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# Hydrogen Gas Dispersion Studies for a Fuel Cell Vessel

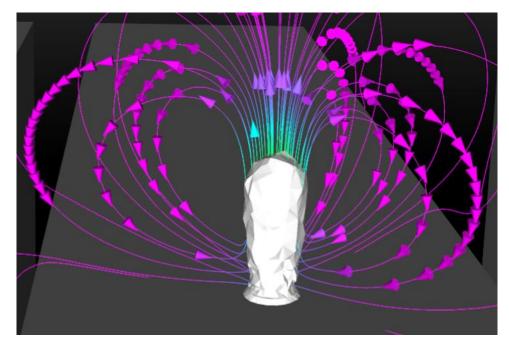
## --Vent Mast, Fuel Cell Room, Bunkering--

Myra L. Blaylock, Kevin M. Gitushi, and Leonard E. Klebanoff

Prepared by:

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Cover Image: Predicted airflow around a flammable hydrogen release (in white).

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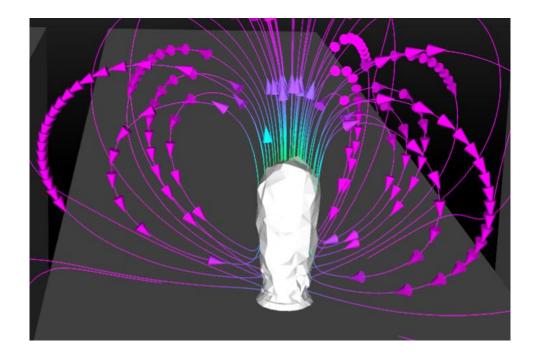
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At a kickoff meeting for the project held at MARAD on August 13, 2019, we received invaluable collaboration, assistance, and feedback from a group of subject matter experts from the Class Societies, as well as MARAD and the U.S. Coast Guard (USCG). This group was affectionately known as The Brain Trust. The Brain Trust consisted of: Joe Pratt (GGZEM), Narendra Pal (GGZEM), Matt Unger (Hornblower), Ed Vaughn (DeJong & Lebet), Rich Delpizzo (ABS), Graeme Hyde (Lloyd's Register), Olav Hansen (Lloyd's Register), Stewart Lee (Class NK), Anthony Teo (DNV GL), Steven Sawhill (DNV GL), Tom Thompson (MARAD), Bryan Vogel (MARAD), Sujit Ghosh (MARAD), Carolyn Junemann (MARAD), Tim Myers (USCG), Cindy Znati (USCG), Patrick Brown (USCG), Pete Bizzaro (USCG), and William Haugh (USCG). We also appreciate the participants giving permission to reproduce their slide presentations in the Appendix to this report.

Thanks are extended to Brian Erhart and Rad Bozinoski, both of Sandia, for assistance with the use of the Hydrogen Risk Assessment Model (HyRAM) and MassTran analysis programs, respectively. We greatly appreciate critical technical comments on this report by our Sandia colleague Gabriela Bran-Anleu.

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Finally, the authors thank Jon Zimmerman, the former Sandia Hydrogen Program Manager, for his helpful suggestions about the project and its execution as well as Kristin Hertz, the current Sandia Hydrogen Program Manager for her recent help.

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# Acronyms:

Abbreviation			
ABS: American Bureau of Shipping			
ACH: Air Changes per Hour			
API: American Petroleum Institute			
CFD: Computational Fluid Dynamics			
CVFEM: Control Value Finite Element Method			
<b>DOT:</b> Department of Transportation			
ESD: Emergency Shutdown			
FC: Fuel Cell			
GGZEM: Golden Gate Zero Emission Marine			
HP: High Pressure			
HyRAM: Hydrogen Risk Assessment Model			
ID: Internal Diameter			
ICE: Internal Combustion Engine			
IEC: International Electrotechnical Commission			
IFC: International Fire Code			
IGF (Code): International Code for Gas Fueled Ships			
LH <sub>2</sub> : Liquid Hydrogen			
LFL: Lower Flammability Limit			
MARAD: Maritime Administration (Department of Transportation)			
META: Maritime Environmental and Technical Assistance			
NFPA: National Fire Protection Association			
PEM: Proton Exchange Membrane			
PRD: Pressure Relief Device			
PRV: Pressure Relief Valve			
RANS: Reynolds-averaged Navier-Stokes			
SIMOPS: Simultaneous Operations			
USCG: United States Coast Guard			

# **Project Summary:**

We report hydrogen gas dispersion modeling results for using hydrogen fuel cell technology on hydrogen vessels. The first topic is the release of hydrogen from highpressure (HP) hydrogen storage tanks through a Vent Mast. Such a release could be routine, for example if the tanks need to be emptied for maintenance purposes. Alternatively, the release could be non-routine in response to an accident scenario involving the threat of fire in the hydrogen storage area. The second topic involves hydrogen release from the interior of a proton exchange membrane (PEM) fuel-cell rack situated in a ventilated Fuel Cell Room. This scenario helps to inform the level of Fuel Cell Room ventilation that is needed as backup in case of a double failure where the ventilation provided within the rack fails and also the hydrogen detector in the fuel-cell rack fails, allowing hydrogen from a fuel-cell leak to enter the ventilated Fuel Cell Room. The third topic involves hydrogen delivery trailer. In all these cases, HP hydrogen gas stored at ambient room temperature is considered.

For the first topic, we successfully extended Sandia's MassTran model to handle the problem of hydrogen release from ten hydrogen tanks, similar to those which will be used on the "Sea Change" and the "Discover Zero" vessels planned for operation in San Francisco Bay. Two hydrogen tanks, with storage capacity of 27.8 kg each, can be emptied within 10 minutes. A ten-tank hydrogen storage system, holding 278 kg, can also be emptied in  $\sim 10$  minutes, with a pressure reduction to half the original pressure (125 bar) realized in 2 minutes. Subsequent computational fluid dynamics (CFD) results show that when the hydrogen is released out of the Vent Mast in a 5-mph wind blowing horizontally, the effect of the wind on the hydrogen dispersion strongly depends on the hydrogen exit speed. For high release speeds ( $\sim 800 - 900$  m/s), the hydrogen flow is strongly momentum-driven, and there is modest cross-wind influence. For slow hydrogen exit speeds (~ 10 m/s), the hydrogen is strongly entrained in the wind flow and blown sideways by the wind, with the downstream flammable envelope rising at a positive angle to the horizontal due to buoyancy. For both high-speed and low-speed releases, the modeling indicates that horizontal wind does not induce significant movement of the hydrogen downward. To capture the influence of wind with a downward component (e.g., created by a downdraft near a building), a study of low-velocity (8.6 m/s) hydrogen release was performed with a 5-mph wind pointed downward at a 45° angle. The results show that despite the buoyancy of hydrogen, the wind blows the hydrogen substantially downward for slow hydrogen speeds exiting the Vent Mast.

For the second topic, hydrogen gas dispersion CFD modeling for several leak sizes within a hydrogen fuel-cell rack inside a Fuel Cell Room revealed interesting findings. In the limiting case of no ventilation, modeling showed that the flammable

region produced by the hydrogen leak is initially limited by self-induced entrainment and recirculation of air, caused by the buoyant rising of the hydrogen release. Locally and at shorter times (minutes), this effect can be even more influential in limiting the size of the flammable envelope than Fuel Cell Room ventilation. With no ventilation, the self-limiting effect eventually transits to a situation where flammable gas fills the Fuel Cell Room.

Modeling results with the Fuel Cell Room ventilation activated show that several seconds after a hydrogen leak is turned on, the flammable region reaches a steady state, with only minor fluctuations due to the air currents in the room created by ventilation. The expected trend with ventilation rate is found, namely that for a given leak size, a smaller and smaller flammable envelope is found as ventilation is increased. For a given level of ventilation, increasing hydrogen leak rate produces a larger flammable region. For early times (< 10 minutes), the local air entraining and recirculation limits the flammable region. However, for longer times, with ventilation, hydrogen is evacuated out of the Fuel Cell Room, preventing the long-term buildup of hydrogen. Thus, the local mixing acts to limit the flammable region for approximately 10 minutes, whereas the active ventilation limits long-term buildup of hydrogen.

For the cases and ventilation rates examined, flammable H<sub>2</sub>/air mixtures greater than 4% clears the Fuel Cell Room within 1.5 sec after the hydrogen leak is turned off. Thus, with ventilation, the physical size of the flammable envelope is very limited (limiting the chances of ignition), and when the leak is terminated (e.g., by a shutoff valve), the room is cleared very quickly of flammable H<sub>2</sub>/air concentrations. Thus, in the event the hydrogen alarm fails in the fuel-cell rack, and the dedicated ventilation within the fuel-cell rack also fails (i.e. a double failure), if the hydrogen alarm in the Fuel Cell Room is triggered and shuts off the hydrogen supply to the rack, the ventilation of the Fuel Cell Room itself clears the flammable mass in less than 1.5 seconds.

The CFD modeling results for the detectable level of hydrogen that would trigger a hydrogen alarm, but is below the lower flammability limit (LFL), showed that higher ventilation rates might have the unintended consequence of making a leak harder to detect, depending on the location of the hydrogen alarm in the Fuel Cell Room. However, a higher ventilation rate does have the positive effect of more rapidly removing hydrogen from the Fuel Cell Room. In the extreme, depending upon ventilation configuration as well as placement and number of sensors, it might be possible to have a leak producing flammable mass without triggering a ceiling-mounted hydrogen detector. We find that for the leak rates investigated in this report, a ventilation rate of 15 ACH provides timely hydrogen evacuation while allowing the leak to be detected by the ceiling-mounted hydrogen monitor (for most monitor locations). While the flammable region is self-limited by the local entrainment of air, the more diffuse detectable (but sub-flammable) region is not self-limited. This is due to the fact that the recirculation pattern required for the self-limiting effect requires a concentration of hydrogen to establish and differentiate the rising hydrogen mass from the surrounding air, thereby establishing the macroscopic recirculation pattern that self-limits the flammable region at short times, even in the absence of ventilation.

For the third topic, calculations using Sandia's MassTran model were performed for filling a marine hydrogen vessel HP hydrogen tank (at 250 bar) from a 350-bar mobile hydrogen refueling trailer. The calculations show that a 250 bar, 27.8 kg capacity Type IV composite tank can be fueled at a maximal rate of 0.005 kg/second subject to the condition that the temperature of the Type IV tank remains below 85 °C (185 °F), resulting in a tank fueling time of ~ 2 hours. Of course, if pre-cooled hydrogen were available, for example from a hydrogen station, the fueling rate could be increased, but pre-cooled hydrogen is not available on mobile HP hydrogen refueling trailers.

If a leak appears in the refueling hose, there is the practical problem of not being able to properly fill the marine tank due to the pressure reduction. Beyond this, there is the safety concern associated with the hose hydrogen leak. When the flow of hydrogen is restricted by a flow orifice (to limit the mass flow rate to keep the boat tank temperature below 85 °C), the pressure in the hose after the flow restrictor is the same all along the length, so the hydrogen plume issuing from the leak is nearly the same whether the leak is located at the trailer end of the hose or the boat end of the hose.

Varying the leak size in the calculation shows that larger leaks produce longer flammable hydrogen plumes as predicted by Sandia's HyRAM+ Toolkit, which uses analytical models of hydrogen behavior (i.e., it is not a CFD code). Plume lengths varied from 13 cm long to 6 meters for the smallest (0.0001 m diameter) to the largest (0.005 m diameter) leaks, respectively. The flammable leak profile did not depend significantly on the temperature of the ambient air or the orientation (vertical, horizontal, angled) of the leak. The pressure backing the leak increases as the fueling takes place; the pressure starts off from 15 bar (the pressure in the boat tank before refueling) and increases to 250 bar. This increase in backing pressure increases the length of the flammable plume, but not linearly with pressure because the flow through the leak is choked.

If the hydrogen plume were to ignite, either explicitly by an ignition source or by spontaneous ignition for pressures above 40 bar, the length of the flame is ~ 40% that of the flammable plume. If ignited, such a jet flame creates around it an exclusion zone that would create a burn injury if a person was within the zone. This zone is generally elliptical but is approximately the size of the length of the jet flame rotated in 3D space about its midpoint.

### Introduction:

Hydrogen is a commodity gas of growing interest for transportation and clean energy production when used with hydrogen internal combustion engines (ICEs) and fuel cells. Hydrogen fuel cells in particular are finding deeper and wider use in our technical society to provide zero-emissions electrical power. The advantages of fuel cells versus diesel engines are higher thermal efficiency (at partial load), dramatically lower noise, reduced maintenance and associated costs, and emissions-free operation at the point of use [1]. In addition, the modularity of fuel cells allows for power architectures that can be more efficiently matched to the power utilization profile of the particular application.

Most major auto manufacturers have designs for light-duty fuel-cell vehicles, with Toyota, Honda and Hyundai already making these vehicles available to the public for sale or lease. Beyond light-duty vehicles, fuel-cell buses have been in service already for many years [2], fuel-cell construction lighting equipment has been demonstrated [3], fuel-cell forklifts are now in routine use by the tens of thousands [4] and the first light rail systems operated by hydrogen fuel cells are now operational [5]. In the last few years the feasibility of using hydrogen fuel cells to replace marine diesel engines in maritime applications has been shown, for example in high-speed ferries [6] and coastal research vessels [7, 8]. A hydrogen fuel-cell ferry called the *Sea Change* (formerly called the Water-Go-Round) has been built for use on the San Francisco Bay beginning in early 2022 [9]. It will be the first commercial hydrogen fuel-cell ferry operating in the Western Hemisphere.

As these various uses of flammable hydrogen gas have been developed, it has been essential that procedures be developed for the safe use of hydrogen based on its physical properties [10]. How hydrogen can be released, mix with air, and disperse has been studied using CFD in order to understand the hazards associated with releases of hydrogen. As part of the general field of using CFD to understand and minimize hazards in industrial processes [11], hydrogen gas dispersion modeling has been an essential ingredient in deploying hydrogen technology safely [12]. In particular, CFD modeling has been used to understand the safety consequences of gaseous hydrogen release in maritime applications [13], for using hydrogen fuel-cell vehicles in tunnels [14], in parking garages [15] and near buildings [16]. The nature of cryogenic releases of hydrogen from liquid hydrogen (LH<sub>2</sub>) spills has also been examined using CFD [17 - 21].

This study is a "follow-on" investigation to prior work in which the release of cold hydrogen gas from the "blowdown" of a LH<sub>2</sub> tank was examined, as well as a pipe rupture in the hydrogen line feeding the fuel-cell rack [22]. Here we report hydrogen gas dispersion CFD modeling results for three particular aspects of using HP hydrogen fuel cell technology to provide primary propulsion or auxiliary power on vessels. The first

aspect, covered in Chapter 1, is the release of hydrogen from HP hydrogen storage tanks through a Vent Mast. Such a release could be planned and routine, for example as part of a maintenance procedure if a tank has to be replaced. Alternatively, the release could be unplanned and non-routine in response to an accident scenario involving the threat of fire in the hydrogen storage area.

The second aspect, covered in Chapter 2, is to examine the case of hydrogen release from the interior of a fuel-cell rack situated in a ventilated Fuel Cell Room. This scenario helps to inform the level of Fuel Cell Room ventilation that is needed as backup in the event of a "double failure" where the ventilation provided within the fuel-cell rack fails and the hydrogen detector in the fuel-cell rack fails, allowing hydrogen from a fuel cell leak to enter the ventilated Fuel Cell Room.

The third aspect, described in Chapter 3, is to understand hydrogen releases that could occur during vessel refueling from a HP hydrogen delivery trailer. In all these cases, HP hydrogen gas is considered, not LH<sub>2</sub>.

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# Kick-off Meeting at MARAD: August 13, 2019

In order to identify the most important hydrogen gas dispersion issues, the Sandia project team (Lennie Klebanoff and Myra Blaylock) consulted with relevant subject matter experts. At the August 13, 2019 face-to-face project kickoff meeting held at MARAD in Washington DC, we received invaluable collaboration, assistance and feedback from subject matter experts from the Class Societies, as well as MARAD and the USCG. This group was affectionately known as The Brain Trust. The Brain Trust consisted of: Joe Pratt (GGZEM), Narendra Pal (GGZEM), Matt Unger (Hornblower), Ed Vaughn (DeJong & Lebet), Rich Delpizzo (ABS), Graeme Hyde (Lloyd's Register), Olav Hansen (Lloyd's Register), Stewart Lee (Class NK), Anthony Teo (DNV GL), Steven Sawhill (DNV GL), Tom Thompson (MARAD), Bryan Vogel (MARAD), Sujit Ghosh (MARAD), Carolyn Junemann (MARAD), Tim Myers (USCG), Cindy Znati (USCG), Patrick Brown (USCG), Pete Bizzaro (USCG), Alex Haugh (USCG) and Sean Karasevicz (USCG). Figure 1 shows a picture of The Brain Trust along with the Sandia project team Lennie Klebanoff and Myra Blaylock, who aspire to be members of the Brain Trust.



