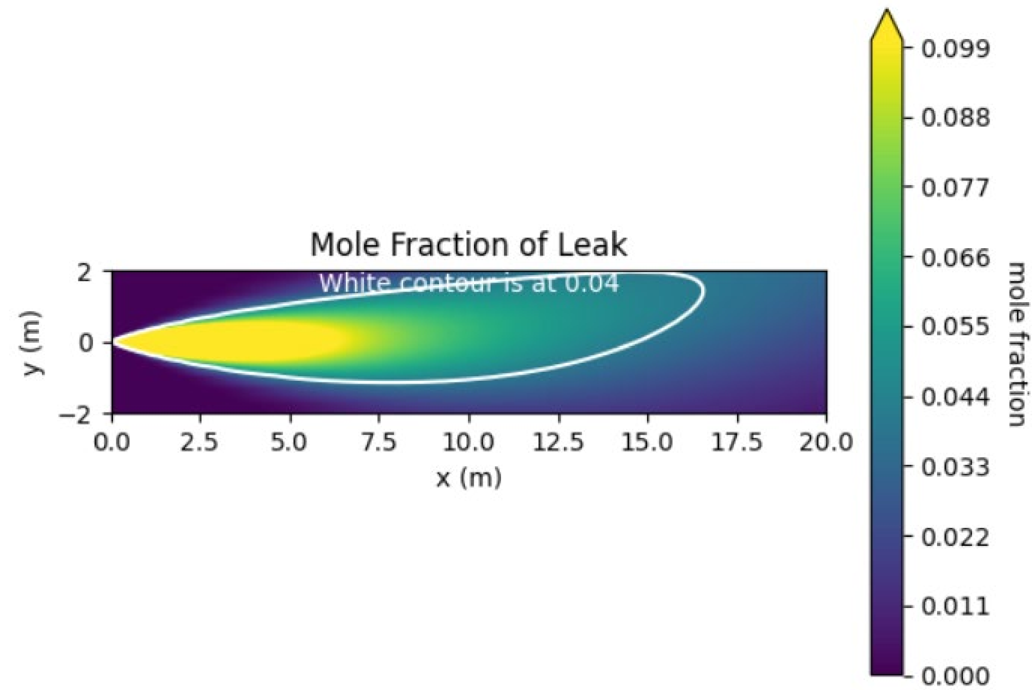


Figure A-89 : Contour at 4% Mole Fraction for LH2 Partial Bore Rupture Case (Before Pump)

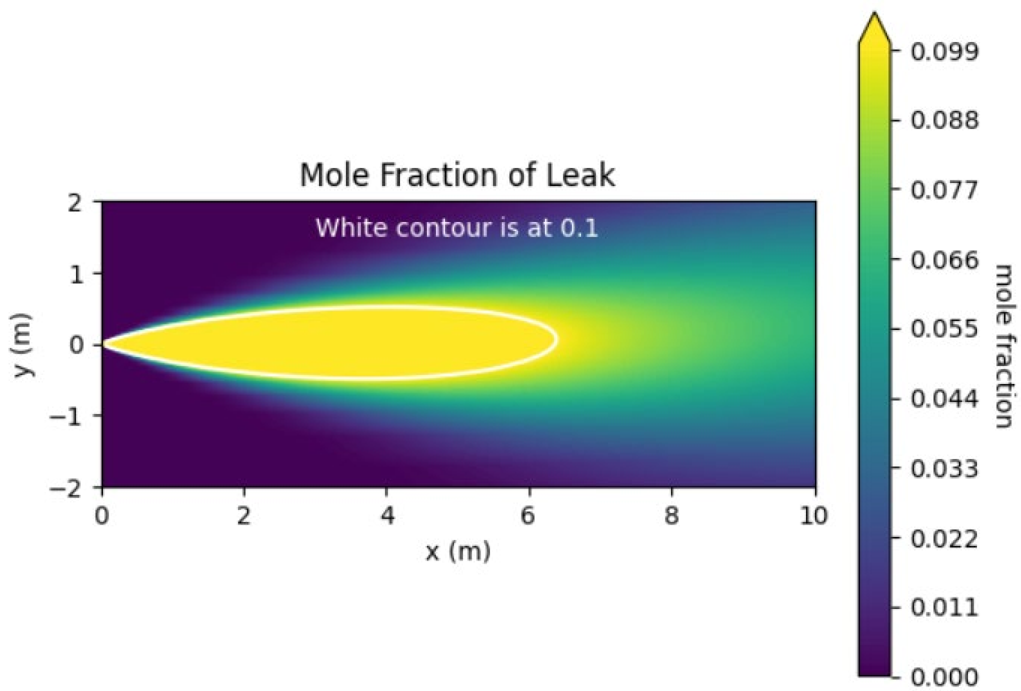


Figure A-90 : Contour at 10% Mole Fraction for LH2 Partial Bore Rupture Case (Before Pump)

Jet Flame/Radiative Heat Flux Model

The jet flame/radiative heat flux model was used to calculate the horizontal distance at which certain heat flux values were reached. Figure A-91 shows the input used in the jet flame/radiative heat flux model calculations.

