SANDIA REPORT
SAND2018-0585
Unlimited Release
Printed January 2018

INFORMING HAZARDOUS ZONES FOR ON-BOARD MARITIME HYDROGEN LIQUID AND GAS SYSTEMS

Myra Blaylock
Joseph Pratt
Gabriela Bran-Anleau
Camron Proctor

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology and Engineering Solutions of Sandia, LLC.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@osti.gov
Online ordering: http://www.osti.gov/scitech

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd
Alexandria, VA 22312

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.gov
Online order: https://classic.ntis.gov/help/order-methods/

SAND2018-0585
Printed January 2018
Unlimited Release

INFORMING HAZARDOUS ZONES FOR ON-BOARD MARITIME HYDROGEN LIQUID AND GAS SYSTEMS

Myra Blaylock, Gabriela Bran-Anleau, and Camron Proctor
Thermal/Fluid Science & Engineering

Joseph Pratt
Energy Innovation

Sandia National Laboratories
7011 East Avenue, MS 9957
Livermore, CA 94550

Abstract

The significantly higher buoyancy of hydrogen compared to natural gas means that hazardous zones defined in the IGF code may be inaccurate if applied to hydrogen. This could place undue burden on ship design or could lead to situations that are unknowingly unsafe.

We present dispersion analyses to examine three vessel case studies: (1) abnormal external vents of full blowdown of a liquid hydrogen tank due to a failed relief device in still air and with crosswind; (2) vents due to naturally-occurring boil-off of liquid within the tank; and (3) a leak from the pipes leading into the fuel cell room.

The size of the hydrogen plumes resulting from a blowdown of the tank depend greatly on the wind conditions. It was also found that for normal operations releasing a small amount of “boil-off” gas to regulate the pressure in the tank does not create flammable concentrations.

ACKNOWLEDGMENTS

The authors are grateful to Sujit Ghosh and Michael Carter at the U.S. Department of Transportation (DOT), Maritime Administration (MARAD) for their support of this work. This project was funded through MARAD's Maritime Environmental and Technical Assistance (META) program pursuant to an interagency agreement.

The authors would also like to thank the following stakeholders for their input in helping to make this work practical and meaningful:

- United States Coast Guard: Tim Meyers, Thane Gilman, Cindy Znati, LT Margaret Woodbridge, and Scott Mercurio
- American Bureau of Shipping: Steve O’Day, Roshan Jacob, Zhongfu Ge
- DNV-GL: Asmund Huser, Gerd-Michael Wursig, Anthony Teo
- Elliott Bay Design Group: Curt Leffers
- Red and White Fleet: Joe Burgard and Tom Escher

Thank you to the following Sandians for their technical contributions: Rad Bozinoski, Lennie Klebanoff, Tricia Gharagozloo, Chris LaFleur, and the members of the Sierra/Fuego support team.

TABLE OF CONTENTS

FIGURES

TABLES

EXECUTIVE SUMMARY

The SF-BREEZE feasibility study* identified a need for better understanding of the behavior of hydrogen releases on-board marine vessels if hydrogen is to be accepted as a viable marine fuel. Stakeholders including the US Coast Guard, American Bureau of Shipping, and DNV-GL were consulted and identified three hydrogen release / gas dispersion scenarios of interest. The first scenario is an abnormal liquid hydrogen tank blowdown through a vent in various wind conditions. The second scenario is the venting "boil-off" to relieve pressure built up under normal operating conditions. The third scenario is a full pipe rupture within the internal fuel cell power room of the vessel.

Two Sandia software packages were used for the leak simulations. MassTran (Mass Transport), a network flow modeling tool developed by Sandia National Labs, was used to calculate the amount and velocity of hydrogen that would be released in a hydrogen release event. Fuego is a low-Mach Computational Fluid Dynamics (CFD) code that uses an approximate projection algorithm with Control Volume Finite Element Method. Reynolds-Averaged Navier-Stokes (RANS) was used to solve the time-dependent Navier-Stokes and energy equations to determine the location and movement of the flammable mass regions.

For the case of a full blowdown in a crosswind, the 5 knot and 30 knot crosswind velocities showed clearly that the hydrogen plume shape is greatly influenced by the wind due to the much lower density of hydrogen compared to that of air. In these simulations, it was also found that the plume is always positively buoyant even when very cold (70 K). The hydrogen will only go downward if there are wind currents that carry it that direction.

For the "boil-off" case, no resulting flammable concentration of gas was present at the vent outlet. The practice of venting small amounts of hydrogen appears to be a safe way to prevent the overpressure of the liquid hydrogen tank on a marine vessel due to a prolonged period of being idle and suggests a hazardous/exclusion zone around such a vent outlet may not be necessary.

For the fuel cell room case, analysis of a large hydrogen release in a confined but ventilated fuel cell power room shows the importance of fast detection and shut-off combined with an adequate and properly designed ventilation system. The low momentum of hydrogen as compared to air as seen in the other release scenarios can be leveraged by the air handling system designer to quickly move hydrogen away from potential ignition sources and out to a safe vent location.

Additional work is recommended to provide the information needed to completely define accurate hazardous zones for hydrogen for open-air releases, and to provide best-practices for ventilation and safety systems in confined spaces. However the understanding obtained from these first results can still be used by regulators to inform the developing design codes, eventually reducing the need for unique gas dispersion studies on every future vessel submitted for approval. It can also lead to codes that avoid placing undue burden on vessel design and layout while avoiding situations that are unsafe. The combination of these results can eventually lead to wider adoption of zero emission hydrogen technology in the maritime sector.

* Pratt, J.W. and L.E. Klebanoff, *Feasibility of the SF-BREEZE: a Zero-Emission, Hydrogen Fuel Cell, High-Speed Passenger Ferry*. 2016, Sandia National Laboratories report SAND2016-9719.

NOMENCLATURE

Abbreviation	Definition
ACH	Air Changes per Hour
Blowdown	Emptying of a pressure vessel until pressure reaches equilibrium with atmosphere
CFD	Computation Fluid Dynamics
DOT	Department of Transportation
IGF Code	International Code of Safety for Ships using Gases or other Low-flashpoint Fuels
LH_2	Liquefied hydrogen
LNG	Liquefied natural gas
RANS	Reynolds Averaged Navier-Stokes
SF-BREEZE	San Francisco Bay Renewable Energy Electric vessel with Zero Emissions

1. INTRODUCTION

The goal for this study is to inform accurate overall hazardous zone requirements for hydrogen when it is used as a fuel for marine vessels. Our hope is to enable faster and easier approval of safe designs by reducing the need for gas dispersion studies on every future vessel submitted for approval, and to avoid placing undue burden on vessel design and layout while also avoiding situations that are unsafe.

The initial stage of this work was a feasibility study conducted by Sandia National Labs, Elliott Bay Design Group, and the Red and White Fleet, a ferry company in the San Francisco Bay, to determine if a zero emissions vessel would be technically possible, accepted by regulators, and commercially viable. The results of this study can be found in the report "Feasibility of the SF-BREEZE: a Zero-Emission, Hydrogen Fuel Cell, High-Speed Passenger Ferry" [1]. The SF-BREEZE ferry has liquid hydrogen stored on the top deck of a 150 passenger boat and is used as a case study for this work.

For this stage of the study, stakeholders including the US Coast Guard, American Bureau of Shipping, and DNV-GL were consulted to help define the most significant potential leak scenarios to analyze. These stakeholders represent design approval authorities so understanding their primary areas of interest is essential to ensure usefulness of the results. Presented here are the results from performing detailed modeling of these initial scenarios. Follow-on studies will examine other scenarios of interest as needed to provide all information necessary to create accurate hazardous zones for hydrogen on-board marine vessels.

This work focuses on the analysis of three main gas dispersion / hydrogen release scenarios. The first scenario is an abnormal liquid hydrogen tank blowdown through a vent in various wind conditions. The second scenario is the venting "boil-off" to relieve pressure built up under normal operating conditions. The third scenario is a full pipe rupture within the internal fuel cell power room of the vessel.

It is important to understand that these hydrogen release scenarios were chosen only to gain insight on the hydrogen dispersion characteristics should such a release be encountered. No attempt was made to predict probability of the release or the resulting hazardous consequence. Appropriate hazardous zone design must consider both of these factors in addition to the gas dispersion characteristics presented herein. Such an analysis will reveal the practical need for hazardous zones, type of zone, size of zone, and mitigation strategies that maritime vessel designers may choose as alternatives to hazardous zones.

2. APPROACH

This chapter describes the approach and setup of the work, beginning with a description of the simulation tools used. Following that are descriptions of the three case studies, and then a discussion of the major assumptions used.

2.1. Simulation Tools

Two software packages were used for the completion of the leak simulations: MassTran to calculate the leak conditions, and Fuego to calculate the flow of the release.

MassTran (Mass Transport), a network flow modeling tool developed by Sandia National Labs, was used to calculate the amount and velocity of hydrogen that would be released in a hydrogen release event. MassTran enables users to model compressible and incompressible flows of multi-species gas mixtures through arbitrary arrangements of pipes, vessels, and flow branches [2]. As the source tank or pipeline empties, MassTran calculates the temperature, pressure, mass, and density of the gas in the source and of the released gas as well as the released mass flow rate and velocity. The equations used for these calculations have been validated in previous work [3] including releases of hydrogen.

Fuego is a robust simulation capability for buoyancy-driven turbulent flow mechanics [4]. This low-Mach Computational Fluid Dynamics (CFD) code is part of Sandia's Sierra Suite [5]. It was validated for hydrogen releases in previous work [3]. Fuego uses an approximate projection algorithm with Control Volume Finite Element Method (CVFEM [6]). Reynolds-Averaged Navier-Stokes (RANS) method was used to solve the time-dependent Navier-Stokes and energy equations. The standard $\kappa - \epsilon$ closure model (a two-equation type model) is used to evaluate the turbulent eddy viscosity for RANS simulations. For the release cases in wind, there are several adjustable parameters for this model can that can be tuned to get more accurate results [7]. For the jet in crossflow class of simulations, the parameters were adjusted appropriately to $C_\mu = 0.1$, $C_{\epsilon 1} = 1.36$, and $C_{\epsilon 1} = 2.0$. For the release case without wind, the typical values were kept: $C_\mu = 0.09$, $C_{\epsilon 1} = 1.44$, and $C_{\epsilon 1} = 1.92$. These were calibrated with air flow [8-10], so if experimental validation ever is done for hydrogen, then these values might be improved. The convection terms in the equations are discretized with a first order upwind differencing scheme although the higher order MUSCL [11] scheme has also been used for some solutions. Transport equations are solved for the mass fractions of each chemical species except for the dominant species which is computed by constraining the sum of the species mass fractions to equal one. The ideal gas equation of state is used to relate the density and pressure of the gas mixture. While the hydrogen is pressurized in the tank, it is in the incompressible regime by the time it is reaches the domain that is under investigation using CFD. Ambient conditions were assumed to be 70° F at 1 atm of pressure.

Changing relative humidity will slightly change the water content of the air, which in turn can affect the density and heat capacity, both important factors in the release modeling work. Two scenarios were examined:

1. Low water content: 10 °C, 40% RH. Water content = 0.2% H_2O by mole
2. High water content: 30 °C, 95% RH. Water content = 1.5% H_2O by mole

The difference in atmospheric water content between these two scenarios is just over 1%. The resulting effect on density and heat capacity is negligible and well within the uncertainty in the modeling results. Hence humidity was not included in the model.

Due to the initial exploratory nature of this project, we chose to use the faster running RANS method instead of the more accurate, but much more computationally expensive Large Eddy Simulations (LES) or Direct Numerical Simulations (DNS). Because of this, the small scale turbulence is averaged, so we expect the dissipation to be under predicted. Thus the predicted fuel concentrations downwind of the release are conservative.

All of the meshes for the simulations were created using the Sandia National Laboratories software tool, Cubit. Mesh sizes range from 60,000 to 2 million nodes.

The open-air scenarios studied use a mole fraction between 8% and 75% for the flammability range of hydrogen rather than the more commonly-used 4%-75% range. It has been experimentally shown that the actual lower limit for a sustained hydrogen flame upon being released as a turbulent jet is 8% by volume at its centerline [12]. The lower limit of 4% continues to be used for still or slowly moving mixtures and is used for the closed room scenario.

2.2. Scenario 1: Abnormal Blowdown due to an Opened Pressure Relief Device from Large LH2 Tank Venting Conditions

The first scenario is a full scale LH_2 tank blowdown which assumes that a pressure relief device abnormally fails open due to a manufacturing or other defect while connected to the vent stack. The tank is modeled to be 4500 gallons operating at 150 psig and holding a mixture of liquid at the bottom and vapor at the top. The worst case scenario would occur when most of the liquid is spent because all of the vapor would be forced out due to the high pressure until an equilibrium is reached with the liquid boiling off and the vapor escaping. At that point the velocity and amount of fuel would be much less than the initial vapor blowdown of the pressurized gas. As a worst case, we assumed the tank to be 90% vapor.