**Figure 1:** The Brain Trust. Front Row (L-R): Rich Delpizzo, Stewart Lee, Tim Myers, Sean Karasevicz, Alex Haugh, Steven Sawhill; Middle Row (L-R): Sujit Ghosh, Myra Blaylock, Narendra Pal, Patrick Brown, Ed Vaughn, Matt Unger, Cindy Znati, Anthony Teo; Back Row (L-R): Lennie Klebanoff, Pete Bizarro, Graeme Hyde.

The Agenda for the meeting is presented in the Final Report Appendix, along with the presentations that were given that day. After presentations from the Class Societies (ABS, Lloyd's Register, Class NK, DNV GL) as well as from boat operators (Hornblower and GGZEM) and the USCG, the Brain Trust brainstormed the most important safety-related hydrogen release scenarios that gas dispersion modeling could examine. The "wish list" included:

- 1. Vent Mast
- 2. Bunkering
- 3. Fuel Cell (FC) Room
- 4. Tanks (fittings/valves) for example in a "tank connection space"
- 5. Fittings/flanges in general

The Brain Trust felt that important model aspects to consider would be weather effects, differences in releases between  $LH_2$  and compressed gas  $H_2$  storage systems, and a comparison of releases on an open deck compared to releases within an enclosed area. The Brain Trust felt the leaks to be studied should be based on definitions for leaks from the International Electrotechnical Commission (IEC).

For the Vent Mast and bunkering scenarios, the ultimate goal should be to specify the shape and size of hazardous zones, and it would be informative if the modeling could examine the differences between  $H_2$  and natural gas, as budget and scope permitted.

Given the budget and schedule limitations of the project, the Sandia project team selected the top 3 topics for study. The Brain Trust recommended the overall scope for each topic:

#### Chapter 1: Vent Mast:

Recommended Activities: examine the range, shape and time behavior of the flammable hydrogen gas envelope released from 278 kg of storage (10 tanks at 250 bar pressure), and exiting the Vent Mast as a function of: rates of release, wind and if possible weather (ambient T, humidity). The Vent Mast should be vertical. In addition to room temperature hydrogen releases, it would be nice to have an analysis of cold (cryogenic, but not liquid)  $H_2$  releases.

#### Chapter 2: Fuel Cell Room:

Recommended Activities: predict the range, shape and time-dependence of the flammable hydrogen gas envelope leaking from a fuel cell rack as a function of leak rate and air-changes per hour (ACH). Examine effect of shape/slant of the roof and the size of the Fuel Cell Room. There is interest in  $H_2$  release from a fitting outside the fuel-cell rack with variable leaks, but <u>not</u> a pipe rupture into the room.

#### Chapter 3: Bunkering:

Recommended Activities: examine the range, shape and time-dependence of the flammable hydrogen gas envelope issuing from a hose leak, examine the size of affected area with hose rupture, determine the sizes and shapes of safety zones and Simultaneous Operations (SIMOPS) zones. Consider full fuel hose rupture, breaking at the midpoint between truck and boat. Consider nominal 250 bar refueling (truck pressure will be higher). Use Table B1 of IEC 60079-10-1 for leak sizes.

The scope of the studies was further limited amongst the three topics due to budget and time constraints. This report describes these hydrogen gas dispersion studies for Topics 1 - 3 as Chapters 1 - 3 below.

### **Chapter 1: Vent Mast**

#### 1.1: Introduction:

Hydrogen fuel-cell vessel designs all have Vent Masts. These masts are vertical pipes that allow planned and unplanned releases of hydrogen to be injected into the air at the highest point on the vessel, so that the hydrogen can rise and safely dissipate. Hydrogen releases from the Vent Mast could be necessary for several reasons. For example in vessels using HP compressed hydrogen, it may be necessary for tank maintenance to remove hydrogen from the tanks (so-called "dumping the tanks"), and passing the hydrogen out to the air through the Vent Mast is the simplest way to do that safely. Alternatively, if there is a leak in the Fuel Cell Room and the room is ventilated, the ventilation exhaust can be connected to the Vent Mast, allowing escape of the hydrogen gas. As an example, a large leak could be a broken hydrogen pipe that is feeding the fuel-cell rack. In another example, purging of excess water out of the fuel cell stack typically requires a burst of hydrogen gas, which is mixed with fuel-cell rack ventilation air and directed to the Vent Mast as well. Other types of Vent Mast releases were considered in an earlier study [1], including boil-off from LH<sub>2</sub> tanks.

Here we examine the physical extent of the hydrogen flammable volume that results when all the vessel's HP hydrogen tanks are opened and vented out the Vent Mast. Comparison is made of releasing hydrogen from one tank versus all of the tanks. The influences of a 5-knot wind, both horizontal and at a 45° downward angle from the horizontal, are included. Finally, the calculations at different points of the venting curve allow an assessment of the flammable region from different hydrogen mass flow rates. This permits an assessment not only of the rapid dumping of the HP hydrogen gas, but also the flammable cloud region that may result from smaller hydrogen releases.

This Chapter is a "follow-on" study from the earlier effort [1] to examine hydrogen Vent Mast releases from the normal "boil-off" of LH<sub>2</sub> tanks, or the rapid release of cold hydrogen gas from the vapor region of a nearly empty LH<sub>2</sub> tank.

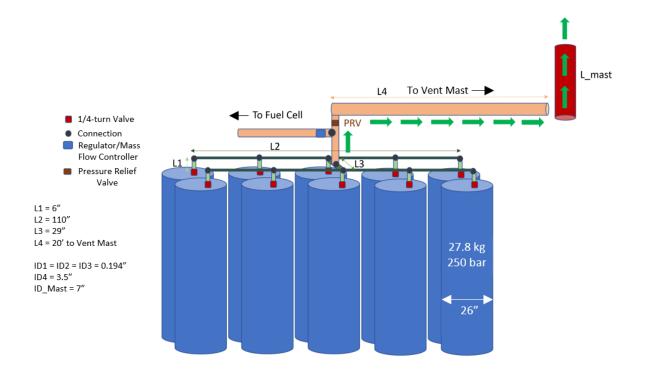
#### 1.2: Approach to Modeling and the Tank and Vent Mast Configuration:

It is useful to know how fast the hydrogen tanks can be emptied for maintenance reasons, or in response to a fire on the vessel in which case it is safer to dump the hydrogen before the hydrogen tanks heat up, preventing hydrogen pressurization to the point of tank rupture. The study of the manifold gas flow was accomplished with Sandia's network flow modeling code, MassTran [2].

MassTran was used to calculate the physical characteristics of the hydrogen release from the tanks, through the tank manifold piping and to the exit plane of the Vent Mast. As such, it is the "input calculation" for the subsequent CFD treatment of the hydrogen dispersion in the open air above the Vent Mast. MassTran enables users to model compressible and incompressible flows of multi-species gas mixtures through arbitrary arrangements of pipes, vessels, and flow branches. As the source tanks empty, MassTran calculates the temperature, pressure, mass, and density of the gas in the tanks, as well as the released mass flow rate and velocity within the gas manifold.

MassTran was used to calculate the mass flow rate and temperature of 278 kg of hydrogen stored in ten 250-bar rated hydrogen tanks should the tanks need to be "dumped" in the event of an emergency. Such a calculation also allows study of slower emptying of the hydrogen tanks for maintenance purposes. The modeled tank configuration is similar to that being adopted for the *Sea Change* Hydrogen Fuel Cell Vessel, the first commercial hydrogen fuel-cell ferry in the Western Hemisphere, and currently undergoing sea trials [3]. The *Sea Change* will be deployed in San Francisco Bay early in 2022. The tank configuration is also similar to that of the Discover Zero vessel, currently in the design process, which will use hydrogen fuel cells for auxiliary power on-board a commercial touring vessel [4].

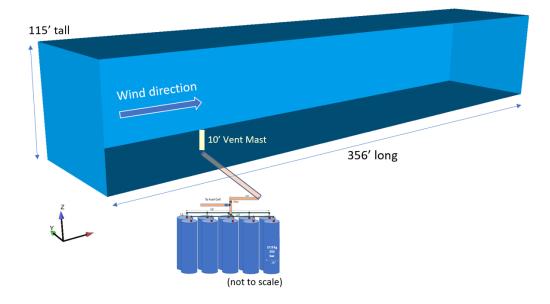
The layout of the tanks, manifold and Vent Mast is shown in Figure 1.1. Each of the ten 1544 L (water volume) tanks holds 27.8 kg of hydrogen at 250 bar. Quarter inch tubing, with internal diameter (ID) of 0.194", connects the ten tanks to larger 3.5" ID tubing that eventually connects to a 7" ID Vent Mast. The calculations take into account heat transfer through the walls of the tanks, the tubing, and the Vent Mast [5]. The Vent Mast was assumed to be 10 feet tall, so that the CGA G-5.5 recommendation of L/D < 60 is met as a strategy to prevent hydrogen detonation [6].



**Figure 1.1:** Layout of the ten-tank configuration. The green arrows mark the vent path for hydrogen. The approximate HP tank dimensions are ~ 26" outer diameter and ~18 feet long. The tanks are based on a commercial Hexagon Purus Type IV tank with hydrogen capacity 27.8 kg at 250 bar. The diagram is not to scale.

#### 1.3: CFD Flow Configuration

MassTran is the "input calculation" for the CFD model (named "Fuego") of the hydrogen release in the open air above the Vent Mast. Fuego is a robust simulation capability for buoyancy-driven turbulent flow mechanics [7]. This low-Mach CFD code is part of Sandia's Sierra Suite [8]. Fuego uses an approximate projection algorithm with a Control Volume Finite Element Method (CVFEM) [9]. The 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. The convection terms in the equations are discretized with a first-order upwind differencing scheme, although the higher order MUSCL [10] 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. 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. The pressure in the CFD domain is sufficiently low to allow the ideal gas equation to properly relate pressure to density. The CFD computational domain for the hydrogen dispersion out of the Vent Mast is shown in Figure 1.2. This domain was formulated with Brain Trust input. The mesh for the simulations was created using the Sandia software tool, Cubit [11]. The mesh has 19,034,701 nodes.



**Figure 1.2:** The CFD domain for the Vent Mast release is 356 feet long x 65 feet wide x 115 feet tall and includes the 10-foot-tall Vent Mast.

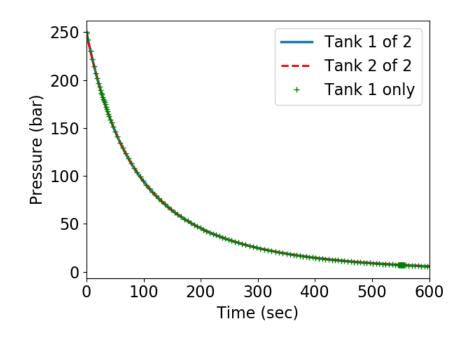
The traditional values given for the flammability range of hydrogen is 4 – 75% (percent by volume) [12]. However, experiments have shown that for a sustained combustion that can propagate in three dimensions, the lower flammability limit (LFL) for hydrogen is closer to 8% [12, 13]. This is true for both combustion of hydrogen in enclosed volumes (like a balloon) [12] and combustion in jet releases [13]. To be conservative, we will assume the hydrogen LFL for all of this study is the traditional 4%.

#### 1.4: MassTran: Comparing a One-tank Release to a Two-tank Release

Our first objective was to understand the flow of hydrogen through the hydrogen storage manifold, as this is required input to the CFD calculation of the release of hydrogen out of the Vent Mast and into the open air. MassTran was originally designed to have only one source tank, so in order to perform the calculations for the venting of multiple tanks, the capabilities of MassTran had to be expanded to facilitate multiple sources (hydrogen tanks) flowing into a single exit vent. To test this new capability we initially compared the MassTran result from venting two tanks simultaneously to that

obtained from venting one tank, as a check before proceeding to studying the 10-tank situation. The two tanks chosen are those closest to the junction of L2 and L3 in Figure 1.1. Results for these "one-tank" and "two-tank" model tests are shown in Figures 1.3 - 1.5. Note: CFD calculations of the hydrogen dispersion in the air above the Vent Mast were not performed for this one-tank versus two-tank study.

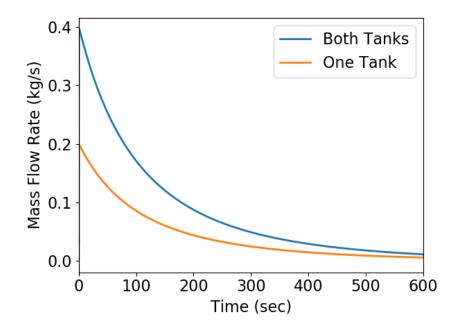
Figure 1.3 presents the "pressure vs. time" results from a one-tank release compared to a two-tank release. The pressure in each tank (Tank 1 of 2, and Tank 2 of 2) is behaving as expected: emptying at the same rate down to one bar pressure. The two-tank "blowdown" (i.e., emptying) is not discernably different from the one-tank result (Tank 1 only). This is because the two tanks have equivalent and parallel vent paths (see Fig. 1.1). After 600 seconds, the pressure remaining in the two-tank scenario is ~ 6 bar.



**Figure 1.3:** Tank pressure during hydrogen venting; Blue Line: pressure inside Tank 1 in a two-tank array; Orange Line: pressure inside Tank 2 in a two-tank array; Green Cross: Pressure inside Tank 1 in a one-tank array. The hydrogen capacity of the two-tank system is 55.6 kg; the hydrogen capacity of one tank is 27.8 kg.

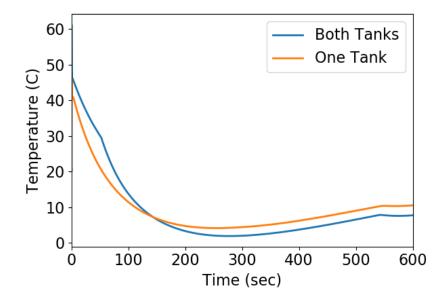
The flows in the one-tank or two-tank arrays are "choked" within the quarter inch tubing L1 right out of the hydrogen tanks (see Fig. 1.1). By "choked" flow we mean that the gas conductance through the tube is limited such that further increases of the upstream gas pressure do not increase flow through the conductance-limited element. Both Tank 1 and Tank 2 have identical L1 tube sections, and therefore empty at the same rate. Also for the 55.6 kg combined quantity of gas, there is no choking downstream of L1 that arises, so the "Tank 1 Only" blowdown is essentially the same as predicted for combined Tanks 1 and 2.

Figure 1.4 shows that the mass flow rate out of the Vent Mast is higher when two tanks are emptied compared to one tank (as one would expect), but the blowdown is still completed in approximately 600 seconds (10 minutes). Note that if the L1 and L2 piping manifold were increased to half-inch tubing, a faster blowdown would be realized. We chose quarter-inch tubing as this is commonly used for such tanks, and is the size used for the *Sea Change* hydrogen vessel.



**Figure 1.4:** Mass flow rate of hydrogen (kg/s) exiting the Vent Mast during hydrogen venting. Blue Line: from a two-tank array; Orange Line: from a one-tank array.

Figure 1.5 shows the temperature of the hydrogen gas at the exit plane of the Vent Mast. There is a small difference in the temperature for the released hydrogen between one-tank and two-tank releases, but the overall results are similar. The hydrogen starts out at 20 °C in the tanks themselves, but the temperature increases by  $\sim 20 - 25$  °C in the process of venting through the system because there is initial compression behind the conductance limitation producing choked flow. A 20 °C temperature rise is of no consequence for the evacuation of the tanks and the release out the Vent Mast. As the venting proceeds, Figure 1.5 shows that the hydrogen temperature at the Vent Mast exit steadily decreases for both the one-tanks and two-tank scenarios.

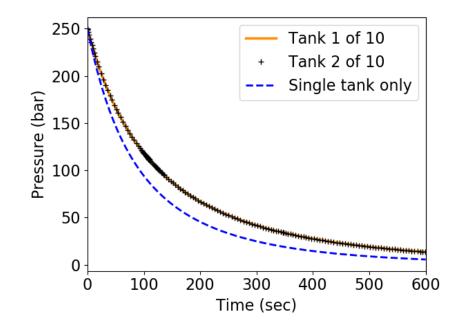


**Figure 1.5:** Temperature of the released hydrogen calculated at the exit plane of the Vent Mast. Blue Line: Two tanks; Orange Line: One tank.

#### 1.5: MassTran: Comparing a One-tank Release to a Ten-tank Release

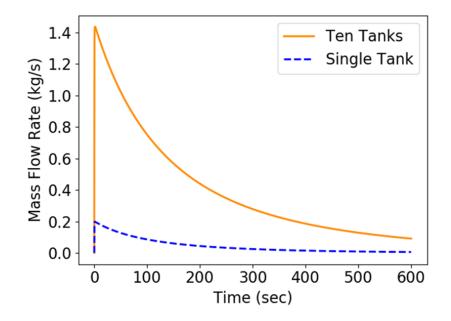
A scenario of practical interest is the ten-tank release for which the pressure in all ten tanks will decrease at the same rate. This would correspond to a "dumping" of the full hydrogen storage load of 278 kg. This dumping could be needed for either maintenance reasons, or needed in the event of some emergency, for example a fire on the vessel. We examined the fastest possible (unconstrained) release because this release not only covers that needed in the event of an accident (fast dumping), but also contains within it information for a slower maintenance release since we predict how mass flow decreases with time.