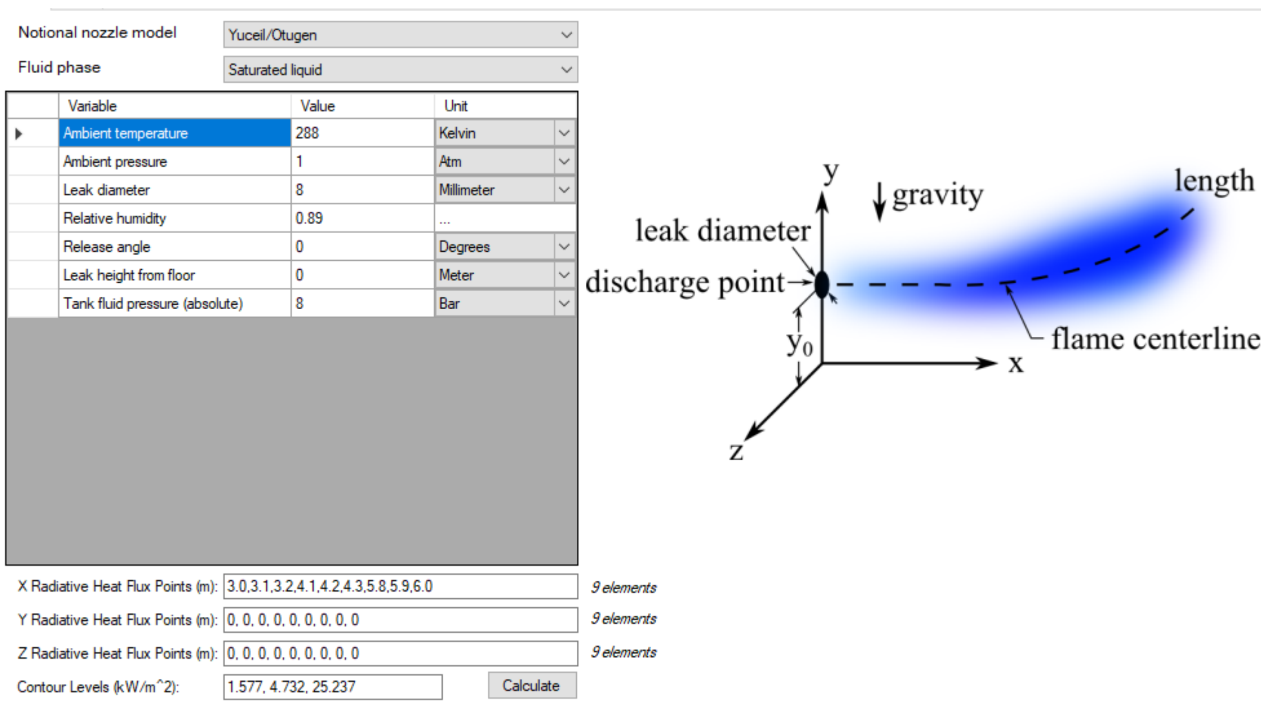


Figure A-91 : Input for the Jet Flame Model Calculation for LH_2 Partial Bore Rupture Case (Before Pump)

Table A-6 shows the radiative heat flux results for the LH_2 partial bore rupture case (before pump). As shown, the horizontal distances at which heat flux of 3, 5, and 8 kW/m^2 are seen are approximately 5.8 meters, 4.3 meters, and 3.1 meters, respectively.

Table A-6: Radiative Heat Flux Results for LH_2 Partial Bore Rupture Case (Before Pump)

X(m)	Y(m)	Z(m)	Flux (kW/m^2)
3.0000	0.0000	0.0000	8.3548
3.1000	0.0000	0.0000	7.9751
3.2000	0.0000	0.0000	7.6226
4.1000	0.0000	0.0000	5.3052
4.2000	0.0000	0.0000	5.1150
4.3000	0.0000	0.0000	4.9345
5.8000	0.0000	0.0000	3.0387
5.9000	0.0000	0.0000	2.9505
6.0000	0.0000	0.0000	2.8658

Figure A-92 shows the flame length for the LH_2 partial bore rupture case (before pump). From this figure, the variable of interest was visually determined to be approximately 3 meters.

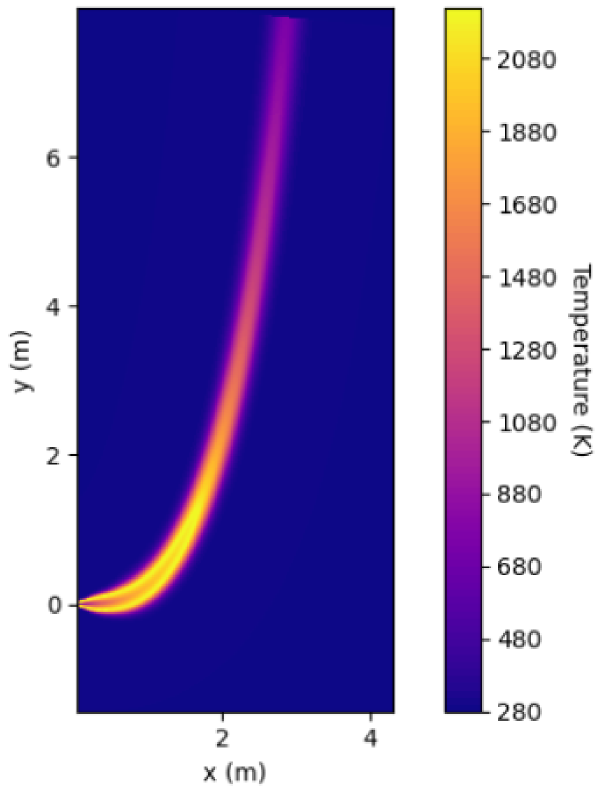


Figure A-92 : Flame Length for LH2 Partial Bore Rupture Case (Before Pump)

A-5.3. Pipe Full Bore Rupture after the Pump

Engineering Toolkit

The engineering toolkit was used to calculate the release mass flow of the liquid hydrogen full bore pipe rupture case. Figure A-93 shows the input parameters used in the calculation. Note, in order to achieve a given mass release rate of 50 kg/hr (14 g/s), the engineering toolkit was used to iteratively change the release pressure with a hydrogen temperature of 70.4 K.