The leak is through a 1 inch orifice in the notional failed relief device near the tank and is choked at that point. As shown in Figure 1, the vent stack reaches 25 feet above the top deck of the ferry and has a 7 inch internal diameter. The height of the stack was selected so that the opening would be above the instrument mast [1]. Due to modeling constraints, the stack was considered to be straight up (instead of at an angle as shown in Figure 1), and the computational domain starts at the top of the opening of the stack. While this choice might slightly influence the modeled location of the plume (i.e. in the model it is prevented from going below the top of the stack) we will show below that this is expected to be a negligible effect.

The size of the assumed 1 inch valve orifice controls how long the leak will last, while the diameter of the vent stack opening controls the velocity of the released gas. Changes in these diameters from what we used here will have an effect on the size and duration of the flammable plume, so what is presented here are representations of an expected plume when the equipment is comparable.

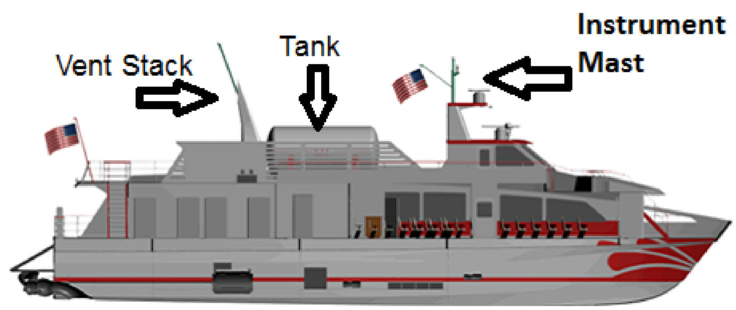

Figure 1. Engineering model of the SF-BREEZE with the locations of the LH_2 tank and the vent stack. Ferry design by Elliott Bay Design Group [1].

While the liquid hydrogen is stored at 20 K, we have assumed that it would heat up to at least 70 K while escaping through the vent. All LH_2 releases were set to 70 K at the outlet of the vent stack.

The tank blowdown was investigated at three different wind speeds: 0 knots to represent a calm day when the ferry is docked, 5 knots which captures normal wind conditions when docked, and 30 knots which could represent either the ferry moving or very windy condition while docked. The wind is assumed constant laminar flow for entire length of the release, which will be shown to have a significant conservative effect of plume length predictions.

2.3. Scenario 2: Normal Venting due to Boil-off

Despite best efforts and innovative designs, all cryogenic storage tanks experience some amount of heat transfer from the environment to the liquid contained inside ("heat leak"). Some cryogenic storage tanks have integrated refrigeration systems or cryo-coolers to maintain cold temperatures in spite of heat leak. For those that do not, over time this heat leak warms the surface of the cryogenic liquid to the boiling point, and it slowly evaporates. In a closed tank system this evolution of gas leads to a pressure rise. At some point, which can take several days or weeks of un-use depending on the tank design and initial conditions, the pressure in the tank will approach the maximum operating pressure, and it is common industrial practice at this point to open a control valve to continually bleed the gas out at a rate equal to the amount being evolved by boiling in order to prevent the pressure from rising higher. This phenomenon is often referred to as "boil-off" and the vented gas as "boil-off gas".

This second scenario examines the dispersion of hydrogen due to boil-off. In the SF-BREEZE report it was estimated that 0.6% of the tank mass would need to be vented or used each day if the vessel has been completely un-used for a long enough time that the pressure in the tank has reached the upper limit of allowable pressure.

Besides the use of tank refrigeration or cryo-cooling systems, another way to eliminate boil-off altogether would be to use the on-board fuel cells to generate a nominal amount of power such as that needed to power the lights. Assuming a conservative 1% mass of a full tank in boil-off per day, in the SF-BREEZE study it was calculated that producing just 7.5 kW of power by the fuel cells (out of 4.96 MW of installed power) would consume all of this gas and there would be no need to vent it.

However, to be conservative, in this study we consider that neither methods are utilized and we model the venting of 1% of the 1200 kg tank over a 24 hour period out of the same vent stack described in the previous scenario. The 7 inch diameter opening results in a 1.29 cm/s velocity release which is simulated with a 5 knot cross wind.

2.4. Scenario 3: Leak Inside Fuel Cell Room

The third scenario shows possible outcomes from a catastrophic rupture of the hydrogen fuel line going into the fuel cell racks located in the interior fuel cell room. The room was assumed to be 24 feet by 16 feet 6 inches and 9 feet 6 inches tall, and have four rows of racks spaced to allow for access and ventilation, as shown in Figure 2. There are nine vents near the floor of the room, each blowing 200 cfm to achieve 30 air changes per hour (ACH) as required by the IGF code for an Emergency Shut Down (ESD) designated space. Since under normal conditions hydrogen naturally rises in air, the outflow vents were located along the center of the ceiling.

The leak assumed that a 1" pipe is completely sheared and pointing upwards from one of the racks. Future studies will include the more likely scenario that there is a hole in the pipe which is some fraction of the pipe diameter instead of the worst case complete shearing of the pipe. The normal pressure in the pipe is expected to be 80 psi, but 100 psi was used for conservatism. It was calculated that a 1" sheared pipe under 100 psi would experience a leak with a velocity of 2500 ft/sec. The fuel system would have sensitive pressure sensors that would detect a drop in pressure due to a leak, and the room will have hydrogen sensors to detect any accumulation above 0.8% hydrogen concentration. Either method will shut off the supply of fuel quickly. Cases where the hydrogen was shut off 0.5 and 2.0 seconds after the beginning of the rupture were analyzed.

2.5. Conservative Assumptions

Throughout the modeling and simulation, several assumptions had to be made, either because the precise information was not available or to allow the simulation to run in a time-efficient manner. The CFD model in particular required multiple days to run on SNL's extensive computing facilities. The assumptions were documented throughout this report, and in all cases, the most conservative assumption was made to ensure the worst cases consequence was analyzed. We would like to state them all in this section to emphasize that more realistic and/or likely scenarios will probably have less extreme results.

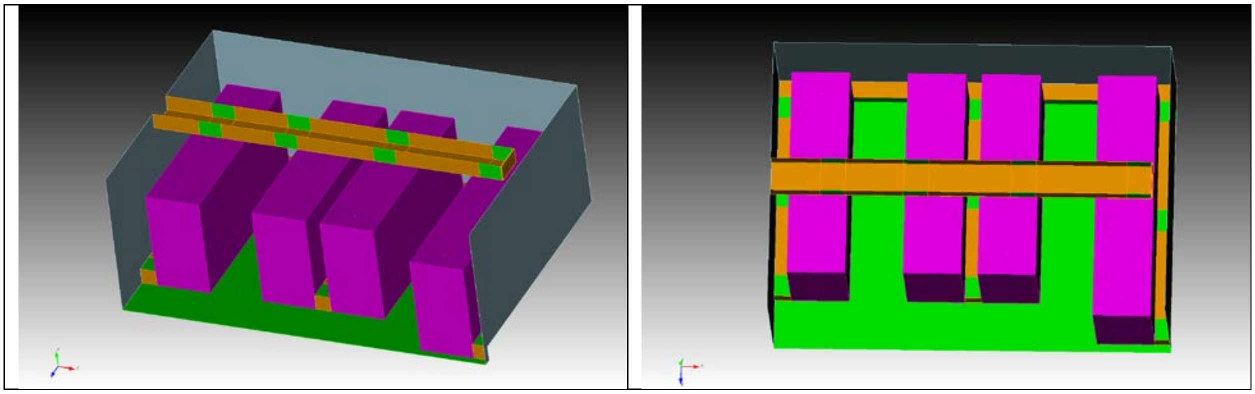

Figure 2. Schematic of the fuel cell room showing the ventilation ducts in orange and the racks in pink. The right hand side shows a top down view.

Assumptions made:

- Under-predicted dissipation due to RANS calculations
- Laminar flow of wind will also under-predict dissipation
- Complete valve failure or pipe shearing instead of more likely 1% diameter leak size
- 90% vapor in tank will have a larger amount of hydrogen released
- 70 K as release temperature throughout entire blowdown and for boiloff

3. RESULTS

3.1. Scenario 1: Abnormal Blowdown due to a Failed-Open Pressure Relief Device from Large LH_2 Tank Venting Conditions

MassTran was used to calculate the venting conditions that are then modeled using CFD. The tank size and conditions described above produce a velocity profile that is shown in Figure 3. The blowdown lasts about 6 minutes. While it is probable that the vapor would heat up as it traverses out the 25 foot vent stack, in this initial study we did not perform a heat transfer analysis of the vent pipe to determine the exit temperature over the blowdown period. It was assumed that the exit temperature is constant at 70 K for the entire release. This was thought to be a reasonable estimate given the starting temperature of the tank (20 K), the length of the vent stack, and the velocity of the gas. If the actual temperature at the outlet is colder, the plume will be less buoyant than shown. If the temperature is warmer, the plume will be more buoyant.

3.1.1. Release without wind

The first case looked at a scenario with no wind, which would be representative of the ferry not moving on a calm day. The domain shown in Figure 4 has a 15-meter x 15-meter footprint and is 80 meters tall. The figure shows the maximum height of the flammable plume is about 50 meters and is reached in 20-35 seconds. The flammable plume has a maximum width of 7 meters at this time. Figure 5 shows images of the entire time-series.

As we will see below with releases in crosswind, hydrogen flow is greatly influenced by air movement. In this case without wind, any air movement in the domain (up to 80 m high) would cause the hydrogen to disperse wider than shown here and have a resulting shorter height of the flammable mass. In other words, these results should be thought of as a theoretical worst-case which would only be encountered when winds are absolutely still.

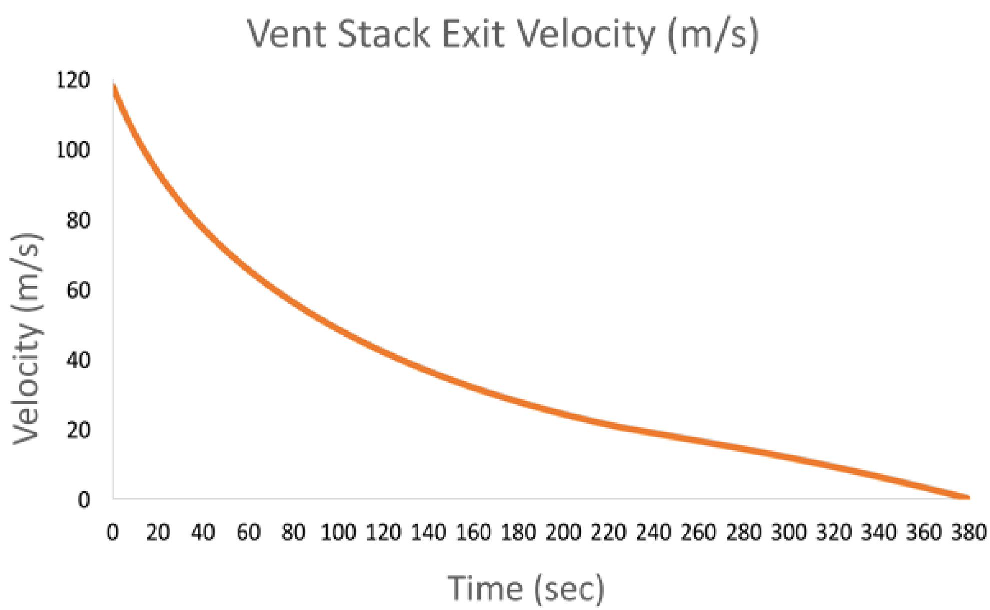

Figure 3. Velocity blowdown profile for a 4500 gallon LH_2 tank starting at 150 psi and 70 K. The initial quality within the tank is 90% vapor and 10% liquid.

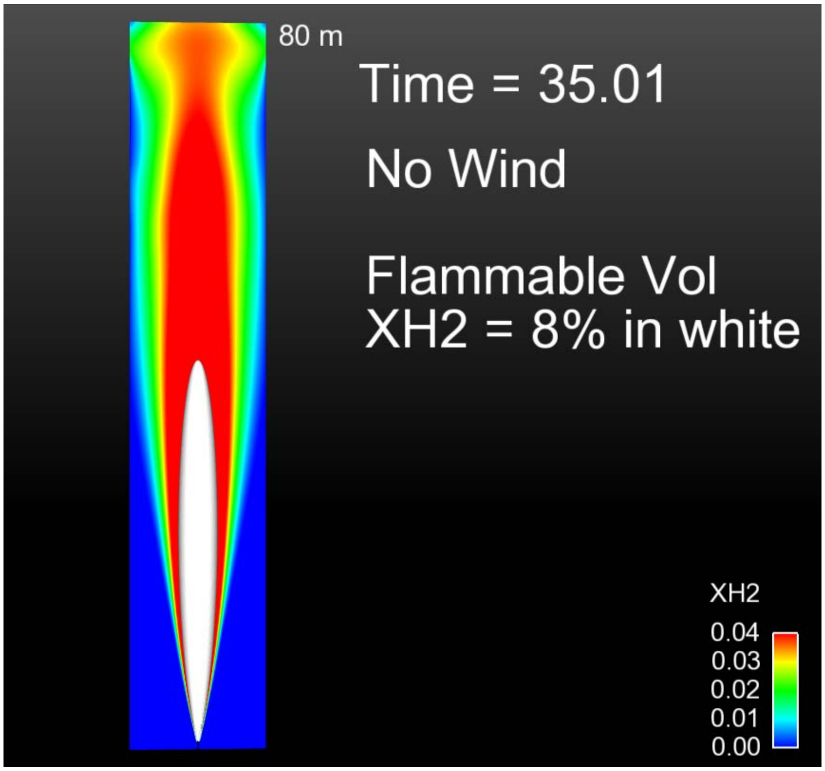

Figure 4. Venting of hydrogen with no wind at the time of maximum height for the flammable range. The colors show the mole faction of hydrogen with the flammable range of 8-75% in white. The domain is 80 m tall and the flammable white region is 50 m tall. The plume has a maximum width of 7 m at this time.