The MassTran results for two of the ten tank pressures are plotted in Figure 1.6. Only two tanks are plotted because the other eight tanks have the same profiles. The pressure in each tank (Tank 1 of 10, and Tank 2 of 10) is behaving as expected: emptying at the same rate down to one bar pressure. The ten-tank "blowdown" (i.e., emptying) takes somewhat longer than the Single Tank Only" result, although they are similar due to the multiplexing of tanks and manifold hardware evident in Figure 1.1. The longer time required for the 10-tank configuration is because the hydrogen has to flow on average through longer sections of tubing L2 which reduces gas conductance. Also, with 10 times more hydrogen (278 kg) being vented, there is some mild choking of this flow downstream. The combined effects make for a longer venting time. Still, after 600 seconds, the pressure within the ten tanks is 13.6 bar, which is about the pressure one would want to leave inside a tank for refueling. Also, such a small residual pressure would eliminate over-pressurizing the tanks in the event the tanks were immersed in a fire. If higher residual tank pressures are acceptable, the tanks can be considered "dumped" faster, as indicated in Figure 1.6.



**Figure 1.6:** Tank pressure during hydrogen venting for one tank compared to tanks in a ten-tank array. Orange Line: Single tank in a one-tank array. Black Cross: Tank 2 of a ten-tank array. Blue Line: Tank 1 in a one-tank array. The total hydrogen load of the ten tanks is 278 kg, and that for the one tank array is 27.8 kg.

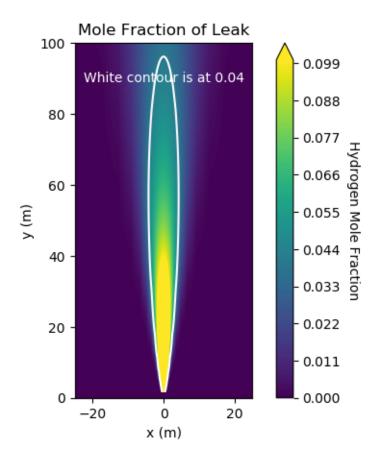
Figure 1.7 shows that the mass flow rate during those 600 seconds is higher as well. The conclusion from Figures 1.6 and 1.7 is that if the hydrogen in the 10 tanks needs to be dumped in the event of an emergency, it can be successfully dumped in ~ 10 minutes. It is also noteworthy that if one wanted to reduce the pressure to about one-half the initial value, to provide some pressure safety margin in the event of a fire but one does not want to dump the entire 278 kg load, this pressure relief can be accomplished in ~ 2 minutes.



**Figure 1.7:** Mass flow rate of hydrogen (kg/s) exiting the Vent Mast during hydrogen venting. Orange Line: from a 10-tank array; Blue Line: from a one-tank array. The total hydrogen load from the 10-tank array is 278 kg; that from one tank is 27.8 kg.

#### 1.6: HyRAM and CFD Analyses for Hydrogen Dispersion Above the Vent Mast for Ten-tank Release

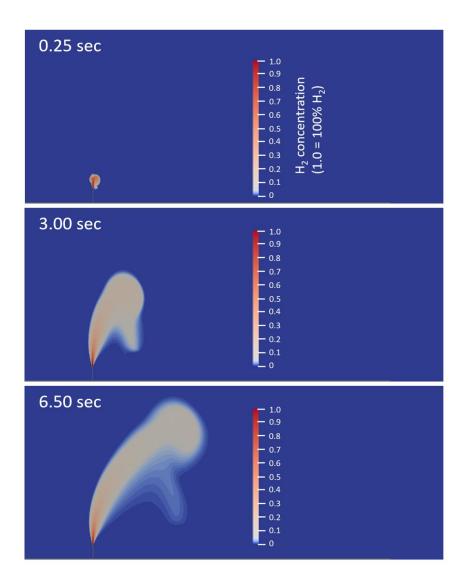
In order to get an idea of the size and shape of the flammable hydrogen envelope exiting the Vent Mast, we first used Sandia's simpler (but less accurate) HyRAM package to calculate the plume length without any wind. Unlike CFD, HyRAM uses a simple plume model to predict the length and concentrations of a release pointing straight up. From MassTran, we know the pressure and the temperature at the opening of the Vent Mast, which is then input into HyRAM's plume calculator along with the 7-inch diameter specification for the Vent Mast. Figure 1.8 shows what the plume height would be if the pressure at the Vent Mast exit were held at its maximum value, instead of decreasing with time as the hydrogen in the tanks are released. Because the pressure is artificially kept at the highest value, this will produce a much taller plume than is observed during a case where the pressure decreases as the hydrogen is released. Nonetheless, it provides a conservative (worst-case) rough estimate for the plume height at the beginning of the 10-tank vent.



**Figure 1.8** The hydrogen mole fraction is shown for the initial pressure (3.24 bar) and temperature ( $66^{\circ}$  F) at the Vent Mast opening for the 10-tank configuration. The 3.24 bar Vent Mast pressure corresponds to a hydrogen tank pressure of 250 bar. Gas within the white contour has hydrogen concentrations 4 % or higher, which includes the flammable range 4 – 75%.

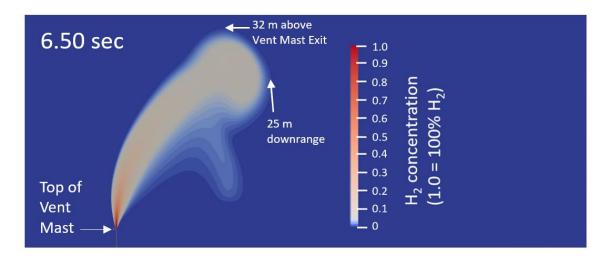
To add the effects of wind and the decreasing pressure on the plume shape, a more sophisticated analysis using CFD modeling is required. The velocity and temperature of the hydrogen exiting the Vent Mast, as calculated by MassTran, are then used as inflow boundary conditions for the CFD domain (Figure 1.2) with a wind flow of 5 knots (2.57 m/s) blowing horizontally. The CFD results are shown in Figure 1.9.

Figure 1.9 shows time-dependent CFD snapshots of the flammable plume that results from the venting of the 10-tank system in a 5-knot horizontal wind blowing to the right. The flammable region is shown in the light beige to red colors, as indicated by the H<sub>2</sub> concentration scale shown on the plot. Since the initial hydrogen direction out of the Vent Mast is vertical, the velocity within the entrained flammable envelope is the combination of the prevailing horizontal windspeed at that location and the higher vertical velocity of the hydrogen. The initial speed of hydrogen out the Vent Mast is 860 m/s. While this is quite fast, it is still less than the speed of sound in hydrogen, which is 1320 m/s, so it is appropriate to use a non-compressible flow solver like Fuego.



**Figure 1.9.** Hydrogen concentration from the 10-foot-tall Vent Mast as a function of time after the venting has started for the 10-tank system. Concentrations above the LFL of 4% are shown in varying shades of beige to red. Time steps for 0.25 seconds, 3.0 seconds and 6.5 seconds (the maximal extent) are shown. The horizontal wind speed is 5-knots (2.57 m/s) towards the right. These figures show an area that is 35 m tall and 96 m long (115' x 315'), which is a cropped section of the full domain to better show the hydrogen release.

Figure 1.10 shows the flammable concentration (> 4 %) of hydrogen in beige/red 6.5 seconds into the vent from the 10-tank array, corresponding to an instantaneous hydrogen mass flow rate of 1.3 kg/s (see Figure 1.7).



**Figure 1.10.** Hydrogen concentration from the 10-foot-tall Vent Mast 6.5 seconds after the venting has started for the 10-tank system. The horizontal wind speed is 5 knots towards the right. The flammable region of hydrogen reaches 32 m high above the Vent Mast exit and is 25 m downrange from the Vent Mast at this time.

The maximal extent of the flammable mass extends 32 m (105 feet) above the Vent Mast exit. Even though Figure 1.7 shows that the maximum release rate is at the very beginning, the flammable plume takes some time to develop, and the peak flammable envelope occurs later, after ~ 6 seconds into the release. Tabular information for the extent of the flammable region is shown in Table 1.1.

**Table 1.1** Extent of the Flammable Plume as a Function of Time for the Vent Mast Release of Figure 1.9. The Plume Length is reported relative to the Vent Mast centerline position, the Plume Height is reported relative to the Vent Mast exit.

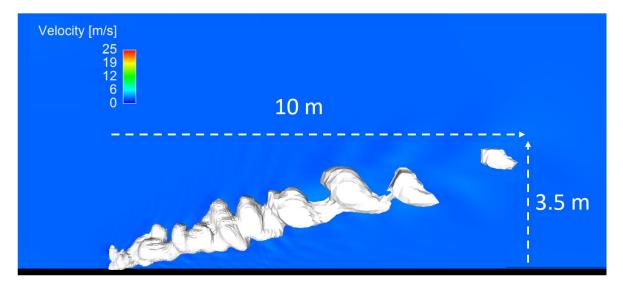
Time (s)	Flammable Plume Length Downrange (m)	Flammable Plume Height Above Release Point (m)
1	4	8.5
2	8	15.5
3	11	20.5
4	14.5	24
5	18	27
6.5	25	32

Figure 1.8 showed that in the absence of wind, the hydrogen would vent directly upwards, but Figures 1.9 and 1.10 show that the horizontal wind will eventually carry the plume sideways as the upward hydrogen momentum dissipates. This is a consequence of hydrogen being low-mass, so that when it encounters a flow of higher-mass gas (air), it tends to be entrained. Right at the Vent Mast exit there is a turbulent encounter between wind and hydrogen, which causes some hydrogen to spiral downward as the flammable envelope mass rises, and the resultant swirl can be seen in Figures 1.9 and 1.10. The flammable region does not extend below the top of the Vent Mast due to the upward momentum of the hydrogen as well as to the natural buoyancy of hydrogen. Note that a comparison of Figure 1.10 with Figure 1.8 shows that the simpler HyRAM model, based on a steady-state flow of hydrogen at maximal release velocity, overpredicts the height of the flammable hydrogen release.

We note here that even at the beginning of the 10-tank venting where the hydrogen pressure is at its highest, the hydrogen pressure at the Vent Mast exit is less than 4 bar. Thus, the Vent Mast releases cannot spontaneously ignite because they are well below the 40-bar threshold of spontaneous hydrogen combustion [12].

Since the release in Figure 1.9 involves a high initial hydrogen velocity (860 m/s), which requires time-consuming small computational time steps for a high-fidelity CFD analysis, only the first ~ 7 seconds of this release could be simulated in a manageable time frame (months). A slower hydrogen release with the same wind speed could be studied with reduced the CFD computation time. Those conditions would be comparable to what one would see towards the end of the larger, 10-tank blowdown. At the end of the blowdown, the hydrogen will have lower vertical momentum and will therefore be blown more easily directly sideways with the wind.

A representative look at such a time is shown in Figure 1.11. This shows a release with a <u>steady-state</u> 13.41 m/s (30 mph) release of hydrogen in a 5-knot crosswind. The hydrogen plume in the flammable range, shown in white, reaches about 10 meters downstream and rises 3.5 meters above the Vent Mast. No velocity information is conveyed in the white envelope.



**Figure 1.11** Hydrogen released with a constant 13.41 m/s (30 mph) hydrogen exit velocity in a 5-knot cross wind. The white color encompasses hydrogen concentrations from 4% to 75 %.

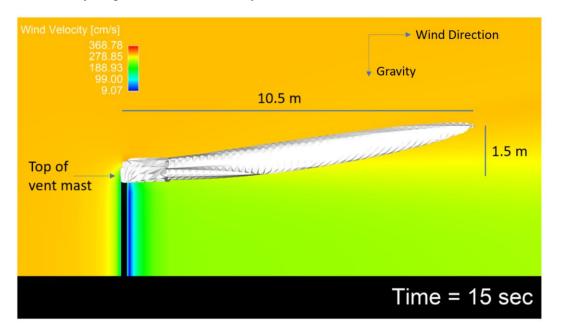
Compared to other Vent Mast releases that could occur on a hydrogen vessel, the 10-minute venting of the 10 hydrogen tanks is a large release, corresponding to an average hydrogen release rate of ~ 0.46 kg/s. It is one of the few types of hydrogen Vent Mast releases that have a flammable plume. For example, in the prior study [1] it was found that the normal boil-off rate for a 1200 kg LH<sub>2</sub> tank was 0.000138 kg/second, producing a hydrogen/air plume with a safe (i.e., not flammable) hydrogen mole fraction of 2.5% or less at the Vent Mast exit. We shall see in Chapter 2 the consideration of hydrogen leaks of a maximum of 3.0 x  $10^{-5}$  kg/s from a fuel cell rack. If ventilated in one second and injected into the Vent Mast without even being diluted by the Fuel Cell Room air (a conservative estimate), this would produce a safe mole fraction out the top of the Vent Mast of 0.5% (using the correspondence 0.000138 kg/second  $\leftrightarrow 2.5\%$  from the prior study [1]). Thus, as far as releases into the Vent Mast from vessel operation, only maintenance dumping of the HP tanks produces a flammable hydrogen release out of the Vent Mast.

# 1.7: CFD for Hydrogen Dispersion Above Vent Mast for Horizontal and 45 Degree Downward Wind Orientations

In the course of this work, we wondered if it is possible out on the open water for the wind to be blowing in any other direction except horizontal, parallel to the water's surface. At the direction of Commander Frank Strom of the USCG Sector San Francisco, on July 17, 2020, we spoke to Mr. Robert Blomerth, who is the Director of Vessel Traffic Services for USCG Sector San Francisco. The Director of Vessel Traffic Services provides a similar service as an Air Traffic Controller, only for the maritime environment, and tracks all wind patterns appearing on San Francisco Bay. Mr. Blomerth reported that on the open water, the wind always blows horizontally. However, we recognize that if the hydrogen vessel is moored near a building, that it may be possible to get some wind propagation at angles other than horizontal.

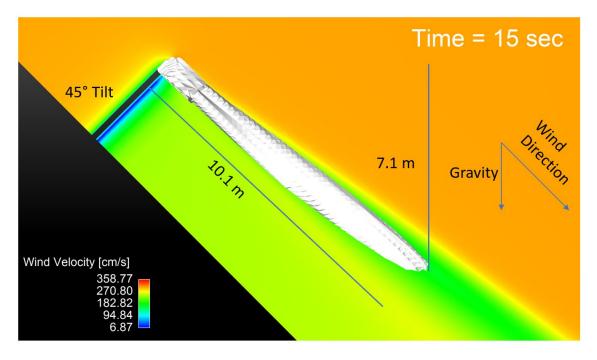
We conducted two hydrogen dispersion Vent Mast calculations with the wind blowing at 5 knots, both horizontally and downward at a 45° angle for a low-speed hydrogen release. This was accomplished, without changing the meshing for the CFD calculation, by changing the angle between the wind direction and the downward pointing gravity vector from 90° (horizontal wind) to 45° (downward pointing wind).

The results 15 seconds after the release for the horizontal wind are shown in Figure 1.12. For this time, the exiting speed of the hydrogen out of the Vent Mast is a relatively slow 8.6 m/s. Figure 1.12 reveals that while the low-speed hydrogen is blown horizontally to the right, it is also rising by buoyancy, since the centerline of the flammable envelope in Figure 1.12 makes a positive angle with the horizontal. Thus, a horizontal wind cannot substantially blow the hydrogen down during the venting for even a smaller low-speed release, although turbulent mixing right at the top of the Vent Mast causes some hydrogen to extend down by about four inches.



**Figure 1.12.** Velocity of the flow field and flammable region of hydrogen concentration (in white) out of the 10-foot-tall Vent Mast 15 seconds after the venting has started corresponding to an initial hydrogen exit velocity of 8.6 m/s. The horizontal wind speed is 5 knots towards the right. The white color encompasses flammable hydrogen concentrations from 4 - 75 %. The flammable region of hydrogen is a narrow horizontal region extending out to 10.5 m (34 feet). The spiral structure within the flammable envelope is an artifact of the meshing algorithm.

The results 15 seconds after the release for the wind angling downward are shown in Figure 1.13. Since the meshing was not changed, the Vent Mast is not properly rendered for the real case in which the Vent Mast and gravity vector are aligned, and the wind is directed downward. Still, the essential effect of wind angle on hydrogen propagation direction will be valid.



**Figure 1.13.** Velocity of the flow field and flammable region of hydrogen concentration (in white) out of the 10-foot-tall Vent Mast 15 seconds after the venting has started for an exit velocity of 8.6 m/s. The wind speed is 5 knots (257 cm/sec) directed towards the right at a  $45^{\circ}$  angle downward with respect to the horizontal. The flammable region of hydrogen in white (4 – 75%) is a narrow horizontal region extending out to 10.1 m (33 feet). No velocity information is presented within the white envelope. The spiral structure within the flammable envelope is an artifact of the meshing algorithm.