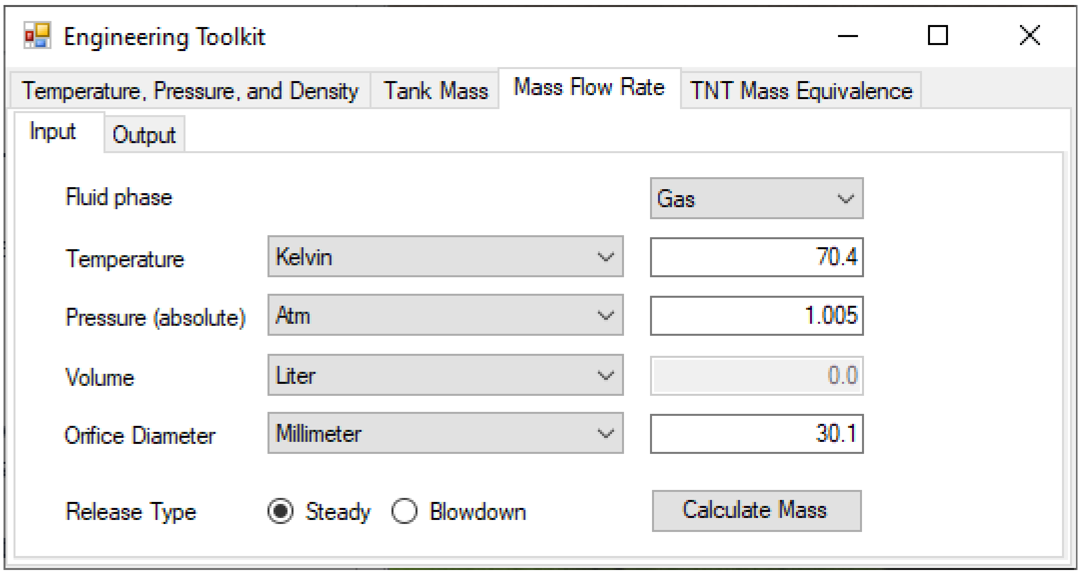


Figure A-93 : Input to Engineering Toolkit for LH_2 Full Bore Rupture Case (After Pump)

Using these inputs, the mass flow rate was calculated (as shown in Figure A-94).

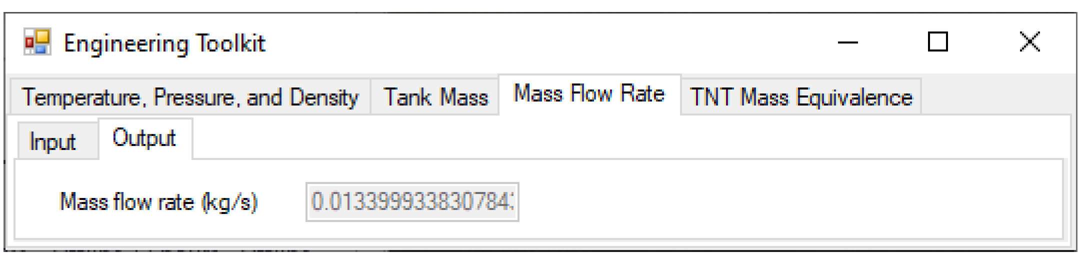


Figure A-94 : Output of Engineering Toolkit Calculation for LH2 Full Bore Rupture Case (After Pump)

Gas Plume Dispersion Model

The gas plume dispersion model was used to calculate the horizontal distance of the hydrogen at different mole fractions. Figure A-95 and Figure A-96 show the input to the gas plume dispersion model for the 4% and 10% mole fraction calculations, respectively.

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	10	Meter
Y lower limit	-2	Meter
Y upper limit	8	Meter
Contours (mole fraction)	0.04	...
Ambient pressure	1	Atm
Ambient temperature	288	Kelvin
Orifice diameter	30.1	Millimeter
Orifice discharge coefficient	1	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	1.005	Atm
Fluid temperature	70.4	Kelvin

Figure A-95 : Input for 4% Mole Fraction Calculation for LH2 Full Bore Rupture Case (After Pump)

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	6	Meter
Y lower limit	-2	Meter
Y upper limit	4	Meter
Contours (mole fraction)	0.1	...
Ambient pressure	1	Atm
Ambient temperature	288	Kelvin
Orifice diameter	30.1	Millimeter
Orifice discharge coefficient	1	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	1.005	Atm
Fluid temperature	70.4	Kelvin

Figure A-96 : Input for 10% Mole Fraction Calculation for LH_2 Full Bore Rupture Case (After Pump)

Figure A-97 and Figure A-98 show the results of the 4% and 10% mole fraction calculations, respectively. From these figures, the variables of interest were visually determined. For the 4% mole fraction case, the horizontal distance was determined to be approximately 7 meters. For the 10% mole fraction case, the horizontal distance was determined to be approximately 5 meter.