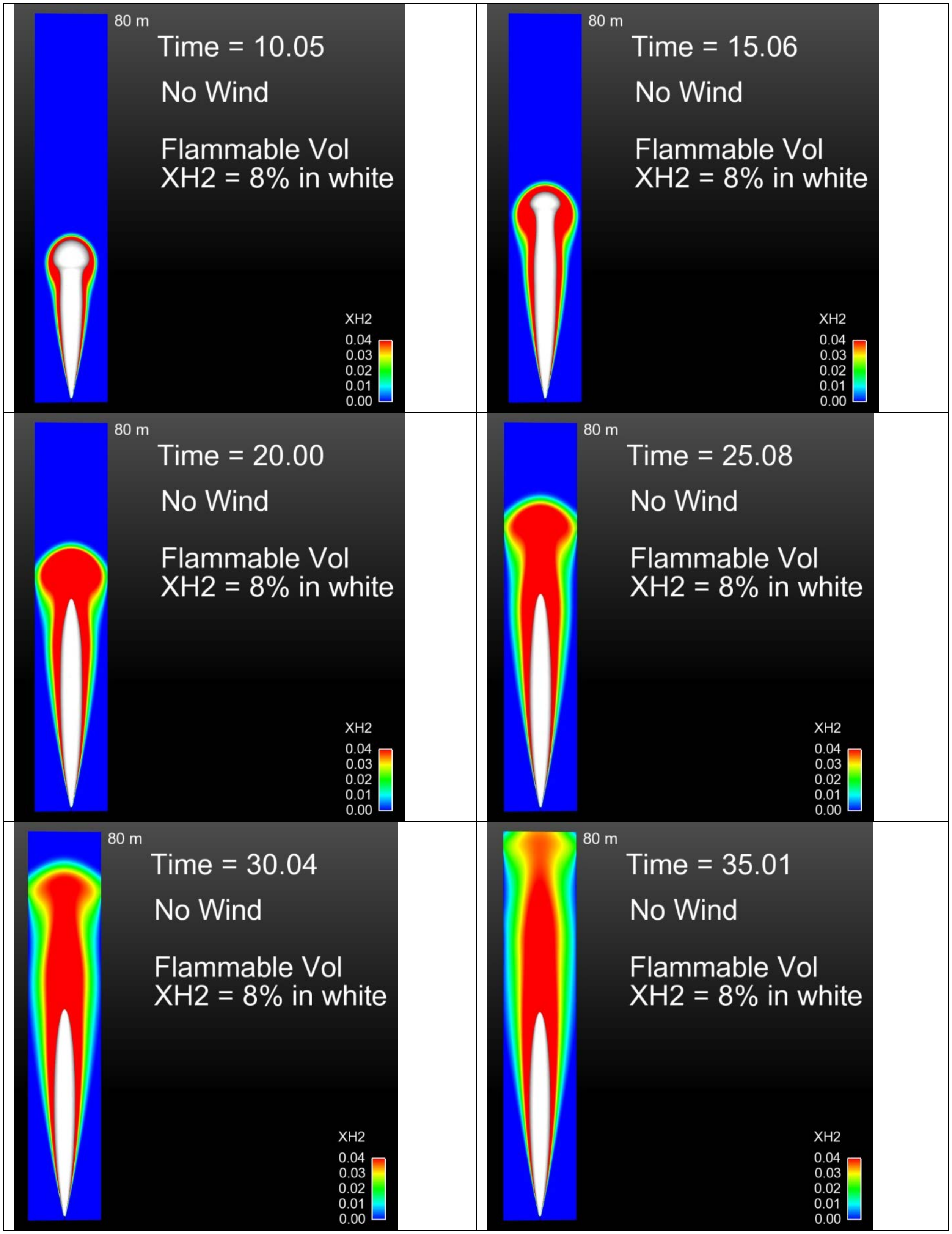

Figure 5: Time series of the no-wind hydrogen venting case. The colors show the mole faction of hydrogen with the flammable range of 8-75% in white.

3.1.2. *Release with 5 knot wind*

The second case explores the resulting plume in a 5 knot laminar flow cross-wind condition. This domain is 80 meters long, 20 meters tall, and 15 meters thick. The plume reaches its maximum length of 20 meters in 14 seconds. Figure 6 shows that the wind has bent the plume so it is only 7.7 meters high. This jet in cross-flow configuration also produces the expected pair of counter rotating vortices [13], shown in Figure 7, which helps dissipate the hydrogen. The time series pictures are shown in Figure 8.

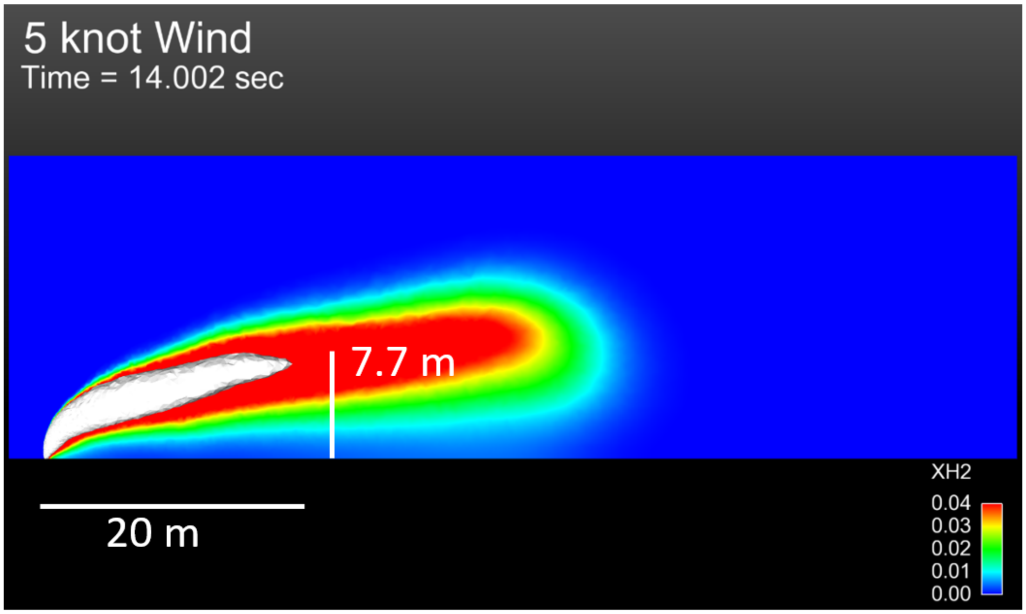

Figure 6. Hydrogen release in a 5 knot wind at time of maximum flammable length (20 m). The colors show the mole faction of hydrogen with the flammable range of 8-75% in white.

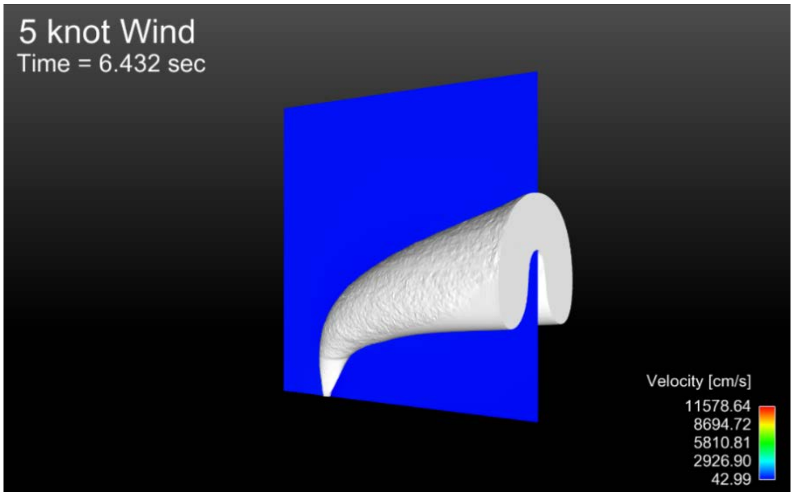

Figure 7. Cut off view of the hydrogen release in a 5 knot wind shows that the flammable mass creates a pair of counter rotating vortices. The flammable range of 8-75% mole fraction is shown in white.

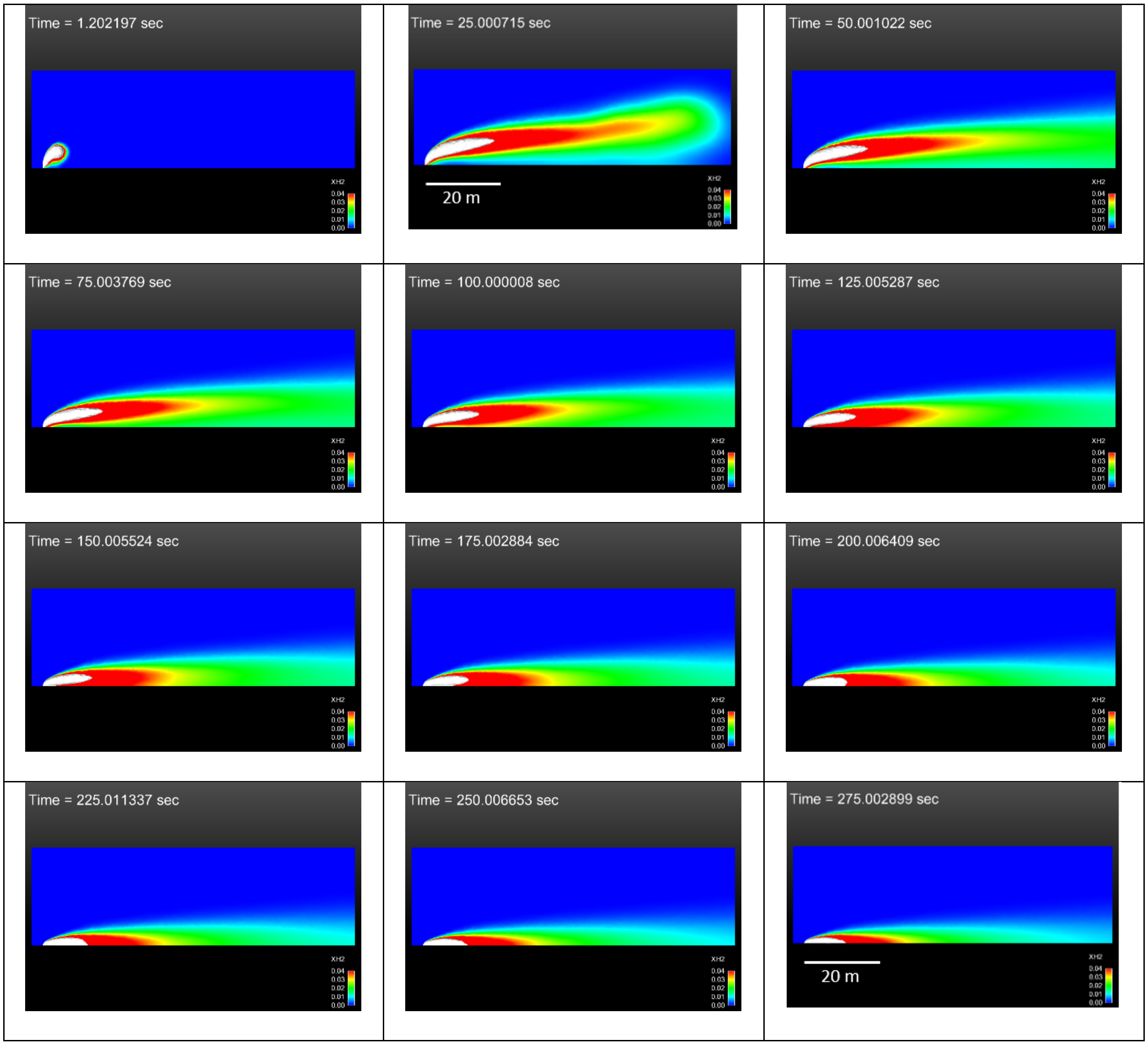

Figure 8: Time series of the hydrogen blowdown venting with a 5 knot crosswind. The flammable range of 8-75% mole fraction is shown in white.