Figure 1.13 shows that a 5-knot wind blowing at a 45° angle downward with respect to the horizontal will carry the low-velocity flammable hydrogen plume downward despite the intrinsic buoyancy of the gas. Again, this is a consequence of hydrogen being lowmass, so that when it encounters a flow of higher-mass gas (air), it is readily entrained. Close inspection of Figure 1.13 reveals that while the hydrogen is blown downwards and to the right, it is also rising since the centerline of the flammable envelope in Figure 1.13 makes a positive angle with the wind direction.

Altogether, the modeling results show that a hydrogen release can be influenced by the wind, with influence being higher the lower the velocity of the hydrogen release. If the wind is directed downwards and the hydrogen velocity is low, then hydrogen can be drawn below the level of the Vent Mast exit. However, if the dumping is done in open water, for which the wind always blows horizontal to the plane of the water's surface, a flammable hydrogen release such as that caused by emergency dumping of the hydrogen tanks cannot be driven downwards by wind on the open water.

However, it can be properly noted that if a hydrogen vessel is moored near a tall building, then it may be possible to get some wind propagation at angles other than horizontal. The nature of wind flows intercepting buildings was the subject of a study by Peterka et al. [14]. In their work, air flow around and over buildings was examined. What was found was that an airflow with downward component can be created by tall buildings, disturbing the normal airflow (in the absence of a building) 1 - 3 building heights downwind from the building location. However, the work also showed that the velocity of the disturbed airflow is only ~ 1/10 of the original (approaching) wind velocity at heights near ground level. In other words, although a downward component can be introduced in the wind flowfield by a tall building downstream from the building, the building dramatically reduces the wind velocity at the likely height (near ground level) of a Vent Mast release.

This Vent Mast hydrogen dispersion work has implications for the hazardous zone that is associated with the use of a Vent Mast on a vessel, as prescribed by the International Code for Gas-fueled Ships (i.e., the "IGF Code") [15]. Since there is currently no applicable code for the use of hydrogen on vessels, the IGF code, written for the use of natural gas on vessels, is the primary regulatory guide for placing hydrogen systems on ships. This is reasonable, since the physical and combustion properties of hydrogen and methane (the primary component of natural gas) are so similar [12]. The IGF code requires a spherical exclusion zone of 10 m radius at the exit of the Vent Mast, anticipating that releases of natural gas can be moved below the Vent Mast exit due to increased density (if cryogenic liquid natural gas is released) or can be blown down by a prevailing wind. The question arises if this spherical exclusion zone is necessary for a hydrogen release, or if instead a hemispherical exclusion zone can be adopted which acknowledges the gas dispersion properties of hydrogen. A hemispherical exclusion zone has been assumed in several hydrogen vessel design studies [16 – 18].

Our sentiment is that the scenario that would argue for a spherical hazardous zone at the Vent Mast exit, namely emergency dumping of the tanks near a tall building experiencing high winds, is not particularly credible and a hemispherical hazardous zone would be sufficient as was assumed previously [16 - 18]. However, further CFD modeling of this question would be needed to determine whether a hemispherical or spherical exclusion zone is needed for credible hydrogen release scenarios.

#### 1.8: Chapter 1 Conclusions

We successfully extended the MassTran model to handle the problem of hydrogen release from ten hydrogen tanks, similar to that which will be used on the Sea Change and the Discover Zero vessels. Two hydrogen tanks, with storage capacity 27.8 kg each, can be emptied within ten minutes. A ten-tank hydrogen storage system, holding 278 kg, can also be dumped in  $\sim 10$  minutes, although a pressure reduction to half the original pressure (125 bar) can be realized in two minutes. CFD results show that when the hydrogen is released out of the Vent Mast in a 5-knot wind, the effect of the wind on the hydrogen release depends strongly on the hydrogen exit velocity. For low-speed hydrogen (~ 10 m/s), for wind that is blowing either horizontally or at a  $45^{\circ}$  downward angle, the hydrogen is entrained in the wind, but the flammable envelope rises at a positive angle to the wind direction vector. If a downward pointing wind from a proximate tall building were to coincide with a tank dumping procedure, the low-velocity part of the hydrogen release could be entrained below the Vent Mast exit. We believe such a coincidence is unlikely, although further study of the issue would be productive. For higher-speed hydrogen flows ( $\sim 800 - 900 \text{ m/s}$ ), the flow is momentum driven with relatively less influence by the 5-knot crosswind.

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3. The California Air Resources Board has recently funded the construction of the *"Water-Go-Round"* hydrogen fuel-cell ferry. Information about the vessel can be found at: <u>https://watergoround.com/.</u> The vessel was recently renamed the *Sea Change*.

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## **Chapter 2: Fuel Cell Room**

#### 2.1: Introduction:

The powerplant envisioned for hydrogen vessels can be either a hydrogen-burning ICE, such as that demonstrated by CMB on the Hydroville hydrogen passenger ferry [1], or a PEM hydrogen fuel cell. The advantage of a hydrogen PEM fuel cell is that it is a truly zero-emissions powerplant, with the only onboard emissions being water. In contrast, a hydrogen ICE engine emits  $NO_x$ . It is important to remember that the "well-to-waves" emissions, that include emissions from the production and delivery of hydrogen fuel, are typically not zero as discussed previously [2].

Hydrogen fuel cells on a vessel would typically be located in Fuel Cell Rooms [3, 4]. In these designs, fuel cell modules (typically ~ 30 kW/module) are combined into fuel-cell racks, with the racks holding ~ 4 fuel cell modules, providing a total rack power of ~ 120 kW. Hydrogen is piped into the room, and into individual fuel-cell racks at a pressure of ~ 7 bar which is reduced even further to about 2 bar before entering the fuel cell modules. The fuel cell modules combine hydrogen and oxygen from the air to produce electricity, waste heat and water (typically as a vapor although liquid water is also produced).

Being in an enclosed space, a leak of hydrogen from one of the fuel cell module fittings can be a concern. This would be a low-pressure (~ 2 bar) hydrogen leak. To mitigate the risks from such a leak, the general safety strategy is to have the rack be fitted with a hydrogen leak detector, with the entire rack subject to ventilation air flow that eventually exhausts out through the Vent Mast of the vessel and does not vent into the Fuel Cell Room. As a secondary safety feature, the Fuel Cell Room itself would have a ventilation system that is independent from that of the fuel-cell rack. A typical value of Fuel Cell Room ventilation could be ~ 30 air changes per hour (ACH).

The results presented in this report complement a prior study [5] of the influence of Fuel Cell Room ventilation on a larger leak involving a rupture of the 7-bar pipe entering the Fuel Cell Room. Though the hydrogen discharge would be momentarily sizeable (0.038 kg), it would be short-lived because the Fuel Cell control system would sense a drop in the pressure of the 7-bar line, and close a shutoff valve within two seconds. The results showed [5] that with a 30 ACH ventilation in the Fuel Cell Room, the hydrogen cleared from the Fuel Cell Room within 7 seconds. The USCG deemed that such a pipe rupture was a low probability accident scenario for a hydrogen fuel cell vessel.

In this study, we focus on the effects of Fuel Cell Room ventilation on three smaller leak amounts emanating from a PEM fuel-cell rack. In this scenario, which was supported by the Brain Trust and in particular the USCG [6], we study the situation where a leak is emanating from one of the low-pressure fittings within the fuel-cell rack. Normally, such a leak would be detected by the rack hydrogen sensor located inside the rack towards the top of the rack. Activation of this hydrogen alarm would activate a shutoff valve on the 7-bar line, cutting off the hydrogen supply to the leak. At the same time, the fuel cell rack ventilation would dilute the hydrogen leak, and carry the diluted hydrogen/air mixture to the Vent Mast for safe release into the atmosphere.

For our scenario, we assume a "double failure" for which the rack hydrogen detector has failed, and also, the ventilation within the rack has failed. Thus, we consider hydrogen building up within the fuel-cell rack, and leaking out the top of the rack through a 4-inch diameter hole. We investigate how the hydrogen leak behaves, and ask how the Fuel Cell Room ventilation influences the hydrogen gas dispersion. Our objective is to understand the nature of the flammable gas risk, particularly how it can be managed with room ventilation and how detectable such leaks are by an in-room hydrogen detector. We simulated the effect that ventilation might have on flammable mass amounts and envelopes in the room and ran five ventilation rates: no ventilation (0 ACH), 15 ACH, 30 ACH, 60 ACH, and 75 ACH.

#### 2.2: Simulation Methods:

All Fuel Cell Room simulations were carried out using Sandia National Laboratories' in-house, incompressible CFD code, Fuego, which was described in Chapter 1. Cantera, a software tool for chemical kinetics, was used to evaluate the species properties [7]. This approach of modeling hydrogen leaks has been validated in previous work [8].

#### 2.3: Mesh and Domain, Leak Rates:

The Fuel Cell Room geometry, which determines the mesh for the calculations, was based on feedback from the Brain Trust and is shown in Figure 2.1. The mesh for the simulations was created using the Sandia National Laboratories software tool, Cubit [9] and has 1,144,314 nodes. The room geometry is very similar to that of the original report [5], with only minor changes in the outflow ventilation system, to make it more realistic. The room was assumed to be 24 feet long x 16 feet 6 inches wide x 9 feet 6 inches tall and have four rows of fuel-cell racks spaced to allow for equipment access and ventilation. There are nine inflow vents near the floor of the room, and the 1 foot x 1 foot outflow vent was located near the center of the ceiling.

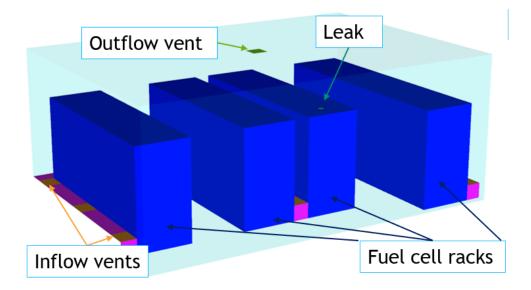


Figure 2.1: The CFD computational domain for hydrogen releases in the Fuel Cell Room.

Three leak release rates were investigated. The lowest rate is the flame quenching release rate [10] which is 18 normal cc/min (Ncc/min) or  $2.58 \times 10^{-8}$  kg/s. We call this "Leak 1." This is the threshold release rate which cannot be ignited, even with an ignition source placed at the leak exit. This is about 100x higher than the allowed leak rate for pressure relief devices (PRDs). To put the  $2.58 \times 10^{-8}$  kg/s hydrogen leak rate into context: if one were to fill a classic model KS-21716 AT&T telephone booth (dimensions H x W x D = 6 feet 11 inches x 2 feet 9 inches x 2 feet 9 inches) with this leakage of hydrogen, it would take 2.35 days to reach the 4% lower flammability limit (LFL) [11]. This results in a very slow velocity of  $3.7 \times 10^{-5}$  m/s out of the four-inch diameter leak orifice, which is assumed to be a hardware opening in the top of the fuel-cell rack (see Fig. 2.1).

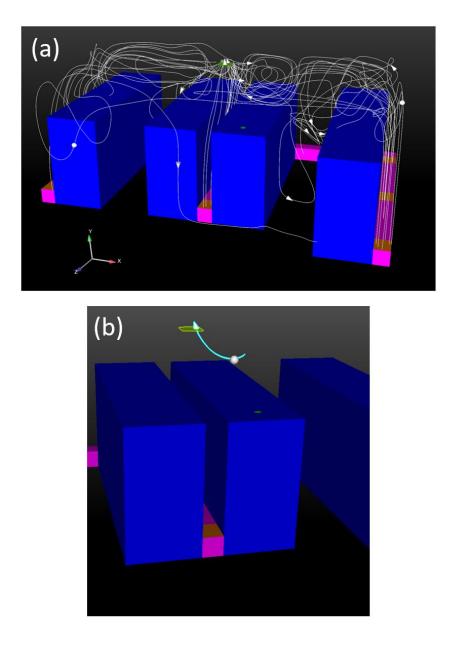
We chose for the highest hydrogen release rate that which a typical fuel-cell rack ventilation system is designed to mitigate. We then added a safety margin, which brought us to a leak rate of  $3.0 \times 10^{-5}$  kg/s, which we call "Leak 3." With this leakage of hydrogen, it would take 3.13 minutes to reach the 4% LFL in our phone booth example. This yields an exit velocity of 0.045 m/s through a 4-inch diameter leak. Finally, we also examined an intermediate hydrogen leak, with a rate of  $1.0 \times 10^{-5}$  kg/s, which gives an exit velocity of 0.015 m/s and would take 9.39 minutes to reach the 4% LFL in our phone booth example. We call this "Leak 2."

#### 2.4: Fuel Cell Room Ventilation and Hydrogen Leak Initiation:

Leaks 2 and 3 were simulated with five different ventilation rates: 0 ACH, 15 ACH, 30 ACH, 60 ACH, and 75 ACH. A ventilation rate of 30 ACH is required by the

IGF code for an Emergency Shut Down (ESD) designated space [12]. For the smallest Leak 1, we ran the simulation for the case of no ventilation (0 ACH) as a limiting case.

Air streamlines for the 30 ACH case without a hydrogen leak are shown in Figure 2.2 (a). As can be seen, the structures in the Fuel Cell Room can have a significant influence on the air flow patterns, as can the location of both the inflow and outflow air vents.



**Figure 2.2:** (a) Air streamlines produced by a ventilation rate of 30 ACH in the Fuel Cell Room without a hydrogen leak. This pattern is for a time index of 10 min; (b) the same air streamlines as in (a) with a streamline shown at the location (white dot) where velocities at different ventilation rates are reported.

The overall flow in the room is as one might expect: air enters the domain from the inflow vents on the floor, flows up the side of the fuel-cell racks, and exits the outlet vent. However, in the space in between the tops of the fuel-cell racks and the outlet vent on the ceiling, the flow can be rather chaotic. We expect such a flow to exist in a practical Fuel Cell Room and its effect on the dispersion of the hydrogen leak is of interest. The velocities at the inflow vents are 0.381 m/s, 0.762 m/s, 1.52 m/s, and 1.91 m/s for the ventilation rates of 15, 30, 60, and 75 ACH, respectively. Velocities of the airflow at the outflow vent in the ceiling range from 2.75 m/s, 5.91 m/s, 9.50 m/s, and 12.0 m/s for 15 through 75 ACH, respectively. Figure 2.2(b) shows a location and the associated airstream for the results of Figure 2.2(a) where we extract air velocities (at the white dot) for different ventilation rates. Those velocities are 0.0921 m/s, 0.288 m/s, 0.710 m/s and 0.842 m/s for 15, 30, 60, and 75 ACH, respectively.

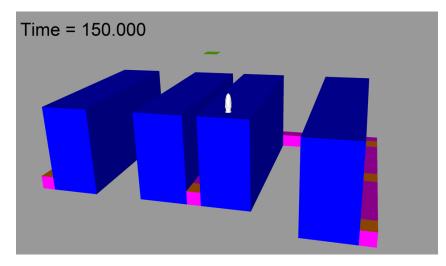
For the hydrogen leak scenarios, the simulations were all run for 600 seconds before the hydrogen leaks were started in order to establish a steady-state ventilation air flow in the room. Then, at 600 seconds, the hydrogen leaks were turned on for 150 seconds to establish a hydrogen leak steady-state, at which point the leaks were shut off. The simulations were all run for an additional 300 seconds after the leak was turned off in order to assess the duration and size of the flammable mass envelope as it is removed by the varying levels of room ventilation. The highest leak rate was also run for several hours in the room with no ventilation to show the buildup that would occur in this extreme situation.

#### 2.5: Fuel Cell Room Results:

#### 2.5.1: Cases with No Ventilation

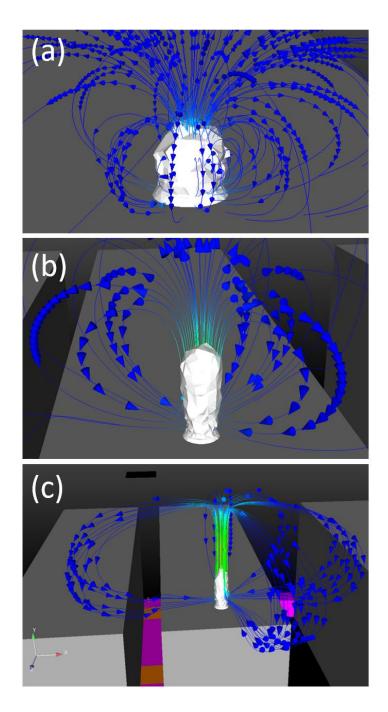
The three leak rates  $(2.58 \times 10^{-8} \text{ kg/s}, 1 \times 10^{-5} \text{ kg/s}, \text{ and } 3 \times 10^{-5} \text{ kg/s})$  were simulated in the Fuel Cell Room with no ventilation as a check of the simulation procedure, to establish a base comparison for the higher ventilation rates and to help develop a physical intuition of how these leaks behave. *Note: we are not recommending that anyone design a Fuel Cell Room without any ventilation for the type of PEM fuel cell rack assumed in this study.* For the figures in this section, the hydrogen in the room that is within the flammable range, 4 - 75% by volume, is shown in white. Since the pressure differential across the leak is below the ~ 40 bar required for spontaneous ignition [11], there is no ignition risk of this flammable envelope unless there is an ignition source located within the white region of release.