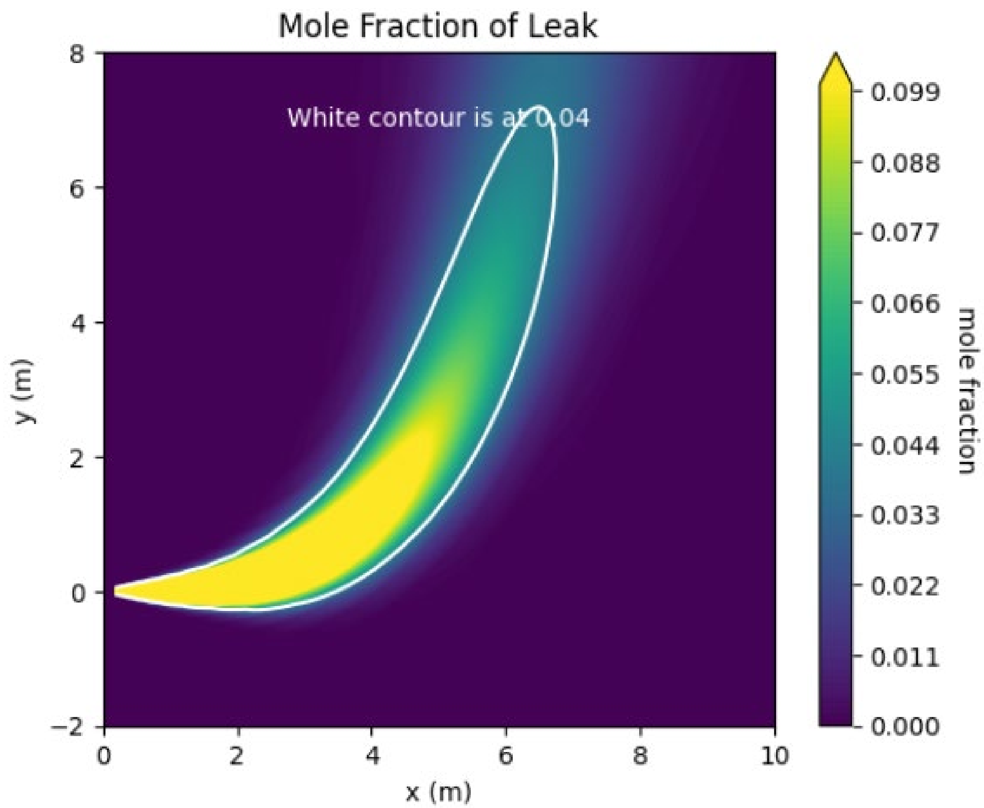


Figure A-97 : Contour at 4% Mole Fraction for LH_2 Full Bore Rupture Case (After Pump)

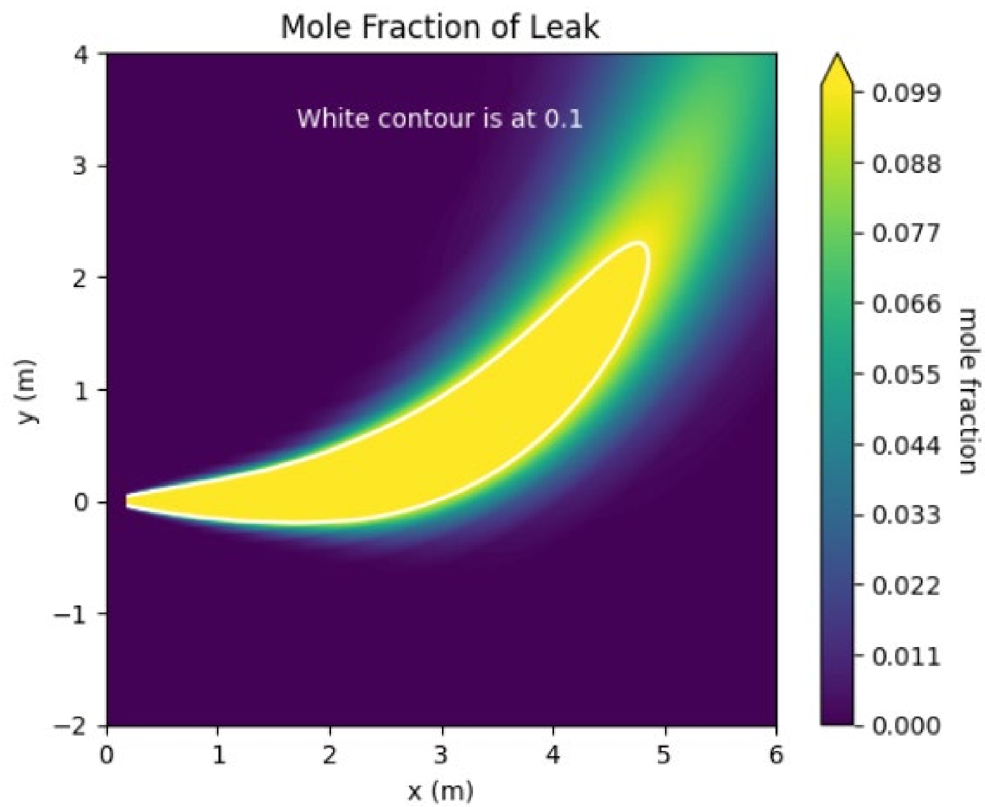


Figure A-98 : Contour at 10% Mole Fraction for LH_2 Full Bore Rupture Case (After Pump)

Jet Flame/Radiative Heat Flux Model

The jet flame/radiative heat flux model was used to calculate the horizontal distance at which certain heat flux values were reached. Figure A-99 shows the input used in the jet flame/radiative heat flux model calculations.