The figures show that even with a modest 5 knot wind, the hydrogen plume is drastically bent over in spite of the high velocity out of the vent stack. This is due to the very low density of hydrogen relative to air even at 70 K, and the resulting momentum differences between the two fluid streams (vertical stream of hydrogen versus cross flow of air). This phenomenon, that the wind direction has a strong, direct influence on the direction and extent of the hydrogen plume, is an important characteristic to consider in establishing hazardous zones for hydrogen.

3.1.3. Release with 30 knot wind

The domain for the 30 knot wind case was made to be 80 meters long, 6.3 meters high, and 6.6 meters thick. As can be seen in Figure 9, the flammable mass leaves the end of the domain after about 30 seconds of simulated time, so we are unable to determine the maximum length of the plume. Figure 10 gives the time series pictures of the release.

Because this RANS simulation only produces laminar flow wind conditions, we would like to point out that in reality a 30 knot wind would most likely be much more turbulent than this simulation shows. It is therefore probable that the flammable concentrations of hydrogen would be dissipated much more easily, making the actual plume much shorter than shown. Future modeling work should examine the effect of large-scale downstream turbulence to better define the practical extent of such a plume.

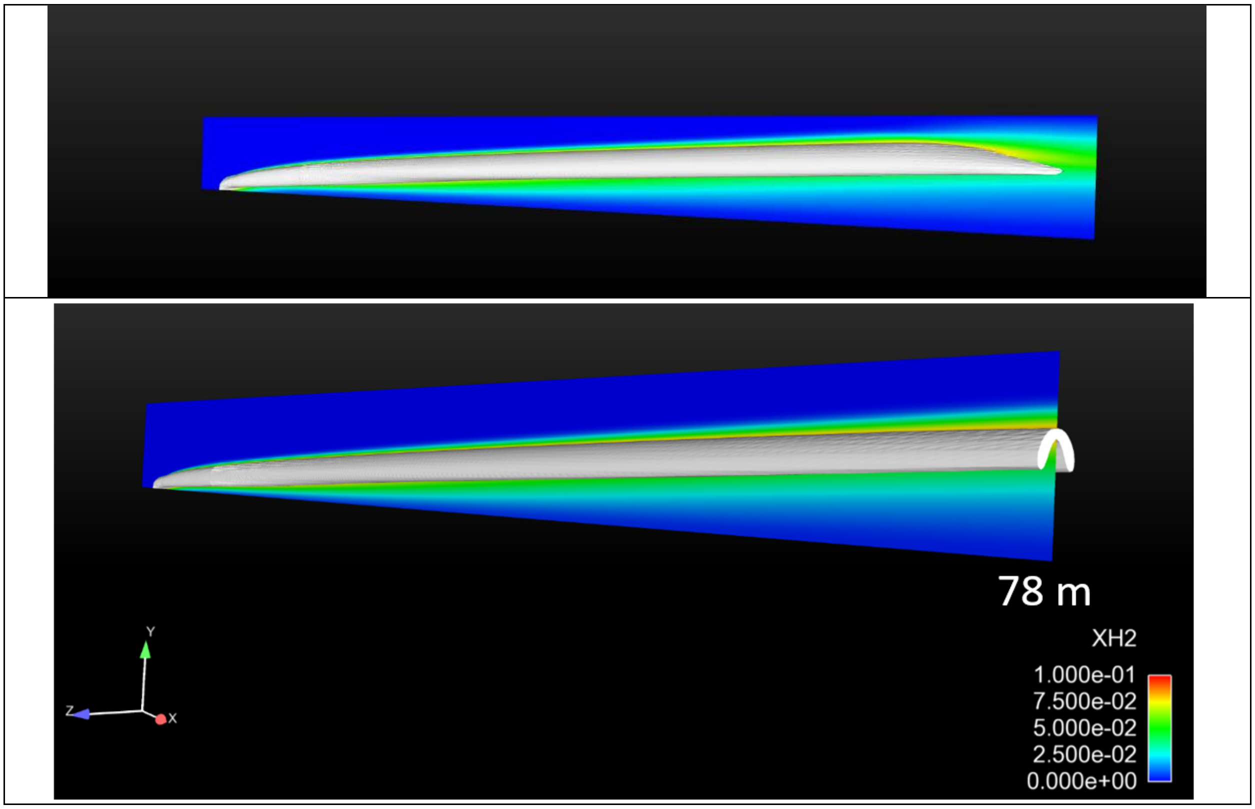

Figure 9. The top panel shows the 30 knot wind case after 26 seconds, and the bottom at 67 seconds. The domain length is 78 m long. The colors show the mole faction of hydrogen with the flammable range of 8-75% in white.

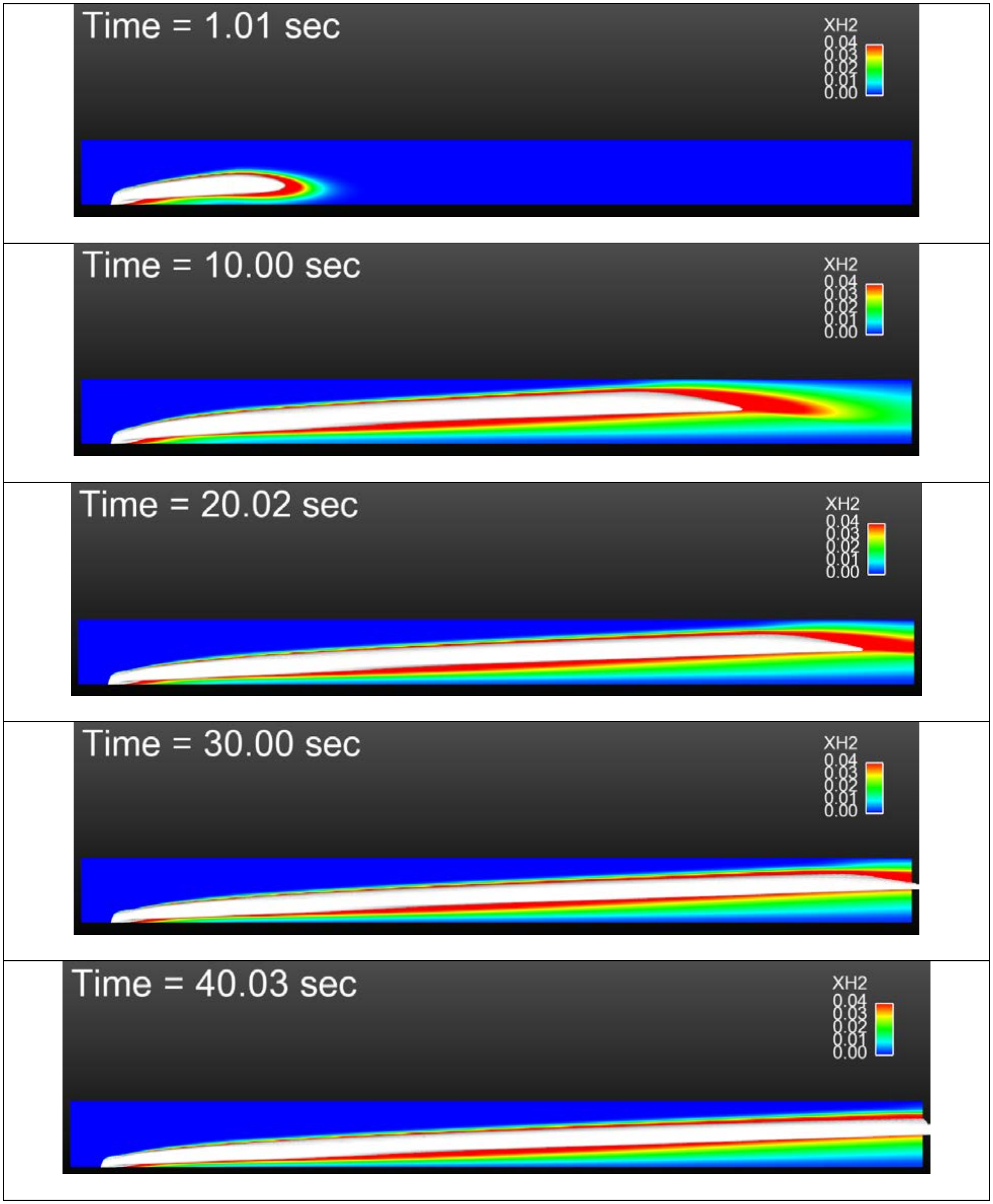

Figure 10: Time series of the hydrogen blowdown venting with a 30 knot crosswind. The domain length is 78 m long. The flammable range of 8-75% mole fraction is shown in white.

3.1.4. Comparison of the different wind scenarios

The three wind cases were compared after three seconds of the release to examine the effects that the wind speed has on the shape of the plume and the amount of flammable mass in the domain. It is shown that the wind has a large effect on the light weight hydrogen. For the case without wind, the plume is 15 meters high and 5 meters across. By adding the 5 knot wind, the plume

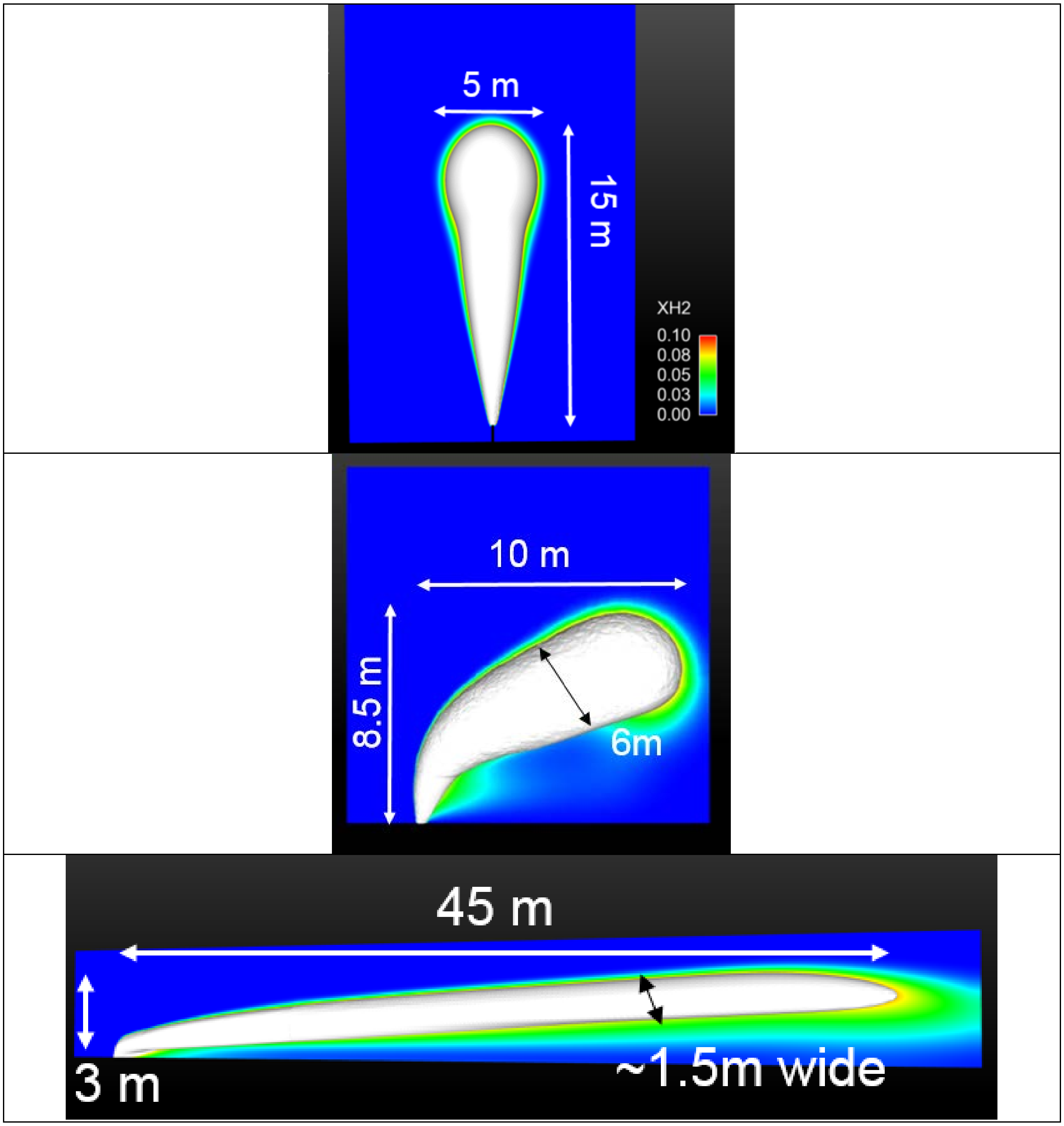

Figure 11. Comparison of the three wind conditions at 3 seconds after release: top panel has no wind, middle panel has a 5 knot wind, and the bottom panel has a 30 knot wind. The colors show the mole faction of hydrogen, with the flammable range of 8-75% in white.

only reaches 8.5 meters, but is 10 meters long and 6 meters wide. The faster 30 knot wind stretches the plume to 45 meters after 3 seconds, but it is only 3 meters high and 1.5 meters across. These effects can be seen in Figure 11.