Figure 2.3 shows the flammable region from Leak 3 ( $3 \times 10^{-5}$  kg/s) after 150 sec of leak time into the unventilated Fuel Cell Room.



**Figure 2.3.** The flammable mass of hydrogen is shown in white for the Leak 3 ( $3 \times 10^{-5}$  kg/s) and no Fuel Cell Room ventilation. The flammable envelope is shown 150 seconds after initiation of the hydrogen leak. The flammable range in white is 4 - 75% by volume.

Interestingly the flammable region is limited by self-induced entrainment of air, caused by the leak momentum and buoyant rising of the hydrogen release, as shown in Figure 2.4.

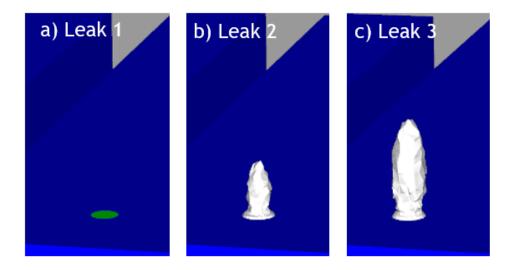


**Figure 2.4:** Airflow around the hydrogen release shown in Figure 2.3 using Leak 3 ( $3 \times 10^{-5}$  kg/s). (a) After 0.537 seconds, (b) after 1.65 seconds and (c) after 4.10 seconds. Flammable mass is in white (4 - 75%); high and low velocity magnitude regions are in green and blue, respectively.

Figure 2.4 shows the airflows around the initial stages of the hydrogen release, which reveals this mixing and why, at least for the duration of the simulation, the entrained air flow dilutes the rising hydrogen release, restricting the flammable region to

the envelope indicated in white, and limited to be relatively close to the leak source. Note that this restriction of the flammable region occurs in the absence of room ventilation, and arises from the local gas dynamics associated with the rising hydrogen leak.

Figure 2.5 compares the flammable regions of the three leak rates after 150 sec of leak time, again for the case of no Fuel Cell Room ventilation. For the smallest Leak 1  $(2.58 \times 10^{-8} \text{ kg/s})$ , there is no hydrogen within the flammable range. This is consistent with the experimental finding that such a leak rate cannot be intentionally ignited even if an ignition source is placed above the leak source [10,11]. Since the lowest leak rate had no flammable mass, even without ventilation in the room, there was no need to model Leak 1 further for cases with room ventilation.



**Figure 2.5:** Comparison of the flammable hydrogen envelope (4 - 75%), shown in white, after 150 sec for a leak rate of a)  $2.58 \times 10^{-8}$  kg/s, b)  $1 \times 10^{-5}$  kg/s, and c)  $3 \times 10^{-5}$  kg/s into the Fuel Cell Room with no ventilation (0 ACH). The flammable envelope has a height of 21.2 cm and 38.3 cm for Leaks 2 and 3, respectively.

As shown by the intermediate Leak 2 and maximal Leak 3 cases, the size of the flammable regions increases with the faster release rate. At 150 sec after the leak has started, the mid-range Leak 2 reached a height of 21.2 cm (8.35 inches) and the largest Leak 3 reached 38.3 cm (15.1 inches). Again, these flammable release envelopes are limited in the early stages of release by the local entrained air flow. If these leaks were allowed to run for very long times, in the absence of ventilation, the room eventually fills with hydrogen. We observed that the flammable region is self-limited for ~ 10 minutes before it starts to grow and eventually reach the ceiling and fill the room.

#### 2.5.2: Cases with Ventilation: During the Leak

The two higher leak rates, Leaks 2 and 3, were modeled with four ventilation rates to compare the shape and amount of the flammable mass at a given time. We also examined the time it takes to clear the room after the hydrogen leak has been turned off. The shapes of the flammable regions after 150 seconds of leak can be seen in Figure 2.6. Although the leak is turned on for 150 seconds, the steady-state situation shown in the figures is established very quickly, several seconds after the hydrogen leak is turned on, with only minor fluctuations due to the air currents in the room created by ventilation. As can be seen in Figure 2.6, there is a trend for a smaller flammable region as the ventilation is increased. For a given level of ventilation, the higher leak rate produces a larger flammable region.

Leak	0 ACH	15 ACH	30 ACH	60 ACH	75 ACH
1.0 x 10⁻⁵ kg/s (Leak 2)	1	1	1	1	•
3.0 x 10 <sup>-5</sup> kg/s (Leak 3)					

**Figure 2.6:** Comparison of the flammable mass (4 - 75%) for Leak 2 and Leak 3 at the ventilation rates indicated 150 seconds after leak initiation. Recall that the leak diameter is 4" diameter for scale and the aspect ratio of the images is 1:1, so the horizontal and vertical directions have the same length scale.

Table 2.1 quantifies these findings by providing the maximum height of the flammable region as well as the mass of hydrogen within the flammable envelope after a steady-state has been established within the first few seconds.

**Table 2.1.** Maximum height of flammable region and the mass of hydrogen within the flammable region for Leak 2 and Leak 3 for the Fuel Cell Room ventilation rates indicated. The time of the gas dispersion pattern is 150 seconds after initiation.

	Max Height of Flammable Region (cm)			Mass of Hydrogen Within the Flammable Region (mg)						
ACH	0	15	30	60	75	0	15	30	60	75
1×10⁻⁵ kg/s Leak 2	21.2	17.9	17.5	16.0	15.3	5.8	5.7	5.8	5.1	4.6
3×10 <sup>-5</sup> kg/s Leak 3	38.3	38.7	37.0	33.2	26.6	22.0	23.0	22.0	20.0	17.0

An interesting finding from this work is that both the height and mass of the flammable volume is only modestly affected by the presence of ventilation. For example, for the  $3\times10^{-5}$  kg/s leak, in the absence of ventilation, the flammable region reaches a self-limiting height of 38.3 cm and contains within the flammable volume 22 mg of hydrogen. With the standard 30 ACH, these values are 37 cm and 22 mg, respectively. It is clear that it is the local air entraining described in Figures 2.4 and 2.5 that is limiting the flammable region in the early stages of leak. However, for longer times, for the case where there is no ventilation, the room eventually fills with hydrogen. In contrast, with ventilation, hydrogen is evacuated out of the Fuel Cell Room, preventing the long-term buildup of hydrogen. Thus, the local mixing acts to limit the flammable region for approximately 10 minutes, whereas the active ventilation limits long term buildup of hydrogen.

#### 2.5.3: Cases with Ventilation: After the Leak Is Stopped

After the hydrogen leak was stopped at 150 s, the simulations were run for an additional 300 s to assess the duration and size of the flammable cloud as it is removed by the varying levels of ventilation. In addition, results are presented for hydrogen levels below that which can be ignited, but greater than the threshold detectable by a hydrogen alarm (typically set to detect 1/10 the LFL or 0.4% by volume). For this discussion, "detectable" means greater than 0.4% and less than the 4% LFL. Note: the minimal level that can be detected by modern gas detection technology is vastly lower than 0.4%.

Table 2.2 provides results for the time to clear both the flammable concentrations of hydrogen and the detectable concentrations. For all the cases and ventilation rates, the flammable mass with concentration greater than 4% clears the Fuel Cell Room within 1.5 sec after the hydrogen leak is turned off. Thus, in the event the hydrogen alarm fails in the fuel-cell rack, and the independent ventilation in the fuel-cell rack fails (i.e. a double failure), if the hydrogen alarm in the Fuel Cell Room is triggered and shuts off the hydrogen supply to the rack, the Fuel Cell Room ventilation very rapidly clears the

flammable mass, in less than 1.5 seconds. Two trends are observed, as expected: smaller leaks are cleared faster for a given level of ventilation and for a given leak rate, the room is cleared faster with higher ventilation rates.

How long hydrogen stays in the room above the level that would trigger a hydrogen alarm (i.e. the detectable level) also depends on both the leak rate and the ventilation rate, as shown by Table 2.2. For Leak 2 ( $1 \times 10^{-5}$  kg/s) at the highest ventilation rate of 75 ACH, the detectable mass is cleared in less than 3 seconds. For the higher leak rate of  $3 \times 10^{-5}$  kg/s and the lowest ventilation rate of 15 ACH, detectable hydrogen lingers for 56 seconds.

Leak/ACH	0	15	30	60	75
Leak 2: 1×10 <sup>-5</sup> kg/s (Flammable)	N/A	1.5	1.25	0.99	0.85
Leak 2: 1×10 <sup>-5</sup> kg/s (Detectable)	N/A	7.5	6.6	2.9	2.8
Leak 3: 3×10 <sup>-5</sup> kg/s (Flammable)	N/A	1.5	1.46	1	1
Leak 3: 3×10 <sup>-5</sup> kg/s (Detectable)	N/A	56	19.6	3.4	3.3

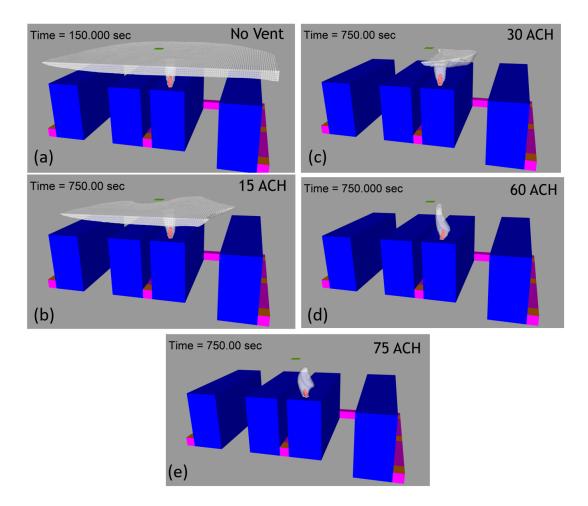
**Table 2.2:** Time to clear out flammable concentrations and detectable concentrations after the hydrogen leak has stopped. Units are in seconds.

#### 2.5.4: The Effect of Ventilation on Hydrogen Alarm Detection

A very important component of hydrogen safety is the use of hydrogen alarms to detect leaks. As discussed above, such monitors are typically set to detect a threshold of 1/10 the LFL or 0.4% by volume. Table 2.2 gives how quickly the detectable mass of hydrogen in the entire Fuel Cell Room is removed by ventilation after the leak is stopped. However, we were also interested in how ventilation affects the pattern of the detectable hydrogen envelope and how this pattern might impact hydrogen detection from a hydrogen alarm fixed to one location.

Figure 2.7 shows five panels giving the spatial behavior of the detectable (but not flammable) hydrogen concentration. The color scheme has been changed so that the hydrogen in the detectable range is colored a transparent white whereas the flammable

range is colored red. Figure 2.7 compares the detectable hydrogen in the room 150 sec after the highest leak rate  $(3 \times 10^{-5} \text{ kg/s})$  starts for all five ventilation cases (0 - 75 ACH).



**Figure 2.7.** Comparison of the effects of different ventilation rates on the detectable (0.4 - 4%) hydrogen (white) and flammable (4 - 75%) hydrogen (red) in the Fuel Cell Room for Leak 3  $(3\times10^{-5} \text{ kg/s})$  150 seconds after leak initiation: a) 0 ACH, b) 15 ACH, c) 30 ACH, d) 60 ACH, and e) 75 ACH. For the cases with ventilation, the leak starts after 600 seconds in order to establish air flow in the room.). Thus, for ventilation, the figure depicts the gas dispersion 150 seconds into the leak, which is 750 seconds into the simulation.

For the case of no ventilation (Fig. 2.7(a)), the detectable hydrogen mass rises, and spreads out over the top of the ceiling. Note that this is for the detectable hydrogen mass, not the flammable mass that was depicted in Figures 2.3 - 2.6, and shown in red in Figure 2.7. Such a leak would be readily detected by a hydrogen monitor placed anywhere on the ceiling of the Fuel Cell Room. As the ventilation is increased to 15 ACH, most of the ceiling is still covered with detectable hydrogen 150 seconds into the leak, although not all of ceiling is covered. For example, a hydrogen monitor located in the top right of the

Fuel Cell Room (Fig. 2.7 (b)) would not detect the leak after 150 seconds. As we progress to 30 ACH, detectable but non-flammable hydrogen is still reaching the ceiling. However, the lateral extent is becoming limited, less likely to be detected by a single hydrogen alarm on the ceiling. For both 60 and 75 ACH cases, the detectable cloud does not reach the ceiling of the room and would not be detected by a hydrogen detector mounted on the ceiling.

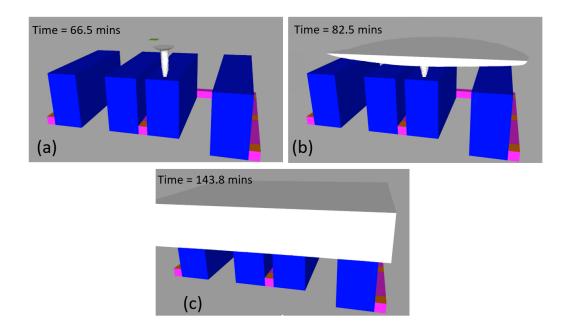
The conclusion from this analysis is that higher ventilation rates might have the unintended consequence of making a leak harder to detect, depending on the placement of the hydrogen alarm, although high ventilation rates would have the positive effect of more rapidly removing hydrogen from the Fuel Cell Room. Since the 15 ACH per hour ventilation rate limits the height of the flammable mass and the overall amount of flammable hydrogen (Table 2.1) in a manner comparable to the higher ventilation rates, while still removing hydrogen (after the leak is stopped) within 1.5 seconds (Table 2.2), a ventilation rate of 15 ACH would still provide hydrogen evacuation while allowing the leak to be detected by the ceiling-mounted hydrogen monitor (for most monitor locations).

It is interesting to note from Figure 2.7 that while the flammable region (indicated in red) is self-limited by the local entrainment of air, as discussed in connection with Figure 2.4, the more diffuse detectable region (indicated in white) is not self-limited. This is due to the fact that the recirculation pattern required for the self-limiting effect requires a high concentration of hydrogen to establish and differentiate the rising hydrogen mass from the surrounding air, thereby establishing the macroscopic recirculation pattern (Fig. 2.4) that self-limits the flammable region at short times, even in the absence of ventilation.

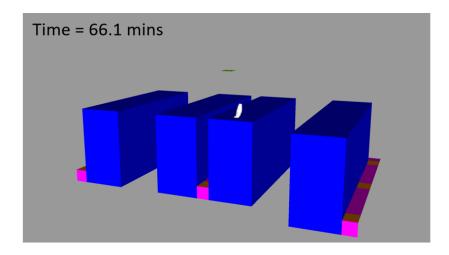
#### 2.5.5: Long Duration Leak

We also compared running the maximal Leak 3 for a longer time, both with no Fuel Cell Room ventilation and with 60 ACH, to make sure we were not focusing on short term effects only in the analyses. The results for no ventilation are shown in Figure 2.8. As expected, the Fuel Cell Room begins to fill with flammable hydrogen. First, it covers the ceiling (Fig. 2.8(a,b)), and then the layer of flammable gas expands downward (Fig. 2.8 (c)).

However, if the Fuel Cell Room is ventilated, the flammable region will reach a steady state size very quickly and will not extend up to the ceiling, or spread out into the rest of the Fuel Cell Room. An example of this for a longer duration hydrogen leak of 66.1 minutes is shown in Figure 2.9.

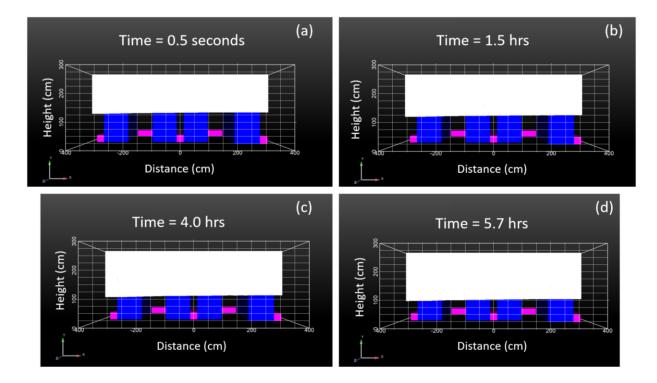


**Figure 2.8.** Flammable (4 - 75%) hydrogen region in white for the case of Leak 3 (3×10<sup>-5</sup> kg/s) with no Fuel Cell Room ventilation at three times during a long-duration leak: a) 66.5 mins, b) 82.5 mins, and c) 143.8 mins.



**Figure 2.9:** Flammable hydrogen region (4 - 75%), in white) for the case of Leak 3 ( $3 \times 10^{-5}$  kg/s) with 60 ACH Fuel Cell Room ventilation at 66.1 minutes into the hydrogen leak.

For the purposes of developing intuition about the behavior of hydrogen releases, we examined the diffusion of hydrogen in the absence of ventilation. First, we start from a point where the hydrogen has filled the upper portion of the room, created by leaving Leak 3 on for 162.2 minutes, then turning the hydrogen leak off. Then, we examine by simulation how the hydrogen, by diffusion, slowly spreads to the remainder of the room. In this way, we can assess the relative contributions of buoyancy (which acts to move the hydrogen up) and diffusion (which acts to move hydrogen in all directions). The result of that calculation is shown in Figure 2.10, with the different panels (a) – (d) showing the flammable hydrogen envelope at the different times sampled.