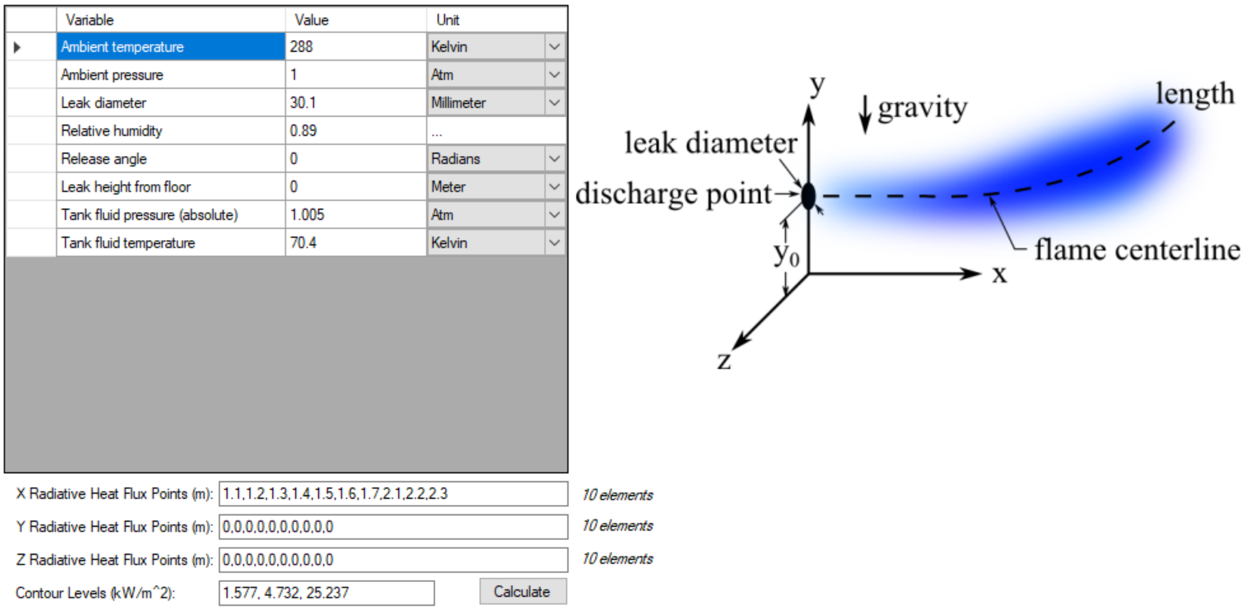


Figure A-99 : Input for the Jet Flame Model Calculation for LH_2 Full Bore Rupture Case (After Pump)

Table A-7 shows the radiative heat flux results for the LH_2 full bore rupture case (after pump). As shown, the horizontal distances at which heat flux of 3, 5, and 8 kW/m^2 are seen are approximately 2.3 meters, 1.7 meter, and 1.2 meters, respectively.

Table A-7: Radiative Heat Flux Results for LH_2 Full Bore Rupture Case (After Pump)

X(m)	Y(m)	Z(m)	Flux (kW/m^2)
1.1000	0.0000	0.0000	9.7279
1.2000	0.0000	0.0000	8.3910
1.3000	0.0000	0.0000	7.3524
1.4000	0.0000	0.0000	6.5208
1.5000	0.0000	0.0000	5.8387
1.6000	0.0000	0.0000	5.2681
1.7000	0.0000	0.0000	4.7830
2.1000	0.0000	0.0000	3.3985
2.2000	0.0000	0.0000	3.1461
2.3000	0.0000	0.0000	2.9197

Figure A-100 shows the flame length for the LH_2 full bore rupture case (after pump). From this figure, the variable of interest was visually determined to be approximately 1.5 meters.

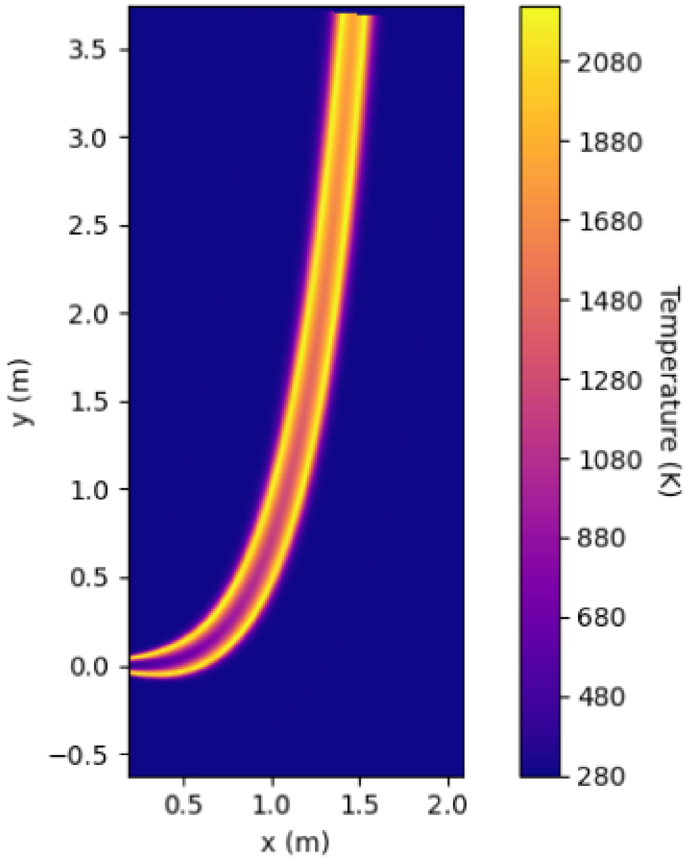


Figure A-100 : Flame Length for LH_2 Full Bore Rupture Case (After Pump)

A-5.4. Pipe Partial Rupture before the Pump

Engineering Toolkit

The engineering toolkit was used to calculate the release mass flow of the liquid hydrogen partial bore pipe rupture case. Figure A-101 shows the input parameters used in the calculation. Note, in order to achieve a given mass release rate of 50 kg/hr (14 g/s), the engineering toolkit was used to iteratively change the release pressure with a hydrogen temperature of 70.4 K.