Increasing the wind velocity also increases the dissipation of the flammable mass, even in these laminar conditions. Table 1 illustrates this by showing how the amount of flammable mass decreases as wind speed increases. The total mass of hydrogen in the domain is shown for reference. [Note: the difference in total mass between wind cases is due to gas flowing out of the open boundary condition on the right for the 30 knot case.]

3.1.5. Buoyancy

One of the most asked questions with regards to releases from a liquid hydrogen tank is whether the extremely cold gas will sink or rise. To address this question we plotted the specific gravity (density of the homogeneous hydrogen/air mixture of the plume divided by the density of air, $\rho_{air} = 0.001196$ kg/m^3) for the 5 knot wind case after 290 seconds. We chose this time because it is relatively late in the release so that the upward momentum due to the initial velocity is minimal, thus giving a somewhat "worst case" result. A specific gravity value less than one indicates that the plume is less dense than air and would therefore be positively buoyant. We found that all of the plume area remains lighter than air. In the center of the plume where the gas is coldest, which might cause a denser mixture, it also has the highest concentrations of hydrogen which counteracts this effect. As seen in Figure 12, the flammable concentrations will remain buoyant.

Table 1. Flammable and total mass of the hydrogen after 3 seconds of venting.

H_2 Mass	No Wind	5 Knots	30 Knots
In the 8%-75% flammable range	25.3 kg	23.8 kg	21.1 kg
Total (for reference)	28.1 kg	28.0 kg	27.6 kg (out end of domain)

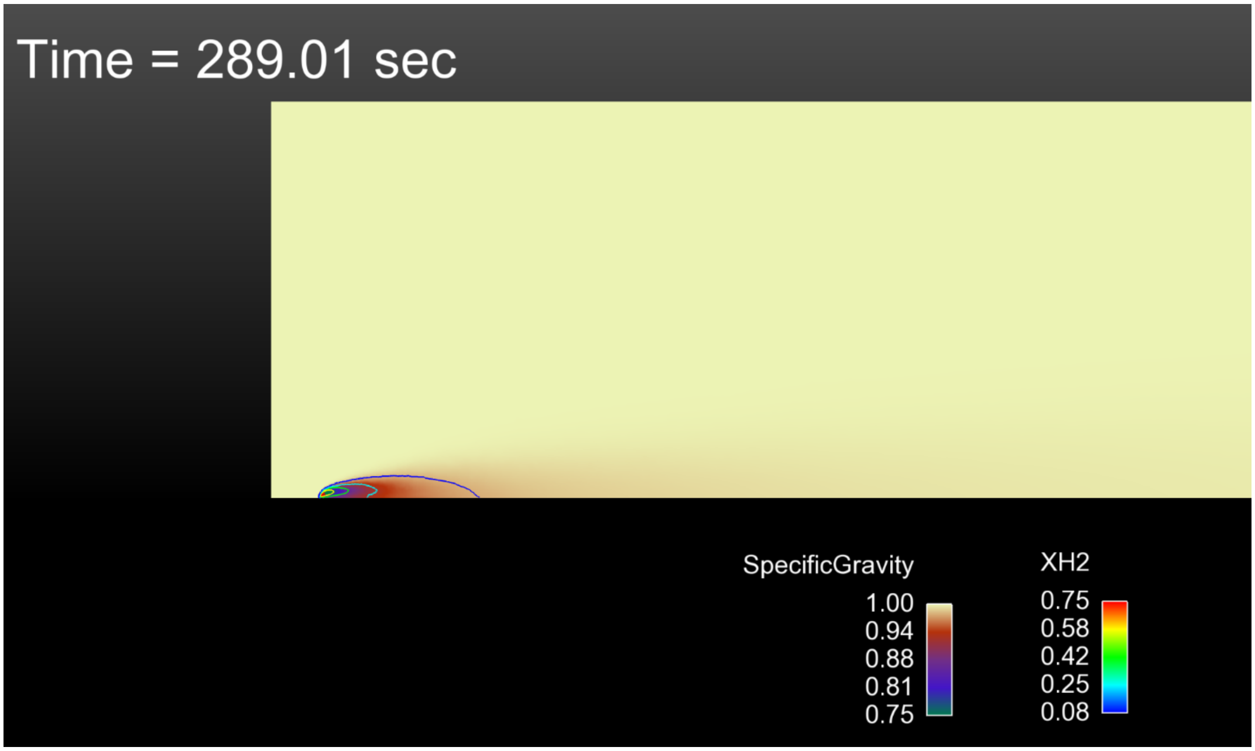

Figure 12. Full blowdown 290 seconds after release in 5 knot wind blowing left-to-right. The shading shows the specific gravity of the plume. A specific gravity less than 1.0 indicates a higher buoyancy than air. Everywhere in the domain the plume mixture is positively buoyant. The contour line colors show the mole fraction. The outermost (purple) line shows the 8% lower flammability limit. It reaches about 10 meters downstream from the release point.

The temperatures profile of the plumes at the three wind speeds are shown in Figure 13, with the mole fractions shown as contour lines. The temperature of the release is coldest where the concentration of hydrogen is highest, so the plumes remain buoyant in these cases as well.

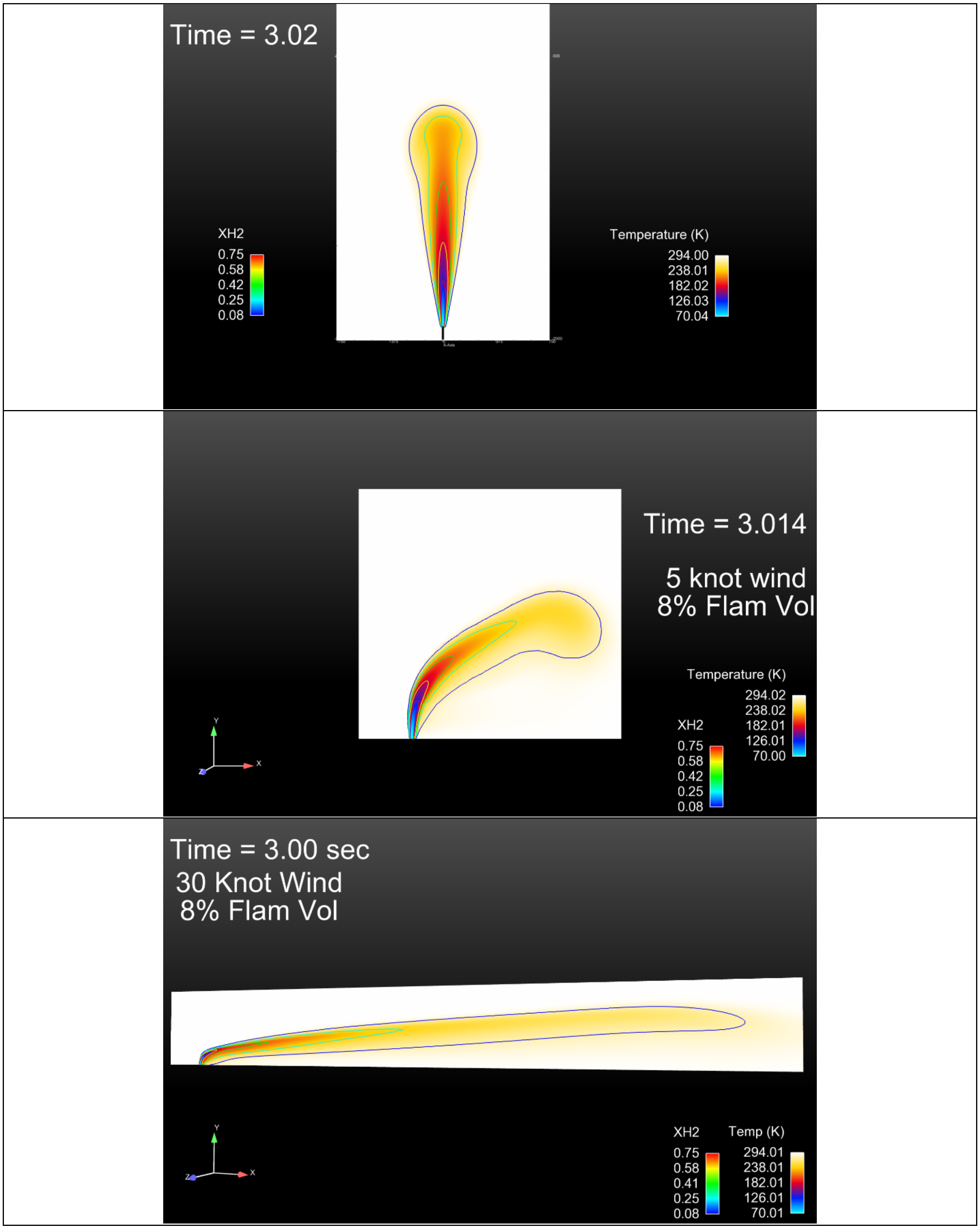

Figure 13. Temperature profiles for the three wind speeds with concentrations shown as contour lines. Shown at a time of 3 seconds after the start of the release. In all cases the plumes remain positively buoyant at all times.

This analysis does not include effects of freezing or condensation of oxygen, nitrogen, or water on the buoyancy of the plume; it only includes the buoyancy of hydrogen. Modeling methods able to address these effects and associated large scale validation experiments are currently either underway (modeling) or planned (experiments) at Sandia National Laboratories. Furthermore, as shown above, wind direction has a large effect on plume direction so that it is possible that a downward wind direction will blow the plume downward in spite of its buoyancy; examining this scenario is recommended for future work.

3.1.6. Comparison to LNG

There are several examples around the world of existing ships that use liquefied natural gas (LNG) as their fuel source. Because LNG is more well-known in the maritime community we believe a comparison of the dispersion characteristics between LNG and LH_2 may be instructive. To do so we modeled an LNG tank with the same volume (4500 gal) and the same pressure (150 psi) as the LH_2 tank. Alternative comparison methods could be to model a different volume LNG tank holding the same amount of mass or energy as the 4500 gallon LH_2 tank, but the same-volume comparison is used here as a means to give a more intuitive feel between the two fuels.

LNG is stored at a temperature of 152 K. For these purposes LNG is assumed to be pure methane. The tank is modeled to start with 95% vapor, which at these conditions has a higher density than that in the modeled liquid hydrogen tank: 18.7 kg/m^3 compared to 17.7 kg/m^3. The initial mass flow rate will also be higher: 5.76 kg/s compared to 1.6 kg/s for the hydrogen system. Figure 14 compares the two resulting blowdown velocities through a 1 inch orifice and exiting the 25 foot vent stack. The LNG blowdown velocity model was not run to completion but from extrapolation of the flow it is clear that the LNG tank will take longer to empty.

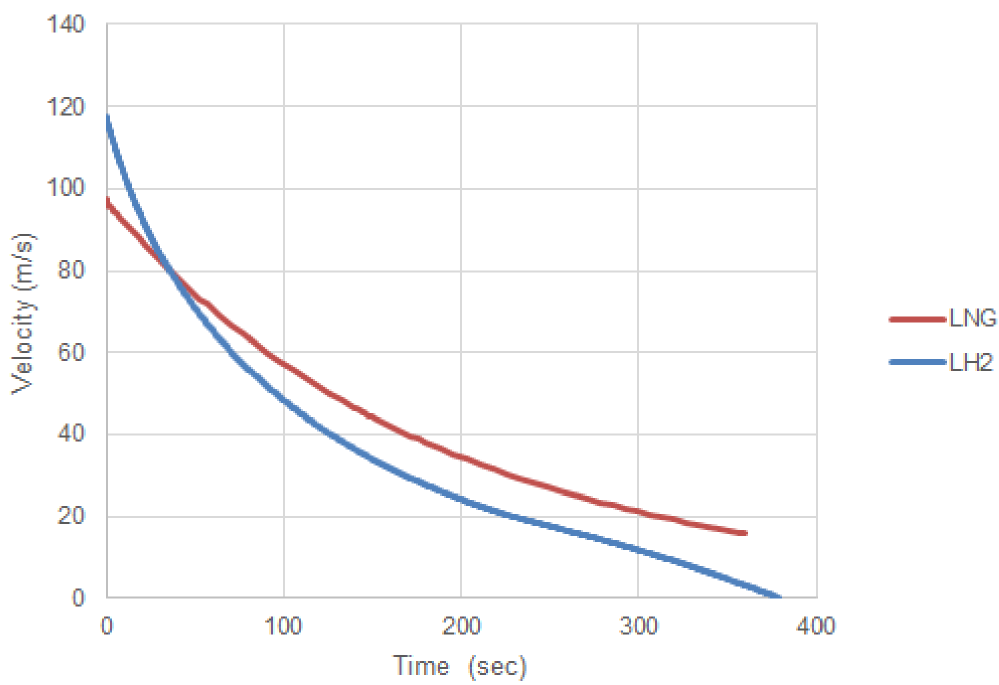

Figure 14. Comparison of the blowdown velocities of the LNG and LH_2 tanks studied.