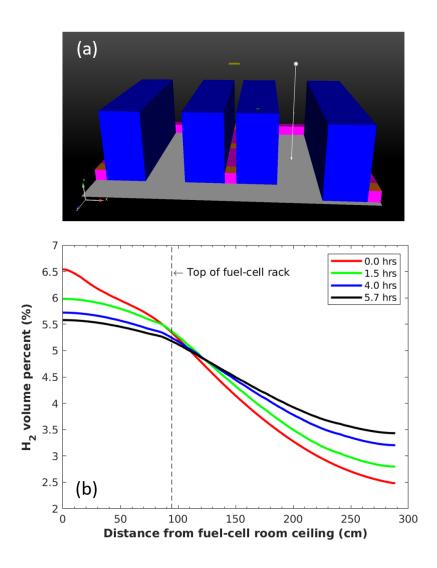


**Figure 2.10.** Flammable hydrogen region (4 - 75%), in white) for the case of Leak 3  $(3 \times 10^{-5} \text{ kg/s})$  having been left on for 162.2 minutes and then stopped with no Fuel Cell Room ventilation. Panels are for (a) 0.5 seconds after the leak is stopped, (b) 1.5 hours after the leak is stopped, (c) 4.0 hours after the leak is stopped and (d) 5.7 hours after the leak is stopped. The lower edge of the white flammable envelope is at 4% in all plots.

At 0.5 seconds after the leak is stopped, the lower edge of the flammable mass is 125.51 cm above floor of the Fuel Cell Room. The hydrogen concentration within this white mass varies from 4 to 32.7% (depending on location), and the flammable hydrogen mass is 285.8 gm. With time, the lower edge of the flammable region extends downward under the action of diffusion.

Figure 2.11 shows the concentration profile from Figure 2.10 at different times along a ceiling-to-floor line as indicated in Figure 2.11(a). Figure 2.11(b) shows that over

the course of ~ 6 hours, hydrogen diffuses out of the white flammable regions of Figure 2.10 near the top of the room, and into regions near the fuel cell room floor located 289.56 cm below the ceiling.



**Figure 2.11:** (a) Location of a vertical line for assessing hydrogen concentrations at different times for the case of Leak 3 ( $3 \times 10^{-5}$  kg/s) with no Fuel Cell Room ventilation, (b) hydrogen concentrations from ceiling (x = 0) to floor (x = 289.56 cm) along the vertical line shown in (a) for 0.5 seconds after the leak is stopped (0 hrs), 1.5 hours after the leak is stopped, 4.0 hours after the leak is stopped and 5.7 hours after the leak is stopped.

## 2.6: Chapter 2 Conclusions

CFD hydrogen gas dispersion modeling for a leak within a hydrogen fuel-cell rack inside a Fuel Cell Room has revealed interesting findings. Analysis of the air flow in the Fuel Cell Room shows that while the overall flow in the room is as one might expect, from bottom to top, in the space in between the tops of the fuel-cell racks and the outlet vent, the flow can be rather chaotic, with velocities of ~ 0.09 m/s, 0.3 m/s, 0.7 m/s and 0.8 m/s for 15, 30, 60, and 75 ACH, respectively. Modeling in the limiting case of no ventilation showed that the flammable region produced by the hydrogen leak is limited by self-induced entrainment of air, caused by the buoyant rising of the hydrogen release. Locally, this effect can be even more influential than the effect of Fuel Cell Room ventilation up to 10 minutes into the release. With no ventilation, the self-limiting effect eventually transits to a situation where hydrogen is filling the Fuel Cell Room.

Modeling results with Fuel Cell Room ventilation activated shows that several seconds after the hydrogen leak is turned on, the flammable region reaches a steady state, with only minor fluctuations due to the air currents in the room created by ventilation. The expected trends are found, namely that for a given leak size, a smaller flammable envelope is found as ventilation is increased. For a given level of ventilation, increasing hydrogen leak rate produces a larger flammable region. The combination of local self-limiting behavior with ventilation develops the following picture: For early times (< 10 minutes), it is the local air entraining and recirculation that limits the flammable region. However, for longer times, with ventilation, hydrogen is evacuated out of the Fuel Cell Room, preventing the long-term buildup of hydrogen. Thus, the local mixing acts to limit the flammable region for approximately 10 minutes, whereas the active ventilation limits long term buildup of hydrogen.

For all the cases and ventilation rates, the flammable mass with concentration from 4 – 75% clears the Fuel Cell Room within 1.5 sec after the hydrogen leak is turned off. Thus, with ventilation, the physical size of the hydrogen leak is very limited (limiting the chances of ignition), and when the leak is terminated (for example by a shutoff valve), the room is cleared very quickly. Thus, in the event of a double failure where the hydrogen alarm fails in the fuel-cell rack, and the independent ventilation in the fuel-cell rack fails, if the hydrogen alarm in the Fuel Cell Room is triggered and shuts off the hydrogen supply to the rack, the Fuel Cell Room ventilation very rapidly clears the flammable mass, in less than 1.5 seconds.

CFD results for the detectable level of hydrogen that would trigger a hydrogen alarm showed that higher ventilation rates have the unintended consequence of making a leak harder to detect, depending on the placement of the hydrogen alarm, although high ventilation rates would have the positive effect of more rapidly removing hydrogen from the Fuel Cell Room. In the extreme, depending upon ventilation configuration as well as placement and number of sensors, it might be possible to have a leak producing flammable mass without triggering a ceiling-mounted hydrogen detector. Since the 15 ACH per hour ventilation rate limits the height of the flammable mass and the overall amount of flammable hydrogen in a manner comparable to the higher ventilation rates, while still removing hydrogen (after the leak is stopped) within 1.5 seconds, a ventilation rate of 15 ACH would provide hydrogen evacuation while allowing the leak to be detected by the ceiling-mounted hydrogen monitor (for most monitor locations). This conclusion applies to the hydrogen leak rates investigated in this report. Larger hydrogen leaks could require larger ventilation rates.

While the flammable region is self-limited by the local entrainment of air, the more diffuse detectable region is not self-limited. This is due to the fact that the recirculation pattern required for the self-limiting effect requires a significant concentration of hydrogen to establish and differentiate the rising hydrogen mass from the surrounding air, thereby establishing the macroscopic recirculation pattern that self-limits the flammable region at short times, even in the absence of ventilation.

Calculations show that for a room partially filled with hydrogen, over the course of ~ 6 hours, hydrogen diffuses out of the white flammable regions near the top of the room, and into regions closer to the fuel cell room floor.

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# **Chapter 3: Bunkering**

# 3.1: Introduction:

In order to apply appropriate safety measures during the bunkering (fueling) of hydrogen fuel-cell vessels at ports, possible leak scenarios that could occur during bunkering need to be understood. One of these scenarios is a leak occurring in the flexible hose connecting the refueling truck (also called a refueling trailer) to the vessel. Here model simulation is used to understand some general characteristic of the hydrogen plume that can result for a variety of hose-related leaks when a hydrogen boat is being refueled from a HP hydrogen transport truck. Several variable hydrogen leak parameters are explored, including the diameter of the leak, the location of the leak along the fueling hose, the leak orientation, and ambient temperature. Initially, we predict the general shape of the flammable (but un-ignited) plumes that would result from such leaks.

The hydrogen releases out of the Vent Mast in Chapter 1, and the leaks out of the Fuel Cell Rack in Chapter 2, could only have been ignited if an explicit ignition source (e.g., match, spark, etc.) had been placed within the flammable envelope of those releases. This is because they were low-pressure releases, below the ~ 40 bar threshold required for spontaneous ignition [1]. However, a leak during fueling of a HP vessel tank to 250 bar will typically be above the 40-bar threshold and can potentially spontaneously ignite. To cover this possible ignition, we predict not only the flammable hydrogen envelope associated with a hose leak, but also the flame profile that results from ignition along with the radiant heat flux emanating from the flame. This study therefore provides insight into the range of possible hose leaks and associated risks that could occur during hydrogen vessel bunkering using HP hydrogen gas.

# 3.2: Modeling Tools:

Two Sandia modeling tools were used to perform these analyses: MassTran and HyRAM.

# 3.2.1: MassTran:

The pressure and temperature of the hydrogen at the various leak locations was calculated using Sandia's network flow modeling tool, MassTran [2]. This code can be used to analyze fully compressible, transonic flows up to high Mach numbers in pipes and networks, and has been rigorously validated for similar applications at Sandia. It is the same software tool that was used in our Chapter 1 studies of hydrogen dispersion from Vent Mast releases.

An example of a hydrogen transport truck is shown in Figure 3.1.



**Figure 3.1:** IGX 350 bar refueling trailer in use at the San Francisco International Airport to refuel hydrogen fuel cell mobile lights, July 23, 2013. *Photo Credit: Lennie Klebanoff.* 

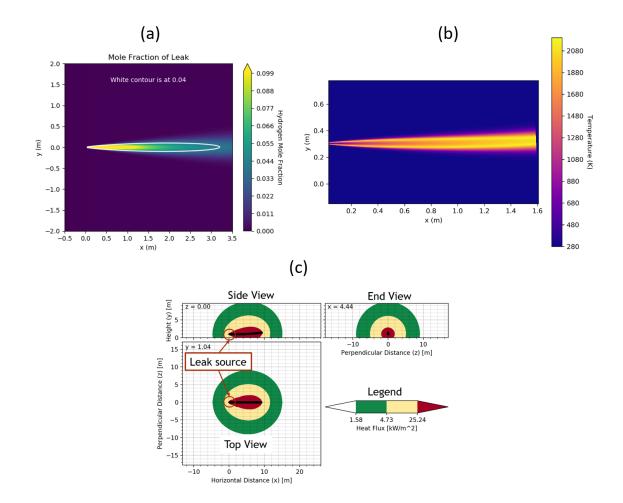
These refueling trailers typically perform "cascade fills" of a customer hydrogen tank. In a cascade fill, the first trailer tank (initially at 350 bar) is opened to the customer hydrogen tank (initially near 0 bar). When the pressure equilibrates, the first trailer tank (now at the lower equilibrium pressure) is valved off and the next trailer tank (at 350 bar) is opened. This procedure is repeated until the customer tank is at the desired pressure, or all the trailer hydrogen tanks have been opened.

This cascade-fill process was deemed too complicated to directly model. Instead, we chose a refueling scenario in which one large hydrogen tank on the refueling truck is used to fuel (by pressure equalization) a much smaller hydrogen tank onboard the vessel via a high-pressure hose. In the absence of leaks, Mass Tran predicts the pressure and temperature of the hydrogen gas in the trailer tank, in the tank aboard the vessel (the boat tank) and in the hose at a given time. This "no-leak" scenario allows us to study how fast a boat tank can be filled before exceeding the 85 °C temperature limit of Type IV tanks. Subsequently, circular holes are introduced at varying positions along the length of the hose to mimic hose leaks. Given this geometry, along with the initial conditions of the leak size and the starting pressures and temperatures in the tanks, MassTran can calculate the pressure and temperature of the hydrogen leaking from the hose at a given time.

The leak temperature and pressure results from MassTran are then input into HyRAM, which calculates the hydrogen plume issuing from the leak as well as the potential flame that could result from either the presence of an explicit ignition source, or from spontaneous ignition. Note that HyRAM is not a CFD calculation.

#### 3.2.2: HyRAM:

Sandia's "Hydrogen Risk Assessment Models (HyRAM) package is a software toolkit that provides a basis for quantitative risk assessment and consequence modeling for hydrogen infrastructure and transportation systems" [3]. Along with the risk assessment, it also provides a "physics mode" where the user can input a single leak case to evaluate the hydrogen plume dispersion of an unignited leak, as well as the temperature of the jet flame and associated radiative heat flux that results if ignition occurs [4, 5]. A generic example of the plume dispersion of an unignited leak is shown in Figure 3.2(a).



**Figure 3.2** (a) Generic example of hydrogen plume dispersion from a leak located at x = 0 showing the mole fraction of hydrogen. In this case, the release is horizontal, (b) a flame plot from HyRAM showing the temperature around the visible flame length if the hydrogen release in panel (a) were to be ignited at the source of the leak and (c) a generic example HyRAM heat flux plot resulting from the flame of panel (b). The black line represents the centerline of the visible flame, with the leak source at the left end. The top left plot shows a Side View of a vertical slice at the plane of the leak. The top right plot shows a End View of a vertical cross-cut of the flame at

about half the length of the flame. The bottom left plot shows a Top View of a horizontal cut at the height of the leak source.

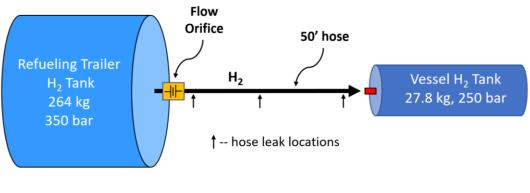
Gravity and buoyancy are included in this model, however wind and any impingements on structures (like walls) are not [6]. The gas plumes are modeled using the Birch plume model [7] and the Able-Nobel equations of state. Figure 3.2(a) (and those like it) shows the molar concentration of hydrogen in air (equivalent to concentration by volume) emanating from a generic leak. Within the enclosed interior region of the white contour lies molar concentrations from 4 % - 100 %. Note that hydrogen cannot ignite for concentrations greater than 75%, so the white contour actually overestimates the flammable region.

Since the backing pressure behind the leak will typically be greater than the  $\sim 40$  bar required for spontaneous ignition [1], spontaneous ignition is possible for these leaks, even in the absence of an explicit ignition source. HyRAM can calculate both gas temperature and a heat flux that would result in the case of ignition of a hydrogen plume. Generic temperature and radiative heat flux plots are shown in Figure 3.2(b) and Figure 3.2(c), respectively for the same generic leak case that was shown in Figure 3.2(a). It can be noted that the flame lengths are typically shorter than the unignited flammable plume and that they are more buoyant because of their higher temperatures. The temperature and radiative heat flux plots show the visible flame length, which is calculated based on the Froude number, hydrogen density, leak orifice, and the velocity of the leak [8, 9]. The steady state calculation does not consider gas thermal conduction, only radiative heat transfer.

The green, yellow, and red ranges in the heat flux plots (Fig. 3.2 (c)) are consistent with NFPA 2. The American Petroleum Institute (API) Standard 521 classifies as  $1.577 - 4.73 \text{ kW/m}^2$  (green region) as the "no-harm' range, with  $4.73 \text{ kW/m}^2$  being the "the heat flux threshold to which personnel with appropriate clothing can be continuously exposed." This is slightly less than the Society of Fire Protection Engineers value of 5.0 kW/m<sup>2</sup> that is the threshold heat flux to which people can be exposed for prolonged periods of time and begin to suffer a burn injury. API 521 defines  $4.732 \text{ kW/m}^2$  (yellow region) as the heat flux threshold in areas where emergency actions lasting several minutes might be required by personnel without shielding but with appropriate clothing, and by the International Fire Code (IFC) as the threshold for exposure to employees for a maximum of 3 minutes. IFC defines  $25.237 \text{ kW/m}^2$  (red region) the exposure limit for non-combustible equipment.

#### 3.3: Problem Specification:

As discussed previously, we chose a refueling scenario in which one large hydrogen tank on the refueling trailer is used to fuel (by pressure equalization) a much smaller hydrogen tank aboard the vessel via a high-pressure hose with theoretical holes for varying leak positions along the hose length. The details of the arrangement, based on guidance from the Brain Trust, are shown in Figure 3.3.



(not to scale)

Figure 3.3: Fueling scenario for hose leak calculations. The diagram is not to scale.

The refueling trailer hydrogen tank is assumed to have a water volume of 11451 L, giving 264 kg of hydrogen storage at 350 bar pressure. With information provided by the hydrogen refueling company IGX [10], the hose was assumed to have a 0.5" outer diameter, with a 0.4" inner diameter (ID) (0.0102 m ID) and a length of 50 feet. The 250 bar Type IV tank on the vessel (boat) is assumed to have the same water volume, 1544 L, as one of the high-pressure hydrogen tanks considered in the Chapter 1 modeling of Vent Mast releases. Recall that such a tank holds 27.8 kg of hydrogen at 250 bar. The large truck hydrogen tank was sized big enough to fill the boat tank completely without a "cascade fill." The fueling tank starts with a pressure of 350 bar, and the empty boat tank being filled is initially at 15 bar, since typically some hydrogen is left in such tanks before they are refilled. The tanks and hoses are modeled including the heat transfer through their walls, as described previously [11].