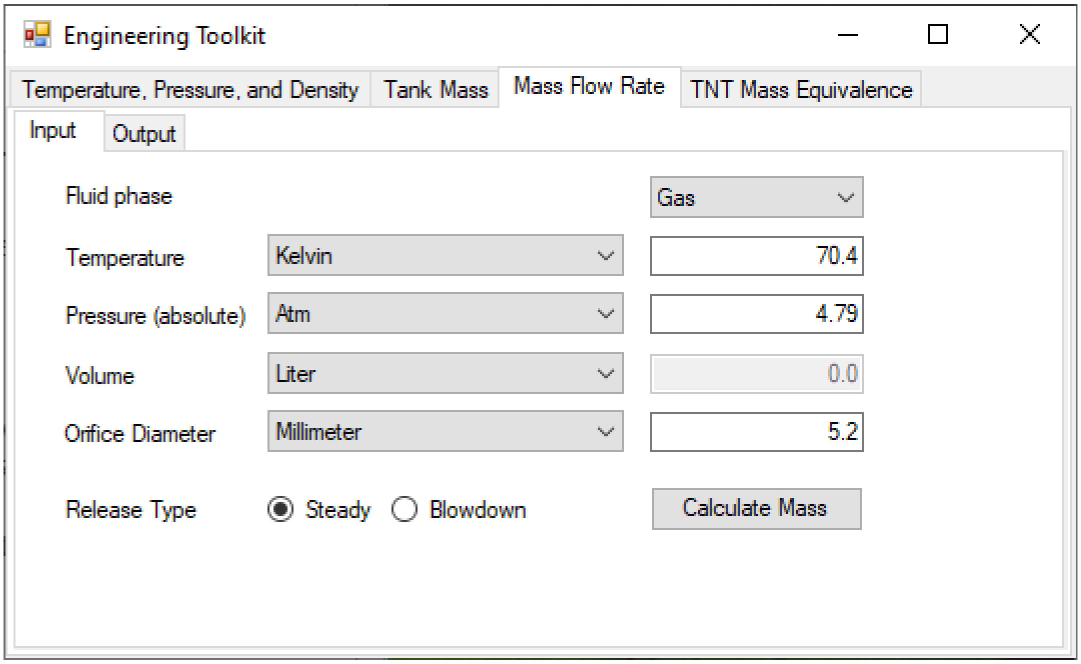


Figure A-101 : Input to Engineering Toolkit for LH_2 Partial Bore Rupture Case (After Pump)

Using these inputs, the mass flow rate was calculated (as shown in Figure A-102).

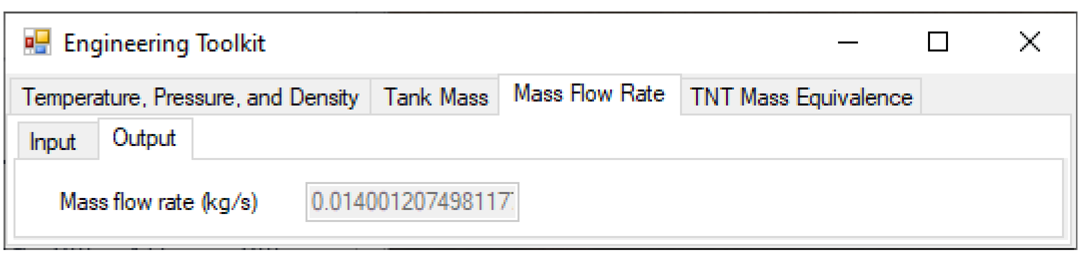


Figure A-102 : Output of Engineering Toolkit Calculation for LH_2 Partial Bore Rupture Case (After Pump)

Gas Plume Dispersion Model

The gas plume dispersion model was used to calculate the horizontal distance of the hydrogen at different mole fractions. Figure A-103 and Figure A-104 show the input to the gas plume dispersion model for the 4% and 10% mole fraction calculations, respectively.

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	8	Meter
Y lower limit	-2	Meter
Y upper limit	2	Meter
Contours (mole fraction)	0.04	...
Ambient pressure	1	Atm
Ambient temperature	288	Kelvin
Orifice diameter	5.2	Millimeter
Orifice discharge coefficient	1	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	4.79	Atm
Fluid temperature	70.4	Kelvin

Figure A-103 : Input for 4% Mole Fraction Calculation for LH2 Partial Bore Rupture Case (After Pump)

Variable	Value	Unit
X lower limit	0	Meter
X upper limit	3	Meter
Y lower limit	-1	Meter
Y upper limit	1	Meter
Contours (mole fraction)	0.1	...
Ambient pressure	1	Atm
Ambient temperature	288	Kelvin
Orifice diameter	5.2	Millimeter
Orifice discharge coefficient	1	...
Angle of jet	0	Degrees
Fluid pressure (absolute)	4.79	Atm
Fluid temperature	70.4	Kelvin

Figure A-104 : Input for 10% Mole Fraction Calculation for LH_2 Partial Bore Rupture Case (After Pump)

Figure A-105 and Figure A-106 show the results of the 4% and 10% mole fraction calculations, respectively. From these figures, the variables of interest were visually determined. For the 4% mole fraction case, the horizontal distance was determined to be approximately 7 meters. For the 10% mole fraction case, the horizontal distance was determined to be approximately 3 meters.