Figure 15(a-c) compares the plumes of methane and hydrogen resulting from a Scenario 1 release, that is, an abnormal venting due to a failed-open relief device on the tank, in a 5 knot crosswind. The top panel shows the hydrogen plume at the time (14 s) of its maximum plume length. The middle panel shows the methane plume at its time of maximum plume length (5 s) for comparison of the maximum plumes of both. The maximum flammable plume for methane reaches 10 meters long and 9.5 meters high. The maximum flammable plume for hydrogen is 20 meters long and 7.7 meters high. For additional insight, the bottom panel shows the methane plume at a comparable time (15 s) of the hydrogen plume for a comparison of the plume size at a given time after release.

The results show that hydrogen flammable plume will be longer in length from the release point, but shorter in height and duration. This is a direct result of the higher momentum of the methane jet, allowing it to penetrate higher vertically into the air than the lower-momentum hydrogen jet. In other words, wind has less of an effect on the methane jet than the hydrogen jet for the same initial conditions (boiling liquid at 150 psig). In addition, the less dense hydrogen will expand more to take up a larger volume at atmospheric pressure.

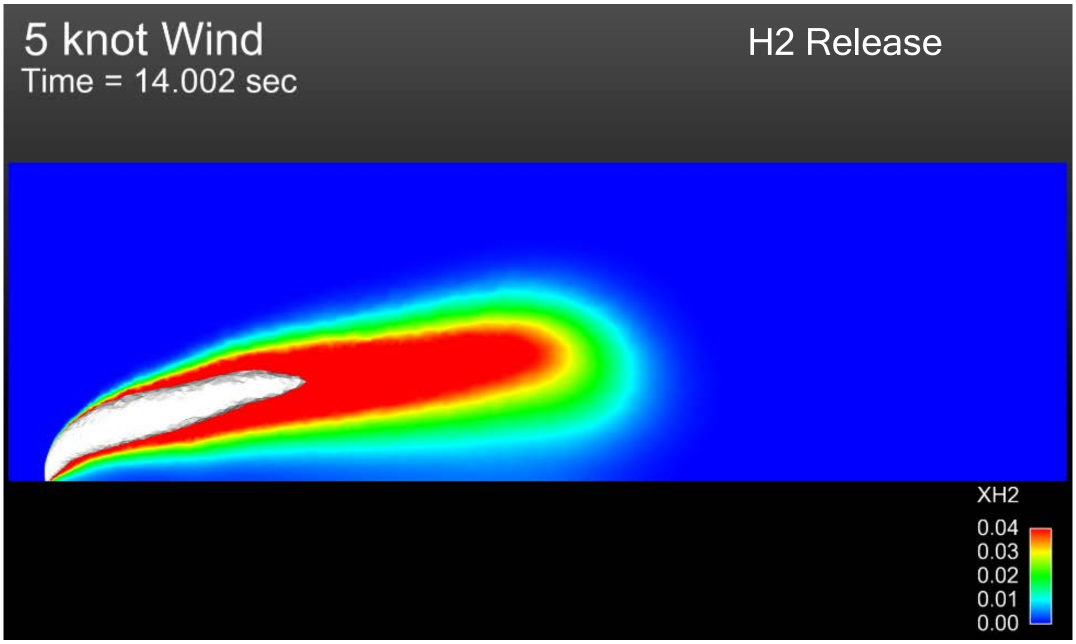

Figure 15(a): Hydrogen release in a 5 knot crosswind at time of maximum plume length (see main caption for additional explanation)

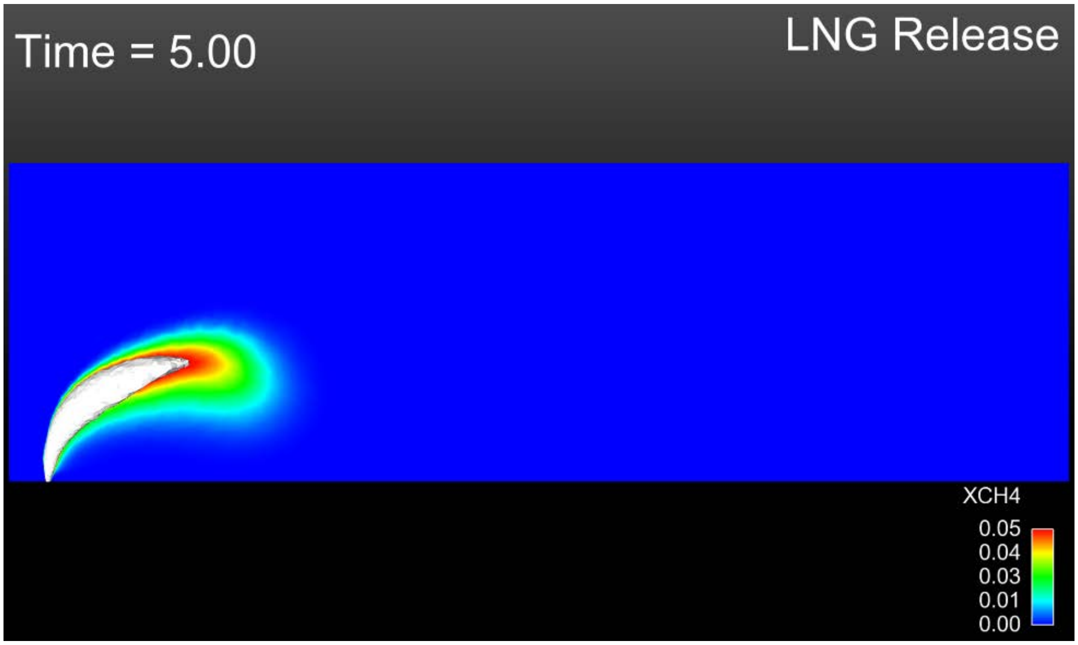

Figure 15(b): Methane release in a 5 knot crosswind at time of maximum plume length (see main caption for additional explanation)

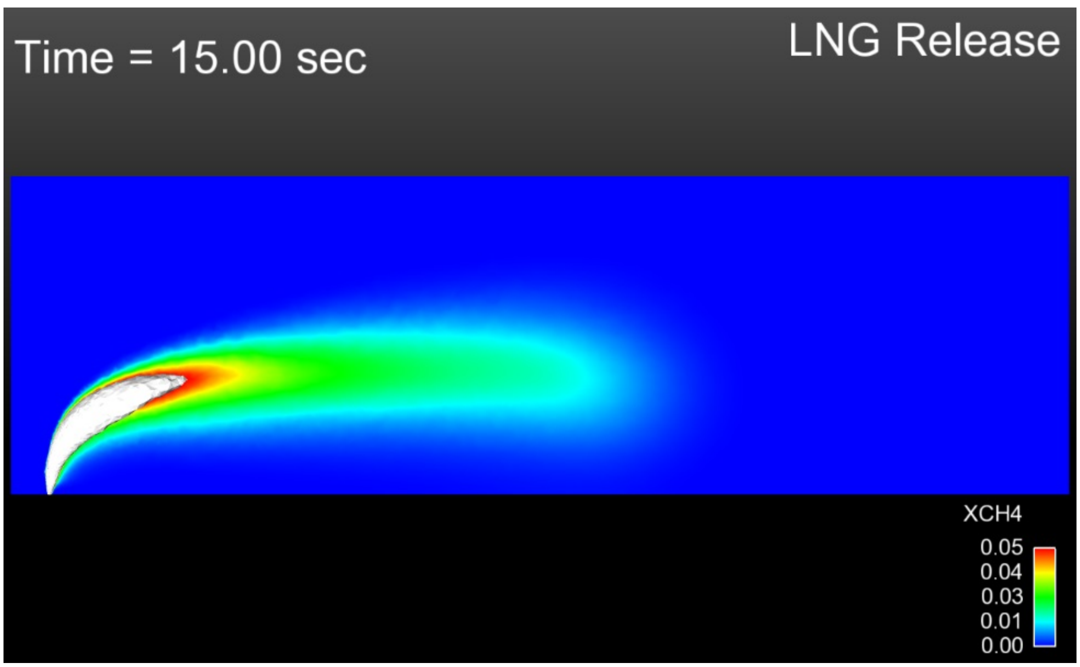

Figure 15(c): Methane release in a 5 knot crosswind at the same time as the maximum hydrogen plume length (Figure 15(a)). (See main caption for additional explanation)

Figure 15(a-c). All domains are 80 meters long and 20 meters tall. The white area designates the gas within the flammable limit for each species, which is 5-15% for methane and 8-75% for hydrogen by volume.

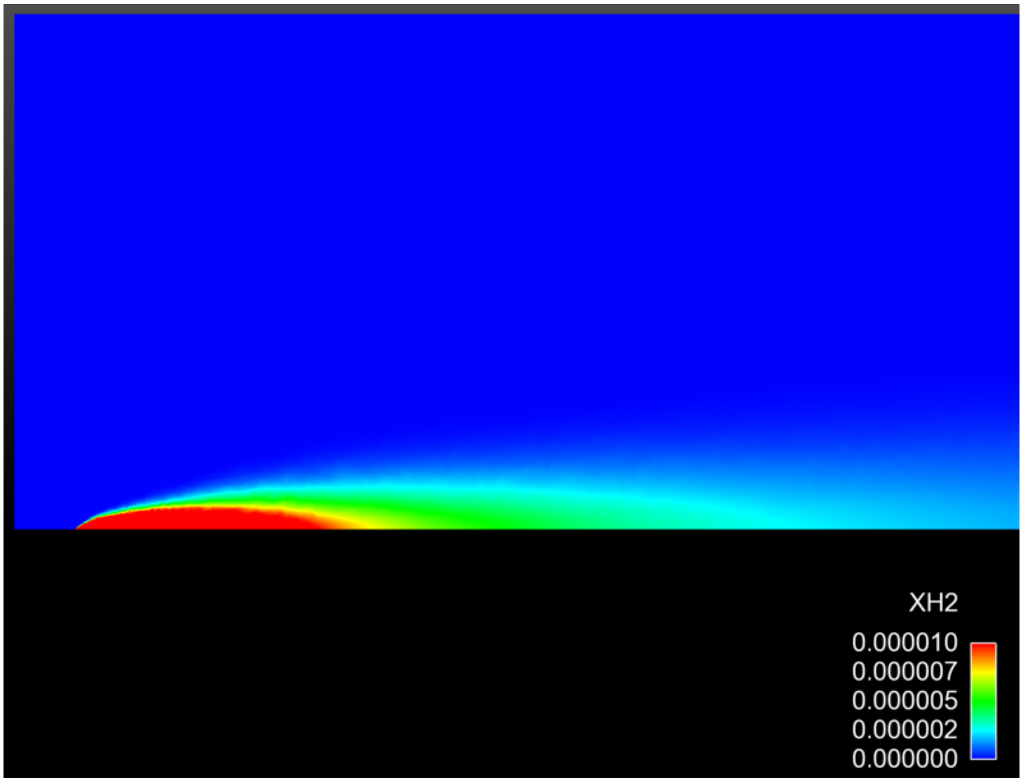

Figure 16. Predicted hydrogen concentration due to boil-off gas exiting the vent pipe. The domain shown in this figure is about 10 meters long. The mole fraction scale is greatly reduced from other images to show the extent of the hydrogen. The released concentrations from this simulation are well under the flammable limit.

3.2. Scenario 2: Normal Venting due to Boil-off

To model the normal operating procedure of venting a small amount of vapor hydrogen to maintain the maximum operating pressure in an idle LH_2 tank, hydrogen was released at a constant rate of 1.29 cm/s, corresponding to a 1% (by mass) leak rate as described in Section 2.3. The small resulting plume builds for about 2 minutes and then reaches steady state. The same mesh and crosswind input conditions were used as the 5 knot case described above. As shown in Figure 16, the hydrogen concentrations from this level of release are much lower than from the full scale tank blowdown, with no visible concentrations above 0.025 (2.5%) within the resolution of the model. The red area in Figure 16 shows the concentrations of 0.0001% and above.

3.3. Scenario 3: Leak Inside Fuel Cell Room

A leak in a ventilated fuel cell room was also modeled. In this scenario, hydrogen was released into the fuel cell room from a full pipe rupture. Two cases were simulated: one where the leak was detected and stopped 0.5 seconds after it began, and one where it was detected and stopped 2.0 seconds after it began. After the leak was stopped, the simulations continued to run to determine how long flammable concentrations would remain in the room with a ventilation rate of 30 ACH.

The simulation was run for 600 seconds before the leak was started to set up the air flow in the room.

For both release times, the flammable mass (with mole fractions between 4% and 75%) increases until the leak is turned off and then dissipates. Figure 17 shows the release after 0.5 seconds and the 12.97 gm of flammable mass is shown in white. Figure 18 shows a 2 second release where the amount of flammable mass is 38.52 gm. For the 0.5 second release, all the flammable mass is gone within 3 seconds, and it takes 6-7 seconds for the room to clear after the 2 second release. A time series of images of the releases can be found in Figure 19 for the 0.5 second case, and Figure 20 for the 2.0 second case.