The hydrogen refueling needs to be compatible with the temperature limits of Type IV composite hydrogen tanks. This means that as hydrogen flows from the refueling trailer to the vessel tank and the gas in the vessel tank heats up due to compression, that gas temperature is prevented from exceeding 85 °C (185 °F). At a vehicular hydrogen station, hydrogen pre-cooling helps mitigate the compression heating, allowing fast fill times. However, pre-cooling of hydrogen is not yet possible for mobile fueling from a hydrogen trailer. This sensitivity to tank temperature is in the spirit of hydrogen refueling protocol J2601 for light duty vehicles [12], although the quantities considered here for the maritime application are considerably higher than the ~ 5 kg relevant to light-duty vehicles. Consequently, no marine hydrogen fueling protocols exist. This flow constraint is achieved using a flow orifice, as shown in Figure 3.3. This

fueling rate information will be of interest for those constructing the first hydrogen vessels and needing to know how fast they can fill their HP hydrogen tanks, and hopefully contribute to the development of marine fueling protocols involving larger hydrogen quantities.

We offer a word of caution regarding Figure 3.3. The refueling scenario was constructed for computational convenience. In a real hydrogen fueling scenario, one would not directly connect a large 350 bar hydrogen tank to a smaller 250-bar rated hydrogen tank out of concern for over-pressurization of the smaller tank. Instead, some means of pressure regulation would be used in between the two tanks and there would be PRDs placed in communication with the vessel tank. These complications were not considered in our modeling work, as we wished to examine some very general aspects of the hydrogen bunkering of vessels. These aspects include how rapidly the Type IV tanks can be fueled with hydrogen and still be kept below the 85 °C (185 °F) limit, the extent of hydrogen plumes from leaks, and the form of jet fires that result if the plumes are ignited.

As suggested in Figure 3.3, three locations along the hose length were simulated: 1 meter from the refueling truck, the middle of the hose, and one meter from the boat tank being filled. We also investigated how the leak size affects the released hydrogen plume. All leaks are assumed to have a circular orifice with a given diameter as given in Table 3.1. The largest leak diameter is 0.005 m, or 0.2 inches, which mimics a large gash in the hose, namely 49% of the hose ID. The other leak sizes are based on IEC standards [13], which characterize set-back distances required based on leak sizes. The smallest leak size, 1% by diameter of the hose, could be considered a "pin prick."

The filling of the vessel hydrogen tank is a dynamic process, with the conditions (temperature, pressure) changing as the hydrogen is transferred from refueling trailer tank to the boat tank. Unless otherwise stated, the leak calculations are reported after 1 second into the fueling scenario for a vessel tank initially at 15 bar. The hose is initially at the pressure of the refueling trailer tank. However, the hose pressure drops quickly as the refueling hose is opened to the boat tank by opening a valve, since there is a flow restrictor present.

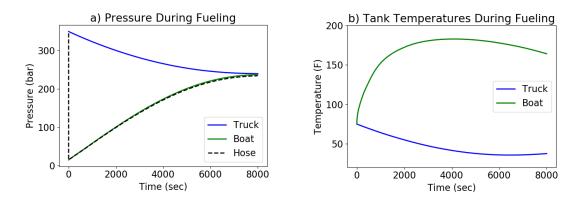
	1% by diameter "pinprick"	Diameter For: 1% by area	Diameter For: 10% by area	Diameter "gash"
Meters	0.0001	0.001	0.0032	0.005
Centimeters	0.01	0.10	0.32	0.50
Inches	0.004	0.04	0.13	0.2

Table 3.1: Leak diameter in meters, centimeters and inches

The ambient air conditions in which the plume is established for most of the simulations were set to have a pressure of 1.01325 bar and 75° F (297 K). The temperature for one case was changed to represent a hot day,  $110^{\circ}$  F (316.5 K), and for another case a cold day,  $-10^{\circ}$  F (250 K). The hydrogen in both the refueling truck and vessel tanks was assumed to be the same temperature as the ambient, although the temperature of the gas will change as it is released from the refueling truck tank and expands in the hose, initially at ambient pressure. The initial pressure of the tank on the boat was sequentially increased to represent a leak occurring at different times during the fueling process, with 15 bar, 125 bar and 240 bar being assumed. All of the HyRAM inputs for the leak were taken 1 second into the fueling process for all of the plume, fire, and heat flux calculations.

#### 3.4: Pressure and Temperature Results

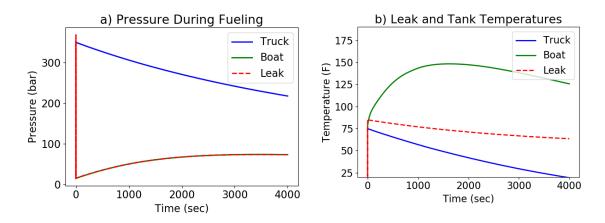
Results for the baseline case of no hose leaks and fueling from the large Refueling Trailer hydrogen tank to the smaller Vessel hydrogen tank on-board the boat are shown in Figure 3.4. Since the refueling rates for tanks this size have not been measured in practice, but will be used on the first hydrogen vessels, these results provide guidance on how fast these tanks can be safely filled while keeping the gas temperature under 85 °C (185 °F). Fueling for a large refueling trailer tank mimics the maintenance of high pressure in a trailer as the cascade proceeds, switching to 350 bar tanks as earlier tanks are emptied.



**Figure 3.4:** (a) Pressure plotted versus time for the interior tank pressures for the hydrogen tank on the refueling truck, on the boat, and inside the hose near the end close to the boat during fueling; (b) Hydrogen gas temperature plotted versus time for hydrogen inside the tank on the refueling truck, and for hydrogen inside the tank on the boat being refueled. The figure assumes no leak from the hose. The water volume of the tank on the boat is assumed to be 1544 L. The fueling tank on the refueling trailer was sized big enough to fill the boat tank completely without a "cascade fill", and is assumed to be 11451 L, consistent with Figure 3.3

The initial pressure in the refueling (trailer) tank is 350 bar and the initial pressure in the refueling hose is also assumed to be 350 bar. As can be seen in Figure 3.4, the pressure in the hose drops to match the pressure in the vessel. The vessel (boat) tank is initially at 15 bar, a residual pressure typically required by refueling services, so a completely empty vessel tank is not being filled. In order to keep the temperature in the boat tank below the required 85 °C (185 °F) [14], the flow out of the fueling tank was restricted with a 0.0005 m diameter orifice. This resulted in a maximum mass flow rate of 0.005 kg/s. Because of this restriction, the pressure in the hose during the fill is very close to the pressure in the tank on the boat. Our results indicate a single boat tank (of the type considered here) can be safely refilled to 250 bar in ~ 2 hours (7200 seconds) with the tank temperature not exceeding 85 °C (185 °F).

Pressure and temperature results when a 0.001 m diameter hose leak is introduced 1 meter from the trailer fueling tank are shown in Figure 3.5. With the presence of the leak, the tank on the boat does not reach the desired 250 bar and instead only reaches  $\sim$  80 bar. Due to the reduced final pressure, the temperature of the boat hydrogen tank only reached  $\sim$  150 °F (65.5 °C). Like the case without the leak (Figure 3.4), the pressure in the hose at the location of the leak is very close to that of the tank being filled.



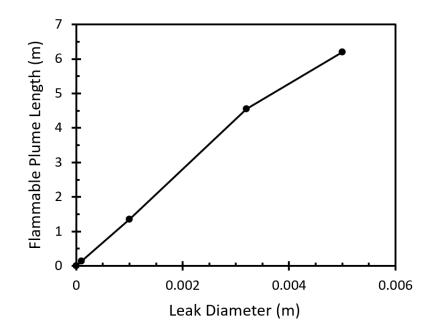
**Figure 3.5:** a) Pressure plotted versus time for the interior tank pressures for the hydrogen tank on the refueling truck, on the boat, and inside the hose at the position of the leak during fueling; (b) Hydrogen gas temperature plotted versus time for hydrogen inside the tank on the refueling truck, inside the tank on the boat being refueled, and in the hose at the leak position. The results are for the 0.001 m leak located 1m from the fueling tank on the truck.

# 3.5: Flammable Leak Plume Results

HyRAM was used to calculate the length and shape of the hydrogen plume within the flammable range (4% or higher) which indicates how far away from the leak source that hydrogen could ignite. All of the plume length figures are presented in Chapter 3 Appendix A. The results for the case 1 second into the hydrogen refueling are tabulated in Table 3.2 with a specific example plotted in Figure 3.6. No wind is assumed in all hose release calculations.

**Table 3.2:** Length of flammable hydrogen envelope (4% or higher) for three leak locations along the hose when the initial tank on the boat is at 15 bar and the Refueling Truck Tank pressure is initially at 350 bar. The leak is established 1 second after the refueling has commenced.

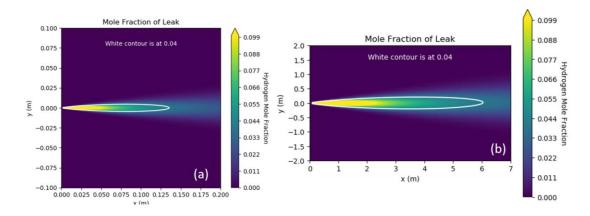
Leak Location	Plume Length 0.0001 m dia.	Plume Length 0.001 m dia.	Plume Length 0.0032 m dia.	Plume Length 0.005 m dia.
1 m from boat	0.14 m	1.35 m	4.25 m	6.5 m
Center of hose	0.14 m	1.35 m	4.55 m	6.2 m
1 m from trailer	0.14 m	1.38 m	4.20 m	6.0 m



**Figure 3.6:** Length of the hydrogen plume within the flammable range (4% or higher) from a leak in the center of the hose. For this calculation, the initial vessel hydrogen tank is at 15 bar, and the fueling trailer hydrogen tank is initially at 350 bar.

As can be seen from Table 3.2 and Figure 3.6, smaller diameter leaks produce smaller plume lengths, all other things being equal. In this configuration with the limited flow rate, the pressure in the hose is nearly the same as the downstream pressure in the tank being filled (close to 15 bar). Therefore, there is little change in the size of the plume as a function of the location along the hose. Auxiliary calculations that were performed without limiting the flow in this way resulted in larger plume length variations with the location of the location be hose.

Figure 3.7 shows the predicted plumes, from the smallest plume (Figure 3.7 (a)) to the largest plume (Figure 3.7 (b)) for the conditions of Table 3.2 and Figure 3.6. Figure 3.7(a) is for the 0.0001 m dia. "pinprick" hose leak located near the boat, versus Figure 3.7 (b) which is for the 0.005 m dia. "gash" leak located near the refueling truck.

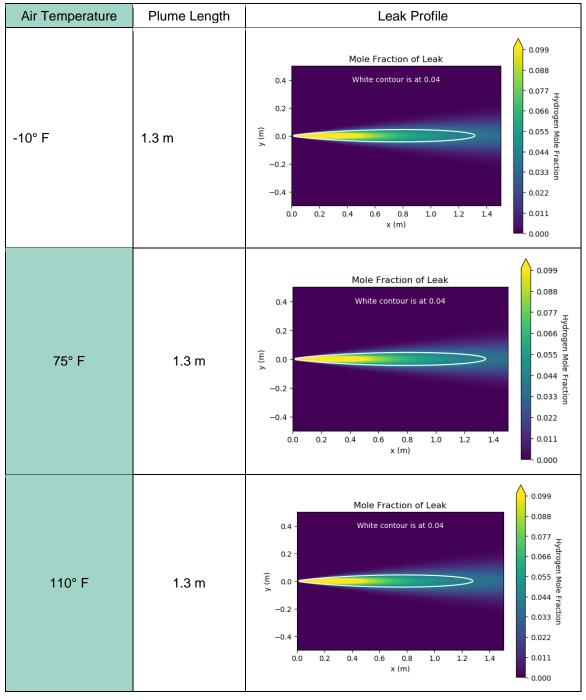


**Figure 3.7:** Calculated plume lengths for (a) the smallest (near boat, diameter = 0.0001 m) to the (b) largest (near truck, diameter = 0.005 m) flammable plume. Note the large change in the plume length scale between these two figures.

The large (0.005 m dia.) leak would only be produced by a hose break which, while possible, is unlikely. In addition, hydrogen hoses have a "break away" feature installed that would limit hydrogen escape in the event of a hose break. The very small (0.0001 m dia.) pinprick leaks are more likely, which could be produced by a defect in the hose, or a problem with the hose connections. In this case, the flammable hydrogen plume emanating from the hose 1 second into the refueling is ~ 13 cm long. The Chapter 3 Appendix gives the flammable plume length for the different combinations of leak size, location and when during the refueling the leak occurs.

The effect of ambient air temperature on plume length was also examined, to explore differences if the leak occurred on a hot or a cold day. Table 3.3 shows that the ambient air temperature has a negligible effect.

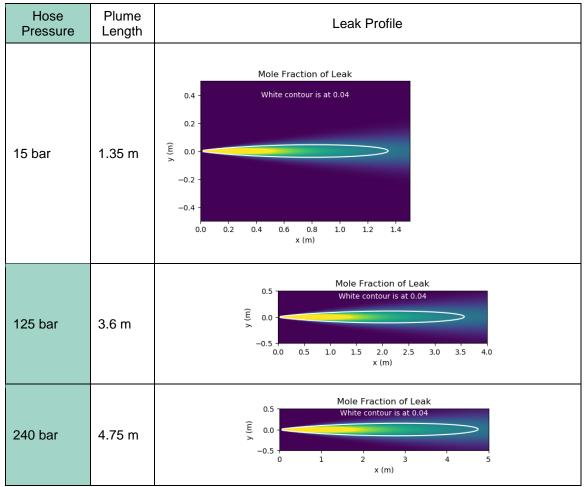
**Table 3.3:** Effect of ambient air temperature on plume length. Leak at hose center. Fueling tank at 350 bar and vessel tank is at 15 bar. Leak diameter of 0.001 m. Leak is established 1 second after the start of refueling.



If a leak in the refueling hose occurs, it could occur anytime during the refueling. If the leak occurs very early in the refueling (Tables 3.2, 3.3 and Figures 3.6, 3.7), the hose pressure will be low (near 15 bar). If the leak occurs in the middle of the fill, the pressure in the hose will be near 125 bar. Towards the end of the fill, the pressure in the hose will

be near 250 bar. Thus, the backing pressure driving the leak could be anywhere from 15 bar to 250 bar, and this pressure will have a significant effect on the length of the plume, with increasing pressure resulting in longer flammable plume lengths.

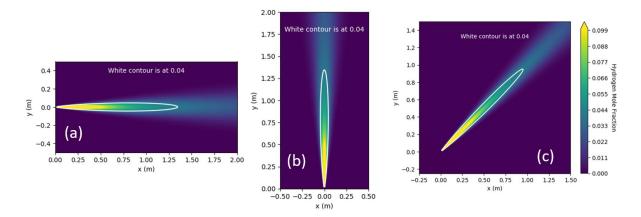
The effect of backing pressure can be seen in Table 3.4, which shows that a 0.001 m diameter leak in the center of the hose, right at the start of boat tank filling (15 bar), will have a flammable plume length of 1.35 m. This is the same result as shown in Table 3.3. Towards the end of the fill, when the tank pressure is at 240 bar, the flammable plume length increases 3.5-fold to 4.75 m. It is interesting that, although the leak backing pressure (i.e., the hose pressure) increases 240/15 = 16 times, the plume length increases only 4.25/1.35 = 3.15 times. This is because the flow through the leak hole is choked, producing the observed non-linearity with backing pressure.



**Table 3.4:** Effect of leak backing pressure on plume length. Leak at hose center. Ambient temperature 75° F. Leak diameter of 0.001 m. Note the changing length scales.

#### 3.6: Variation with Leak Direction:

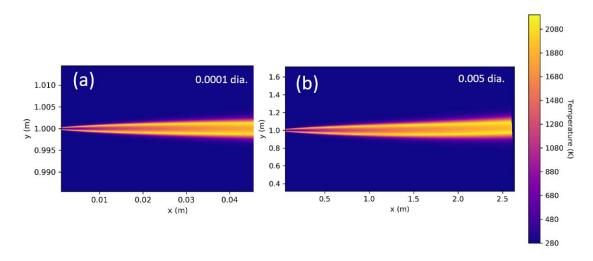
To investigate the effect of orientation on the flammable plume lengths, three release directions were examined: horizontal, vertical, and at a 45° angle. For all orientations, the calculations were performed for the leak case at the center of the hose with a 0.001m diameter leak orifice for an initial boat hydrogen pressure of 15 bar, giving a hose pressure of 15 bar. The results are shown in Figure 3.8. The orientation of the leak has little effect on the length or width of the flammable region produced by the leak because the plume is momentum dominated in these cases. Gravity is in the negative y direction for all plots.



**Figure 3.8:** Plume length for leak at hose center; ambient temperature 75° F; filling tank pressure 350 bar; vessel tank pressure 15 bar; leak diameter of 0.001 m. Release direction is (a) horizontal, (b) upward (vertical) and (c) 45° upward. Gravity points in the negative y direction for all plots.

## 3.7: In the Event of Ignition: Flame Length and Heat Flux

Ignition of a flammable hydrogen cloud issuing from a leak can be caused by explicit ignition from an ignition source (spark, hot surface) or from spontaneous ignition if the backing pressure behind the leak is greater than 40 bar [1], which it can be depending on if the leak occurs during the early stages of tank filling (low pressure) or later stages (higher pressure). Assuming the plumes described thus far are ignited, the resulting flame lengths can be taken from the HyRAM temperature plots. An example is shown in Figure 3.9 with results tabulated in Table 3.5.