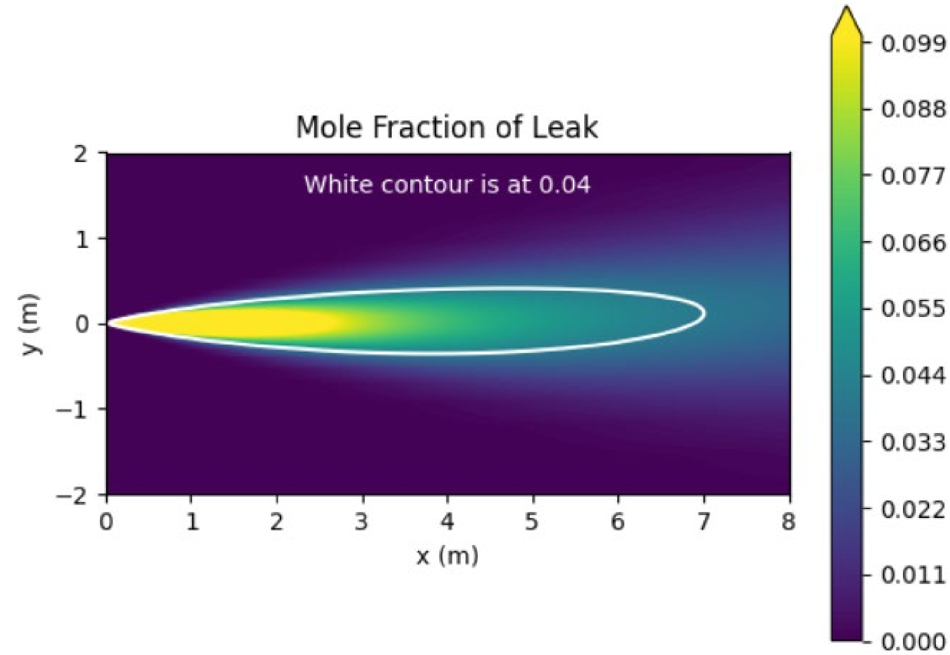


Figure A-105 : Contour at 4% Mole Fraction for LH_2 Partial Bore Rupture Case (After Pump)

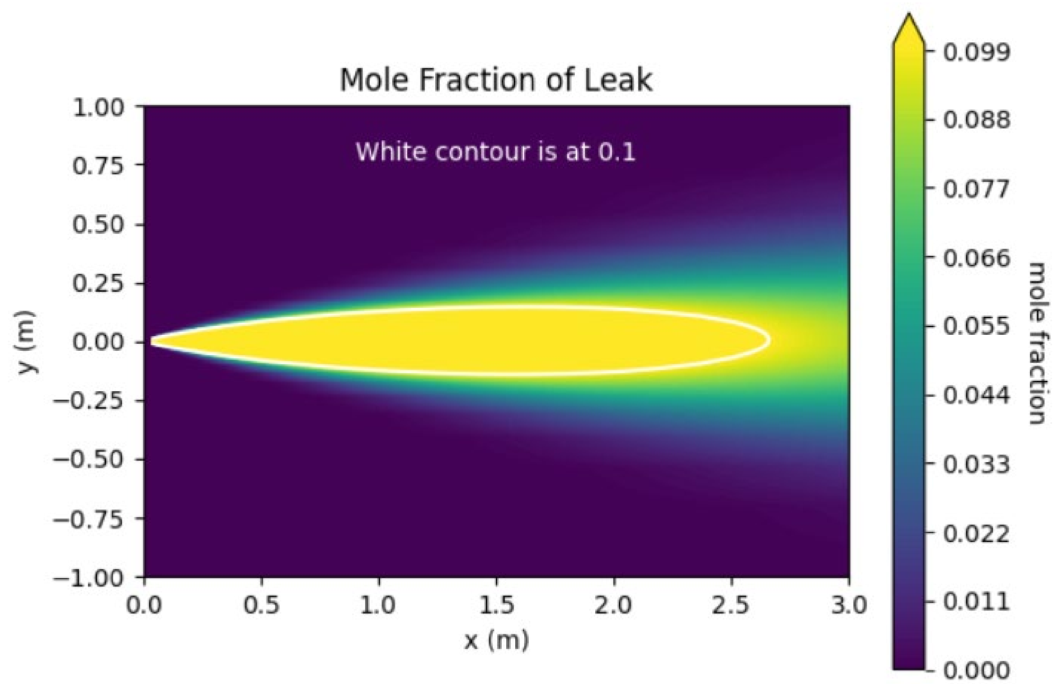


Figure A-106 : Contour at 10% Mole Fraction for LH_2 Partial Bore Rupture Case (After Pump)

Jet Flame/Radiative Heat Flux Model

The jet flame/radiative heat flux model was used to calculate the horizontal distance at which certain heat flux values were reached. Figure A-107 shows the input used in the jet flame/radiative heat flux model calculations.