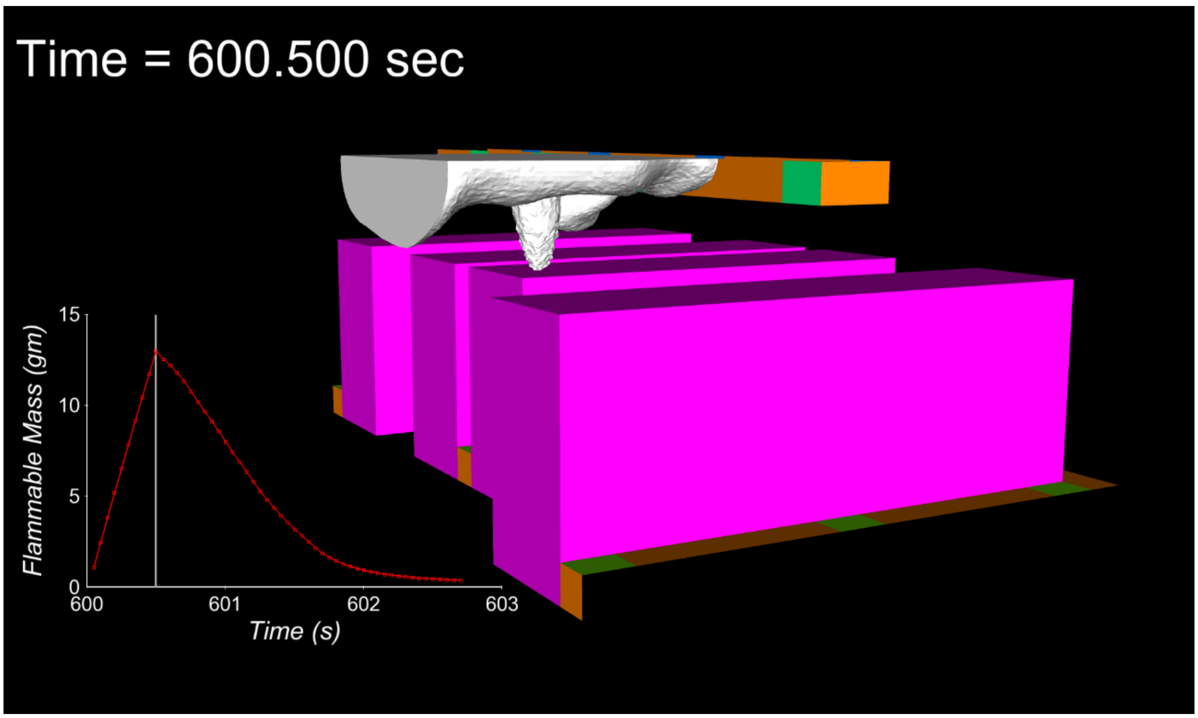

Figure 17. The 3D model shows the maximum extent of the plume in the fuel cell room after a release of 0.5 seconds, which contains 12.97 gm of flammable mass (shown in white). The inset graph (lower left) shows the flammable mass over time.

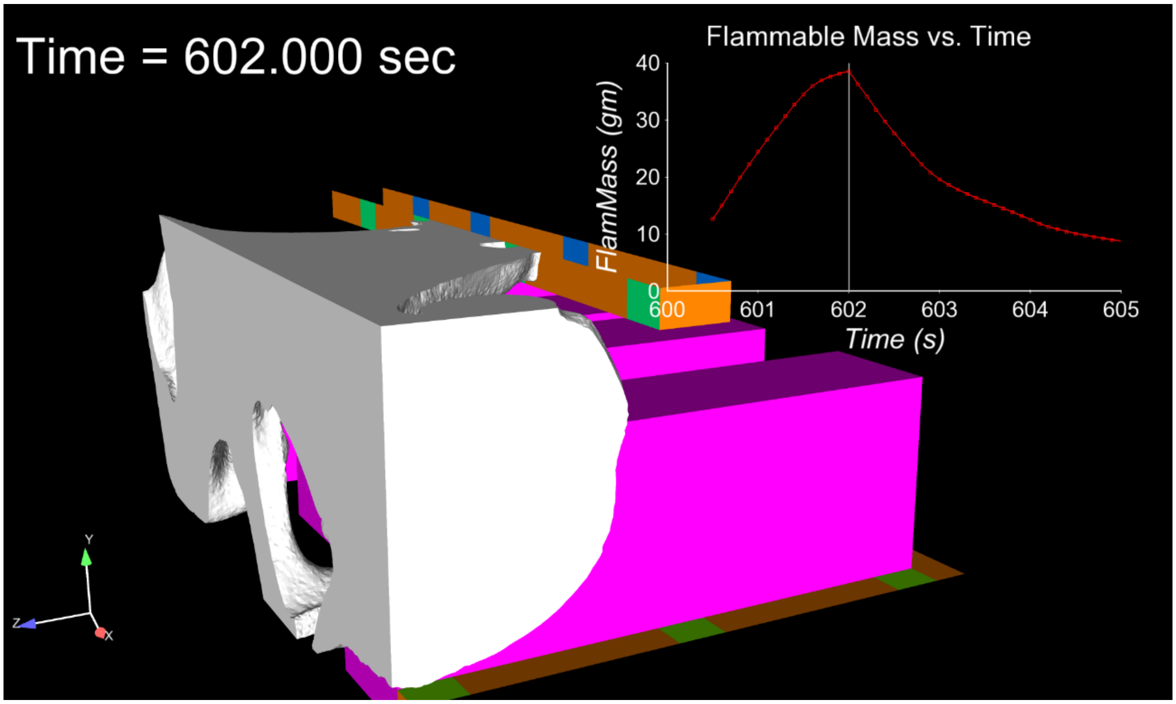

Figure 18. The 3D model shows the maximum extent of the plume in the fuel cell room after a release of 2.0 seconds, which contains 38.52 gm of flammable mass (shown in white). The inset graph (upper right) shows the flammable mass over time.

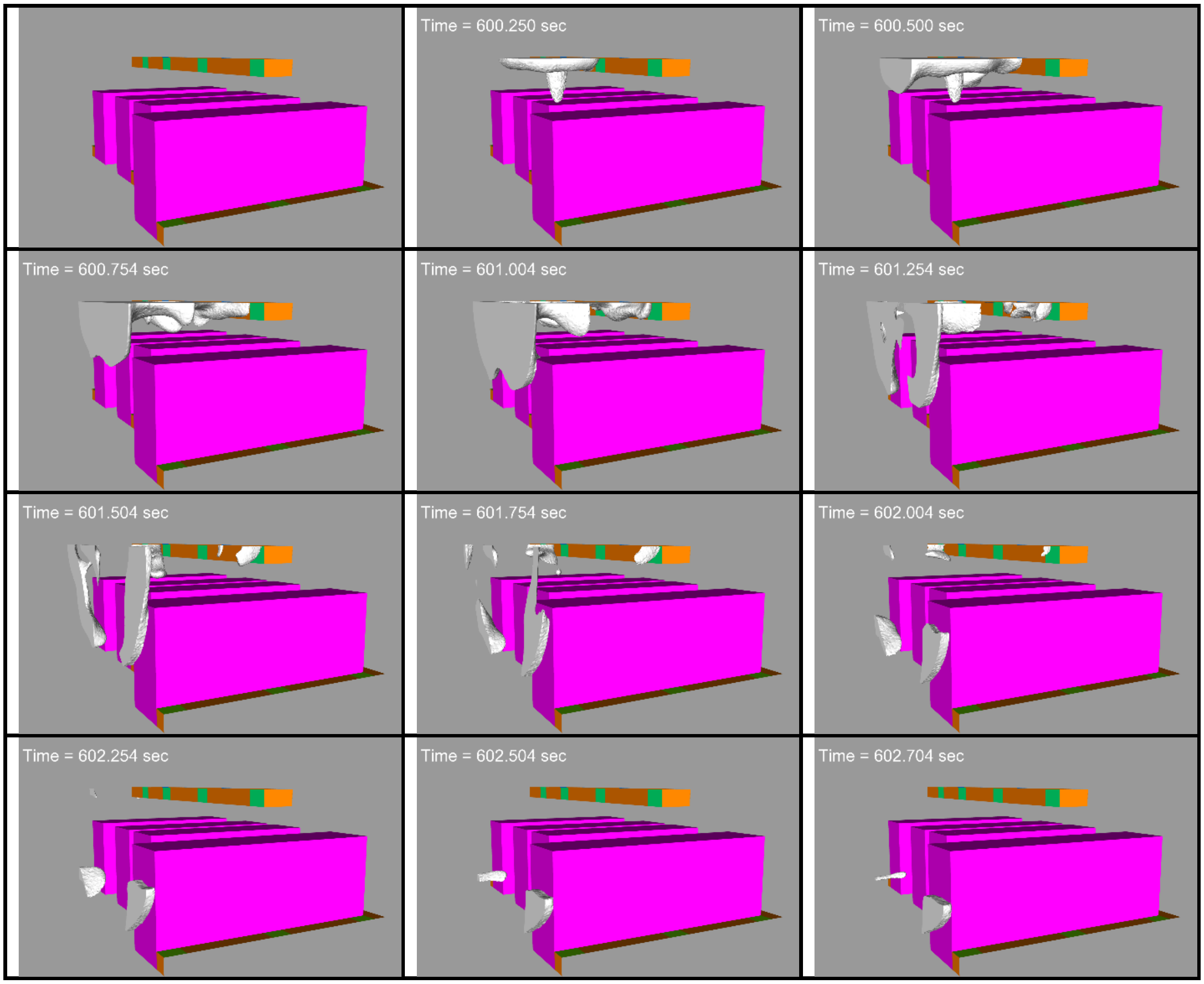

Figure 19: Time series of images of the fuel cell room leak with 0.5 second shutoff time. The flammable region of 4%-75% is shown in white.

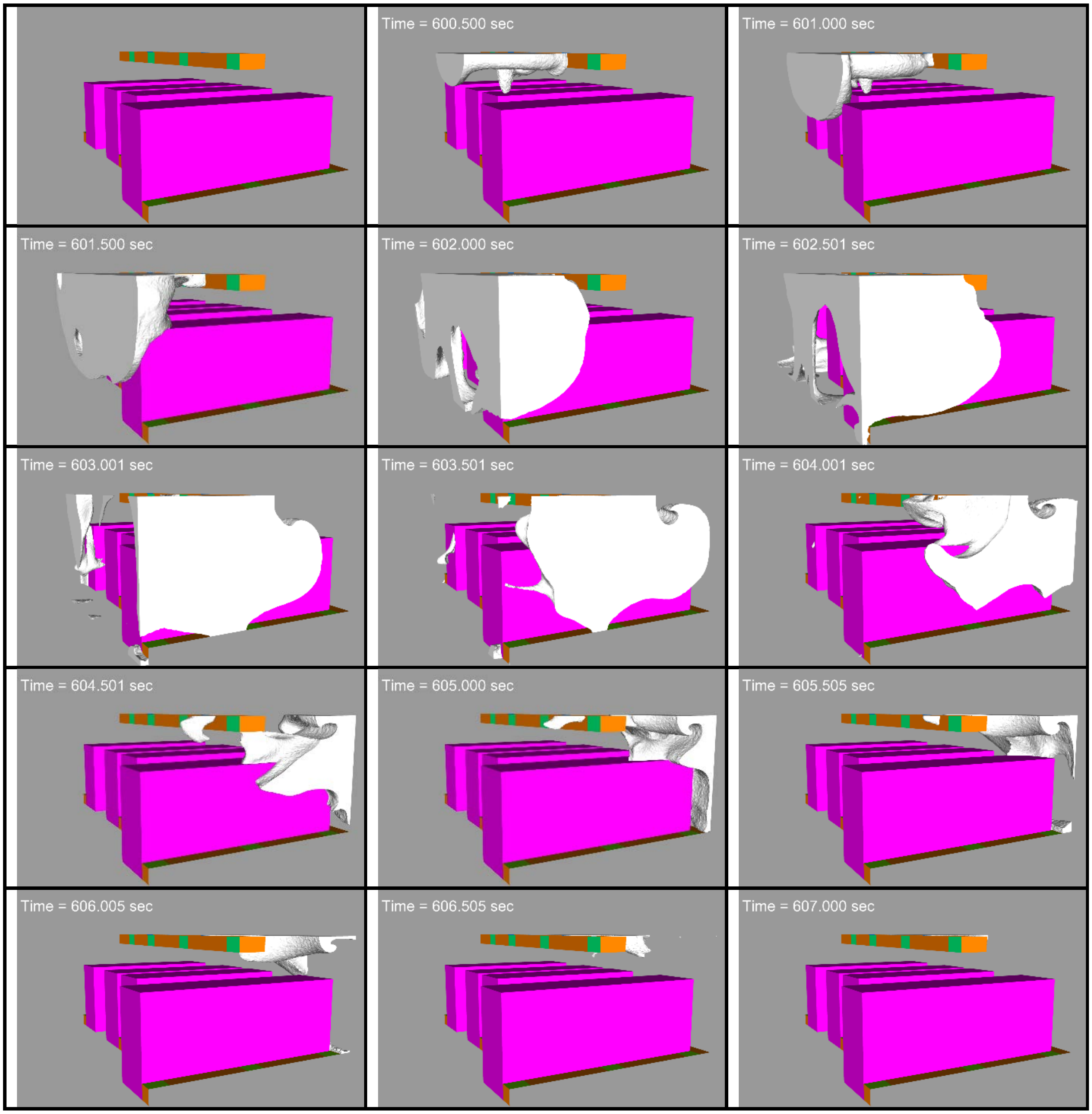

Figure 20: Time series of images of the fuel cell room leak with 2.0 second shutoff time. The flammable region of 4%-75% is shown in white.