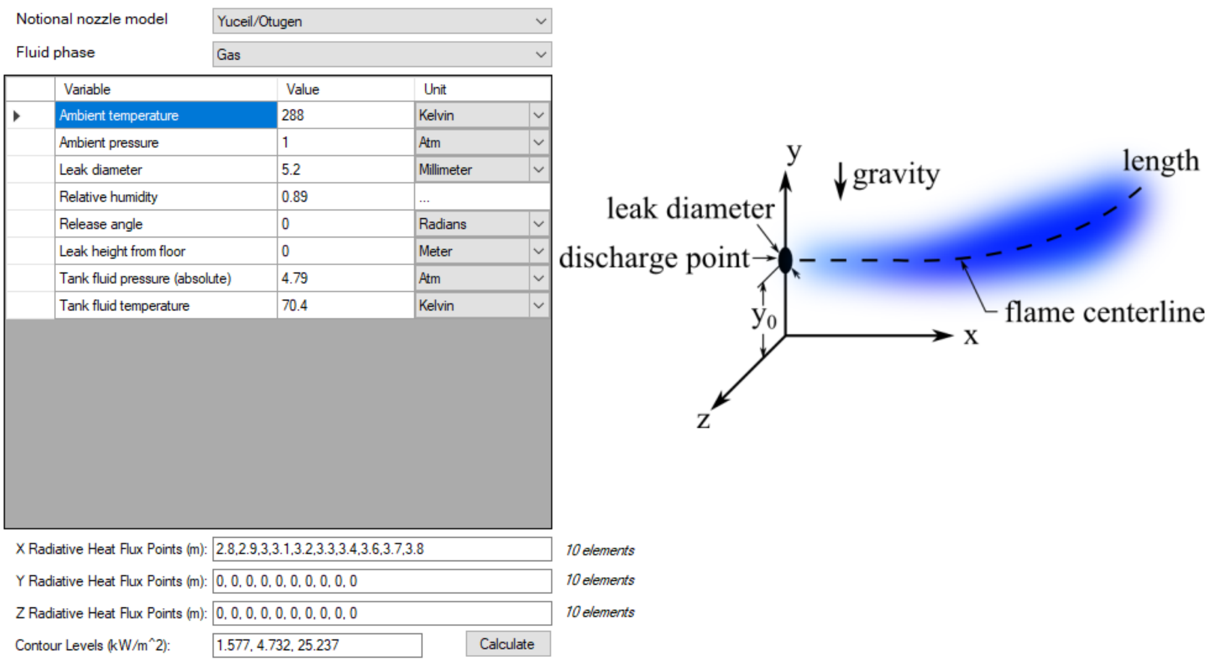


Figure A-107 : Input for the Jet Flame Model Calculation for LH_2 Partial Bore Rupture Case (After Pump)

Table A-8 shows the radiative heat flux results for the LH_2 partial bore rupture case (after pump). As shown, the horizontal distances at which heat flux of 3, 5, and 8 kW/m^2 are seen are approximately 3.7 meters, 3.3 meter, and 2.9 meters, respectively.

Table A-8: Radiative Heat Flux Results for LH_2 Partial Bore Rupture Case (After Pump)

X(m)	Y(m)	Z(m)	Flux (kW/m^2)
2.8000	0.0000	0.0000	9.6933
2.9000	0.0000	0.0000	8.4332
3.0000	0.0000	0.0000	7.3500
3.1000	0.0000	0.0000	6.4218
3.2000	0.0000	0.0000	5.6280
3.3000	0.0000	0.0000	4.9498
3.4000	0.0000	0.0000	4.3701
3.6000	0.0000	0.0000	3.4487
3.7000	0.0000	0.0000	3.0829
3.8000	0.0000	0.0000	2.7674

Figure A-108 shows the flame length for the LH_2 partial bore rupture case (after pump). From this figure, the variable of interest was visually determined to be approximately 3 meters.

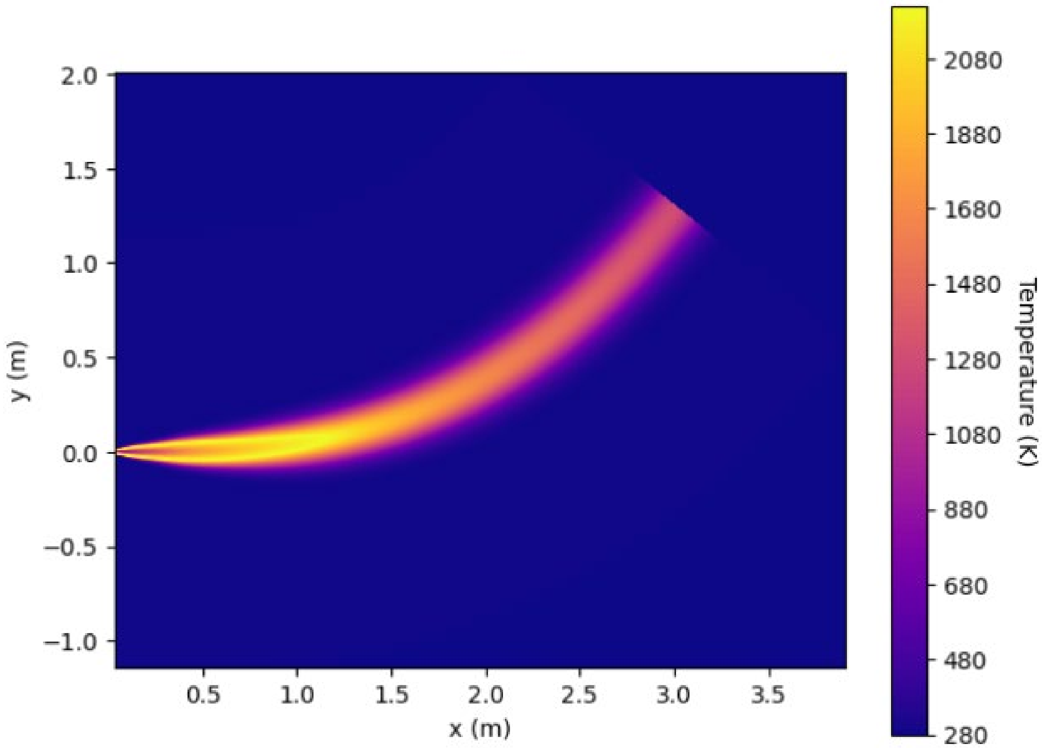


Figure A-108 : Flame Length for LH_2 Partial Bore Rupture Case (After Pump)

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