3.3.1. Overpressure Calculations

If hydrogen is ignited in a confined space it can produce a detonation or deflagration with a resulting pressure wave ("overpressure"). Fuel cell room designs incorporating well-designed and functioning ventilation, elimination of ignition sources, and well-placed leak detection would not allow such a combustion event, but failure of systems could lead to the possibility and thus the consequences of a detonation are explored here for insight.

Conveniently, Bauwens and Dorofeev [14] have developed an analytic model to estimate overpressure which only considers the flammable mass quantities and enclosure volumes, and assumes perfect mixing. Model results yielded good agreement with peak overpressure measurements from large-scale hydrogen release and deflagration experiments by Ekoto et al. [15]. Accordingly, the model was used here to estimate peak overpressure hazards based on the flammable mass prediction from the CFD simulations; pressure impulse was not considered. Note that the model assumes no instability enhancement of the flame front (e.g., acoustic) and that local blast waves are relatively minor, which are reasonable assumptions for leaks with small flammable volumes. Equation 1 describes how the adiabatic increase in pressure depends on the mass of hydrogen consumed:

Eq. 1. $$\Delta p = p_0 \left\{ \left[\frac{V_T + V_{H2}}{V_T} \frac{V_T + V_{H2}/\chi_{stoich}(\sigma - 1)}{V_T} \right]^{\gamma} - 1 \right\}$$

where p_0 was the ambient pressure, V_T was the total facility volume of open space in the room (i.e., not including the fuel cell racks and vents) and V_{H2} was the volume of a notional cloud of pure hydrogen at ambient temperature and pressure with a mass corresponding to the total hydrogen mass in the flammable hydrogen air mixture range (4%-75%), χ_{stoich} was the hydrogen-air stoichiometric mole fraction, σ was the expansion ratio for stoichiometric hydrogen-air combustion (7.199), and γ was the air specific heat ratio (1.4). Note that it was convenient to define V_{H2} as the quotient of total flammable hydrogen mass—which was a ready output from the FUEGO CFD simulations—divided by the known ambient density of pure hydrogen.

This overpressure correlation as developed only considers the sudden combustion of all flammable contents. The equation assumes the enclosure to be perfectly sealed, no heat transfer out, and a constant flammable volume throughout the entire burn. The presence of ventilation, wall heat transfer, and the fact that the mixtures will continually lean out will mean that the actual overpressure may be much lower than is calculated.

On the other hand, the flame front might become increasingly turbulent due to obstacles such as the racks, perturbing the flame-front making and making it even more turbulent, which would result in an increase in the turbulent flame speed. It is possible that the burn velocity could become fast enough that it could transition into a detonation, in which case the overpressures will be much greater. These factors are brought to the attention of the reader so that the assumptions in the calculation are clear, and it is known that the result should be taken as an estimate only.

For the 0.5 second release, our post processing tools showed that the 12.97 gm of hydrogen in the flammable range has a volume V_{H2} of 0.155 m^3. When entered into Eq. 1, this results in an overpressure of 7.0 kPa. For the 2 second release case, 38.52 gm corresponds to a volume V_{H2} of 0.46 m^3, resulting in an overpressure of 21.2 kPa. Jeffries, et al. [16, 17], shows the resulting consequences for a range of overpressures as shown in Table 2. It can be seen that the overpressure from the 2 second release would reach levels that could cause serious damage to the structure as well as severe harm to anyone in the room.

Table 2. Consequences of overpressures in an enclosed space [16, 17].

Overpressure (kPa)	Consequence
6.9	Injuries due to projected missiles
13.8	Fatality from projection against obstacles
13.8	Eardrum rupture
15-20	Unreinforced concrete wall collapse

While the scenario of a full pipe rupture during normal operation may be an unrealistic occurrence, the results presented here help with understanding of impact of such a leak. These results can be used to understand important factors and consider mitigation strategies for the fuel cell room or other rooms with potential for hydrogen leaks. For example, automated leak detection and shutoff, flow limiting devices, minimum ventilation rates, and ventilation design can be considered along with secondary mitigation strategies such as blow-off panels to reduce or eliminate the harmful consequences of a hydrogen leak.

4. CONCLUSIONS

Results from a 1D gas transfer code were coupled with CFD modeling to investigate the outcome of a 4500 gallon LH_2 tank blowdown in three wind conditions that cover a wide range of conditions that a hydrogen fuel cell powered vessel is likely to experience. For the 5 knot and 30 knot wind velocities, it is clear that the hydrogen plume shape is greatly influenced by the wind due to large density difference compared to air. In these simulations, it was also found that the plume is always positively buoyant even when very cold (70 K). The hydrogen will only go downward if there are wind currents that carry it that direction.

In comparing the release of hydrogen to methane (used to simulate LNG) in a 5 knot wind, the plume of flammable H_2 will be longer than plume of flammable methane but not as tall. This can be attributed to the lower momentum of the hydrogen jet relative to the methane jet and subsequently the influence that air movement can have on the plumes.

It was found that during normal “boil off” venting to reduce the pressure of the tank that there is no resulting flammable concentration of gas at the vent outlet. This practice appears to be a safe way to prevent the overpressure of the liquid hydrogen tank on a marine vessel due to a prolonged period of being idle and suggests a hazardous/exclusion zone around such a vent outlet dedicated for this purpose may not be necessary.

Analysis of a large hydrogen release in a confined but ventilated fuel cell power room shows the importance of fast detection and shut-off combined with an adequate and properly designed ventilation system. The low momentum of hydrogen as compared to air as seen in the other release scenarios can be leveraged by the air handling system designer to quickly move hydrogen away from potential ignition sources and out to a safe vent location.

5. FUTURE WORK

This initial study has shown that there are several addition scenarios where further investigation would be insightful. Below is a list of possible follow on studies that would help answer questions concerning the safety of this type of vessel.

Vent stack releases:

- Explore the effect of downdrafts of external flows to show if this is an important issue or not. Superimpose air patters simulated by CFD around a boat and simulate an area below the release point going below the vent mast.
- Investigate whether hazardous zones should be completely spherical.
- Compare turbulent simulations to laminar ones.
- More in-depth modeling of release through the vent to calculate the release temperature.
- Simulate ignition of the plume and calculate the extent of the harm regions.

Fuel Cell Room releases:

- Investigate different directions of leak with and without impingements.
- Change ventilation configurations.
- Vary the leak rate and duration including smaller leaks with longer duration and leak size ranging from 0.1% to full rupture.
- Have additional models to move towards a recommended design. Perhaps simulations can specify maximum volume/mass of gas downstream of shutoff valve, dependent on room volume and ventilation.
- Perform explosion simulations with a safety tool to examine effects of blow out panels.
- Show result comparing methane versus hydrogen overpressures.
- Investigate the effects ignition on large flammable turbulent clouds.
- Conduct experiments with dispersion and explosion in a mockup of a fuel cell room is recommended to validate models and mostly to establish limiting volumes of hydrogen when it can cause too high pressures, and to design the release panels with the needed opening times and areas.

REFERENCES

1. Pratt, J.W. and L.E. Klebanoff, *Feasibility of the SF-BREEZE: a Zero-Emission, Hydrogen Fuel Cell, High-Speed Passenger Ferry*. 2016, Sandia National Laboratories.
2. Bozinoski, R., *MassTran Documentation: Release 0.9.0.* 2017.
3. Houf, W.G., et al., *Hydrogen fuel-cell forklift vehicle releases in enclosed spaces.* International Journal of Hydrogen Energy, 2012.
4. Moen, C., et al. *A multi-mechanics approach to computational heat transfer*. in *ASME 2002 International Mechanical Engineering Congress and Exposition*. 2002. American Society of Mechanical Engineers.
5. Edwards, H.C. and J.R. Stewart, *Sierra: A Software Environment for Developing Complex Multi-Physics Applications*, in *First MIT Conference on Computational Fluid and Solid Mechanics*, K.J. Bathe, Editor. 2001, Elsevier Scientific.
6. Ferziger, J.H. and M. Peric, *Computational methods for fluid dynamics*. 2012: Springer Science & Business Media.
7. Ray, J., et al., *Bayesian Parameter Estimation of a k-ε Model for Accurate Jet-in-Crossflow Simulations.* AIAA Journal, 2016. **54**(8): p. pp. 2432-2448.
8. Beresh, S.J., et al., *Penetration of a Transverse Supersonic Jet into a Subsonic Compressible Crossflow.* AIAA Journal, 2005. **43**(2): p. 379-389.
9. Beresh, S.J., et al., *Turbulent Characteristics of a Transverse Supersonic Jet in a Subsonic Compressible Crossflow.* AIAA Journal, 2005. **43**(11): p. 2385-2394.
10. Beresh, S.J., et al., *Crossplane Velocimetry of a Transverse Supersonic Jet in a Transonic Crossflow.* AIAA Journal, 2006. **44**(12): p. 3051-3061.
11. Barth, T.J. and D.C. Jespersen, *The design and application of upwind schemes on unstructured meshes.* 1989.
12. Schefer, R.W., et al., *Ignitability limits for combustion of unintended hydrogen releases: Experimental and theoretical results.* International Journal of Hydrogen Energy, 2011. **36**(3): p. 2426-2435.
13. Blevins, R.D., *Applied fluid dynamics handbook.* 1984: Van Nostrand Reinhold Co.
14. Bauwens, C.R. and S. Dorofeev. *CFD Modeling and Consequence Analysis of an Accidental Hydrogen Release in a Large Scale Facility*. in *International Conference on Hydrogen Safety 5*. 2013. Brussels, Belgium.
15. Ekoto, I.W., et al., *Experimental investigation of hydrogen release and ignition from fuel cell powered forklifts in enclosed spaces.* International Journal of Hydrogen Energy, 2012. **37**(22): p. 17446-17456.
16. Mueller, J.T. and P.M. Urban, *Characterization of direct methanol fuel cells by ac impedance spectroscopy.* Journal of Power Sources, 1998. **75**(1): p. 139-143.
17. Jeffries, R.M., S.J. Hunt, and L. Gould, *Derivation of fatality of probability function for occupant buildings subject to blast loads*, W.A.S. Technology, Editor. 1997, Health and Safety Executive.

DISTRIBUTION

2 U.S. Department of Transportation, Maritime Administration
Attn: Sujit Ghosh
Attn: Michael Carter
MAR-410, W28-216
1200 New Jersey Ave SE
Washington, D.C. 20590

3 US Coast Guard, Design and Engineering Standards
Attn: Tim Meyers
Attn: Thane Gilman
Attn: Cindy Znati
USCG HQ (ENG-3)-Room 5R19
2703 Martin Luther King Jr. Ave. SE
Washington DC 20593-7509

1 US Coast Guard, Marine Safety Center
Attn: LT Margaret Woodbridge
US Coast Guard Stop 7430
2703 Martin Luther King Jr. Ave SE
Washington DC 20593-7430

1 US Coast Guard, Liquefied Gas Carrier National Center of Expertise
Attn: Scott Mercurio
2901 Turtle Creek Drive
Port Arthur, TX 77642

1 American Bureau of Shipping
Attn: Zhongfu Ge
16855 Northchase Drive
Houston, TX 77060

1 DNV-GL
Attn: Asmund Huser
Veritasveien 1, 1363
Hovik, Norway

1 Elliott Bay Design Group
Attn: Curt Leffers
5305 Shilshole Ave NW, Suite 100
Seattle, WA 98107

1 Red and White Fleet
Attn: Joe Burgard
Pier 45 Shed C
San Francisco, California 94133

1 U.S. Department of Energy
Attn: Laura Hill
1000 Independence Ave., SW
Washington, D.C. 20585-0121

1	MS0748	Chris LaFleur	06231
1	MS9052	Amanda Dodd	08366 (electronic copy)
1	MS9052	Joseph Pratt	08366
1	MS9052	Ethan Hecht	08367 (electronic copy)
1	MS9054	Bob Hwang	08300 (electronic copy)
1	MS9054	Chris Moen	08360 (electronic copy)
1	MS9161	Leonard Klebanoff	08367
1	MS9161	Jon Zimmerman	08367 (electronic copy)
1	MS9406	Camron Proctor	08250
2	MS9957	Myra Blaylock	08253
1	MS9957	Gaby Bran-Anleu	08253
1	MS9957	Radoslav Bozinoski	08253
1	MS9957	Patricia Gharagozloo	08253 (electronic copy)
1	MS0899	Technical Library	09536 (electronic copy)
1	MS9018	Central Technical Files	08944

Sandia National Laboratories