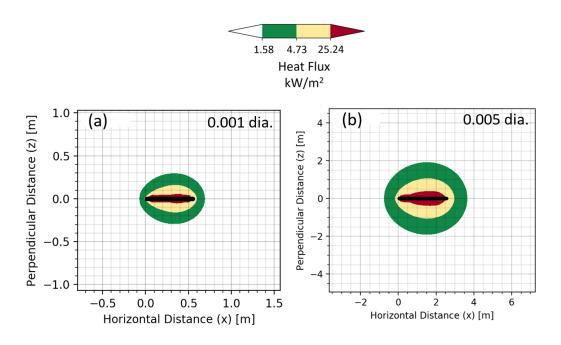


**Figure 3.9:** Temperature and length comparison for (a) the 0.0001m diameter leak and (b) the 0.005 m diameter leak. Leaks are located at the center of the hose Note the large change in length scale for these two figures. The refueling trailer tank pressure is initially 350 bar and the hose and vessel tank pressure are initially 15 bar.

<b>Table 3.5:</b> Flame Length in meters with ambient temperature 75° F; filling tank pressure 350
bar; vessel tank pressure 15 bar.

Leak	Flame Length:	Flame Length:	Flame Length:
Location	0.001 m dia.	0.0032 m dia.	0.005 m dia.
1 m from boat	0.60 m	1.70 m	2.60 m
Center of hose	0.55	1.85	2.55
1 m from truck	0.58	1.70	2.500

The flame lengths are about 40% shorter than the flammable (but unignited) plume lengths. The reason for this is that for the case if ignition, the hydrogen is being consumed by the combustion to non-combustible products as it exits the leak. Thus, the "flammable region" is truncated by burning for the ignited flame case relative to the analogous unignited hydrogen plume.

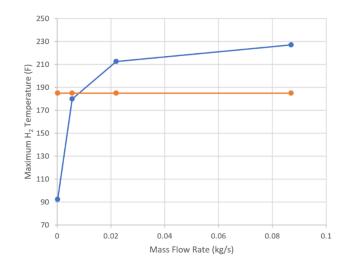


**Figure 3.10:** Comparison of the heat flux for 0.001 m dia. (a) and the 0.005 m dia. (b) leaks located at the center of the hose. These are "top views" of the thermal map. The refueling trailer tank pressure is initially 350 bar and the vessel tank pressure is initially 15 bar.

Figure 3.10 shows that the size of the leak will have a large influence in size of the area where it would be harmful to be in the event of an ignited leak. For the leak diameter of 0.001 m, the area of danger (shown in yellow and red) would be about half a meter from the leak source. However, for a gash in the hose (0.005 m), there would be a burn hazard out to 3.5 meters downstream from the ignited leak. The hazardous zone (red, yellow) where one can suffer a skin injury is generally elliptical but is approximately the size of the length of the jet flame rotated in 3D space about its midpoint.

# 3.8: Hydrogen Mass Flow Rate to Limit Tank Temperature During Cascade Refueling

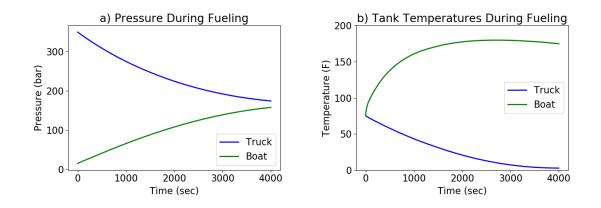
As determined by Figure 3.4, one of the 27.8 kg capacity boat hydrogen tanks can be refueled from a much larger 350 bar refueling trailer tank in ~ 2 hours while keeping the boat tank temperature below 85 °C (185 °F). This requires limiting the hydrogen mass flow rate to 0.005 kg/hr. In a real cascade fill, the first trailer hydrogen tank is opened to the customer tank, and these two tanks may be more similar in size. Here we consider the scenario where the fueling tank on the truck is the same size as the boat tank, and the filling would be done in a cascade with many (15) tanks on the refueling truck. Using MassTran, we examine the hydrogen transfer in the first cascade fill step, where we assess hydrogen transfer from the first truck tank set at 350 bar and the empty boat tank starting at 15 bar. A range of what the maximum gas temperature in the boat tank would be as a function of the mass flow rate is shown in Figure 3.11. This figure shows that for the case of equally sized tanks, the mass flow rate would have to be limited to 0.0056 kg/s.



**Figure 3.11:** Plot of the temperature of the hydrogen gas inside the boat tank versus maximum hydrogen mass flow rate. To keep the temperature in the tank less than 185 °F (orange line) the mass flow rate needs to be 0.0056 kg/s or lower. The hydrogen tank on the refueling trailer is assumed to be the same size as on the vessel, with 27.8 kg capacity. Mass flow rate was regulated with a variable size valve.

This number corresponds well with the 0.005 kg/sec mass flow limit determined in connection with Figure 3.4. This makes sense since ultimately, the temperature of the boat tank is determined by the mass flow rate into it, regardless of the type (small or large) on the refueling truck. The size of the first tank in the cascade fill from the refueling truck determines how much hydrogen is transferred in the pressure equalization.

The pressure and temperature of the refueling truck and boat tanks during the hydrogen transfer is shown in Figure 3.12. To keep the boat tank temperature below 185  $^{\circ}$ F, the refueling needs to be conducted over 4000 seconds, or ~ 1 hour. Note that the boat tank is filled only to ~ 150 bar in this first step of the cascade fill.



**Figure 3.12:** Pressure and Temperature for the filling of a boat tank from the same size tank on the truck.

Since the boat tank is being filled to only ~ 150 bar, less hydrogen is being transferred. Therefore, the time to transfer this reduced amount of hydrogen can be reduced while still holding to the 0.0056 kg/sec mass flow limit required to keep the boat tank temperature below 85 °C (185 °F).

#### 3.9: Chapter 3 Conclusions

Calculations were conducted of refueling a marine hydrogen vessel HP hydrogen tank (at 250 bar) with a 350-bar mobile hydrogen refueling trailer. The calculations show that a 250 bar, 27.8 kg capacity Type IV composite tank can be fully fueled at a maximal rate of 0.005 kg/second so that the temperature of the Type IV tank remains below 85 °C (185 °F), resulting in a tank fueling time of ~ 2 hours with fueling from a large refueling truck tank. We also considered the first step of cascade refueling, examining hydrogen transfer to the same boat tank from a trailer tank of equal size. In that case, the boat tank is incompletely filled in that first step, achieving a final pressure of ~ 150 bar. That first step can be accomplished in about 1 hour and still keep the hydrogen temperature in the boat tank to 85 °C (185 °F). Of course, if pre-cooled hydrogen were available, for example from a hydrogen station, the fueling rate could be increased, but pre-cooled hydrogen is not yet available on mobile HP hydrogen refueling trailers.

If a leak appears in the refueling hose, there is the problem of not being able to properly fill the marine tank due to the pressure reduction. Beyond this, there is the safety concern associated with the hose hydrogen leak. When the flow of hydrogen is restricted by a flow orifice (to limit the mass flow rate to keep the boat tank temperature below 185 °F), the pressure in the hose after the flow restrictor is the same all along the

length, so the hydrogen plume issuing from the leak is nearly the same whether the leak is located at the trailer end of the hose or the boat end of the hose.

Varying the leak size in the calculation shows that larger leaks produce longer flammable hydrogen plumes. Plume lengths varied from 0.13 m to 6 m long for the smallest (0.0001 m diameter) to the largest (0.005 m diameter) leaks. The flammable leak profile did not depend significantly on the temperature of the ambient air or the orientation (vertical, horizontal, angled) of the leak.

The pressure backing the leak increases as the fueling takes place, and the pressure starts off from 15 bar (the residual pressure in the boat tank before refueling) and increases to 250 bar. This increase in backing pressure increases the length of the flammable plume, but not linearly with pressure because the flow through the leak is choked.

If the hydrogen plume were to ignite, either explicitly by an ignition source or by spontaneous ignition for pressures above 40 bar, the length of the flame is only 40% that of the flammable plume. If ignited, such a jet flame creates around it a zone of exclusion that would create a burn injury if a person was within the zone. This zone is generally elliptical but is approximately the size of the length of the jet flame rotated in 3D space about its midpoint.

# 3.10: Chapter 3 References

1. L.E. Klebanoff, J.W. Pratt and C.B. LaFleur, "Comparison of the Safety-related Physical and Combustion Properties of Liquid Hydrogen and Liquid Natural Gas in the Context of the SF-BREEZE High-Speed Fuel-Cell Ferry," Int. J. of Hydrogen Energy **42** (2017) 757 - 774.

2. R. Bozinoski, "*MassTran (v0.19.1) Theory Guide,*" Sandia National Laboratories, Livermore, CA, 2019. Sandia Report: SAND2019-7163.

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4. B.D. Ehrhart, C. Sims, E. Hecht, A.B. Muna, K.M. Groth, J.T. Reynolds, M.L. Blaylock et al., *HyRAM (Hydrogen Risk Assessment Models), Version 3.0*, in *Sandia National Laboratories, Albuquerque, NM*. 2020, software available at <a href="http://hyram.sandia.gov">http://hyram.sandia.gov</a>.

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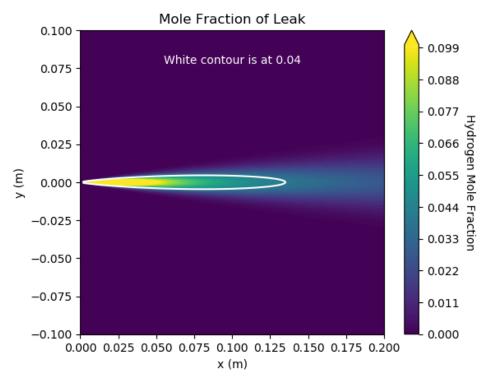
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8. A. Molina, R.W. Schefer and W. G. Houf, "*Radiative Fraction and Optical Thickness in Large-scale Hydrogen-jet Fires*," Proceedings of the Combustion Institute, **31** (2007) 2565–2572.

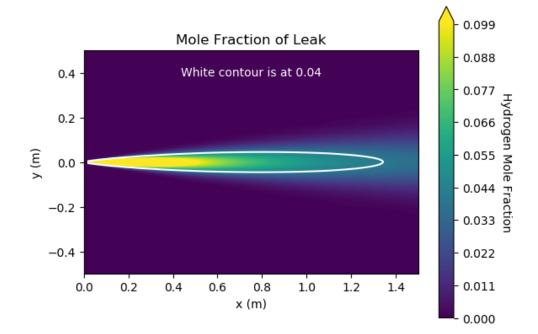
- R.W. Schefer, W.G. Houf, B. Bourne and J. Colton, "Spatial and Radiative Properties of an Open-flame Hydrogen Plume," Int. J. of Hydrogen Energy 31 (2006) 1332-1340.
- 10. Private communication from D. Leighton (IGX) to L.E. Klebanoff on 11/2/2020.
- 11. R. Bozinoski and W. Winters, Netflow Theory Manual. 2016. SAND2016- 0515R.
- 12. A description of the J2601 Fueling Protocol can be found at: https://www.energy.gov/sites/prod/files/2014/03/f10/webinarslides\_h2\_refueling\_ protocols\_022213.pdf
- 13. IEC 60079-10-1 "Explosive atmospheres –Part 10-1: Classification of areas Explosive gas atmospheres." Edition 2.0 2015-09
- 14. Private communication from Kevin Harris (Hexagon) to L.E. Klebanoff.

# 3.11: Chapter 3 Appendix 3A: Plume Figures

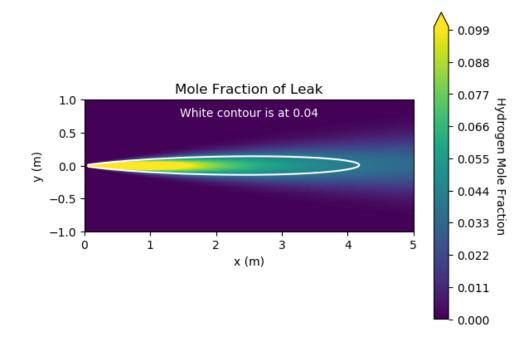
The unignited dispersion plume figures are presented here. The filling tank initial pressure is 350 bar. The empty tank on the boat has a pressure of 15 bar. The initial temperature of the hydrogen and the ambient temperature are 297 K (23.9 °C, 75 °F). The time that the leak occurs is 1 second after the fueling has started.



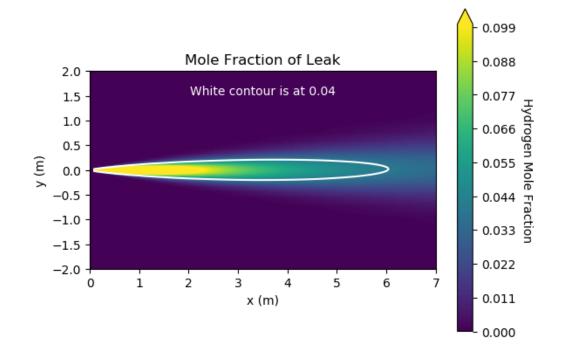
**Figure 3A1:** Diameter = 0.0001m; 1 meter from truck



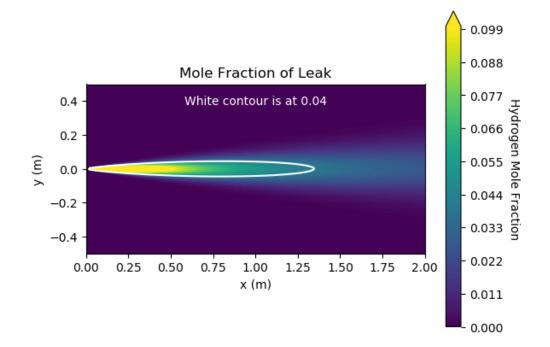
**Figure 3A2:** Diameter = 0.001m; 1 meter from truck



**Figure 3A3:** Diameter = 0.0032m; 1 meter from truck



**Figure 3A4:** Diameter = 0.005m; 1 meter from truck



**Figure 3A5:** Diameter = 0.001m; 25 feet from truck (center of hose).

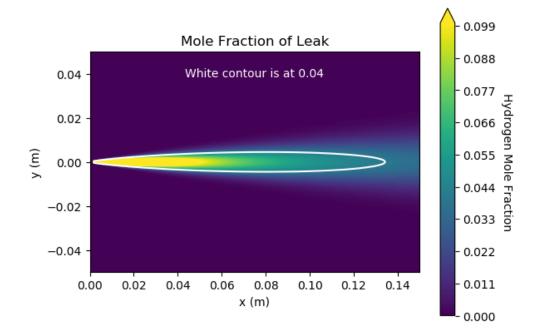
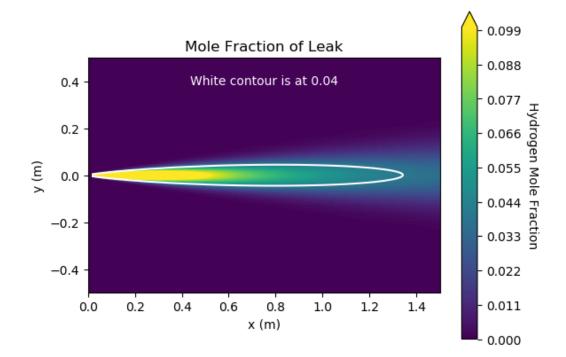
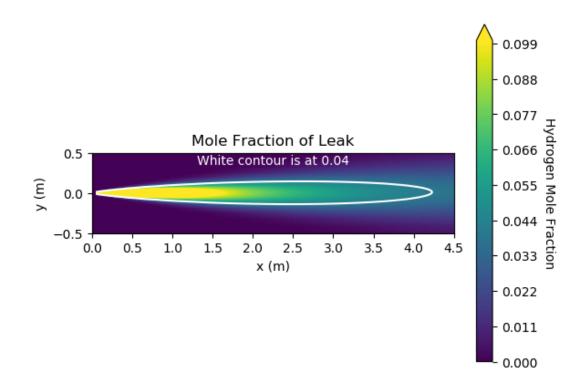


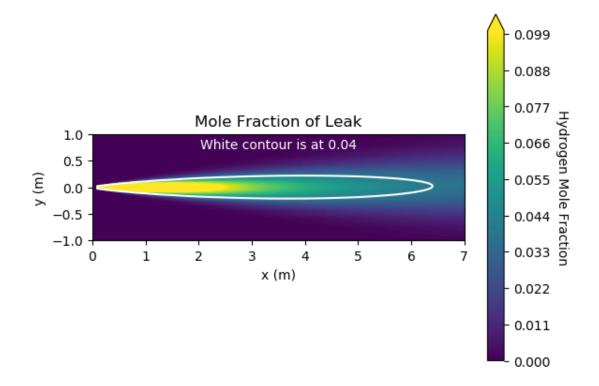
Figure 3A6: Diameter = 0.0001m; 1 meter from boat.



**Figure 3A7:** Diameter = 0.001m; 1 meter from boat



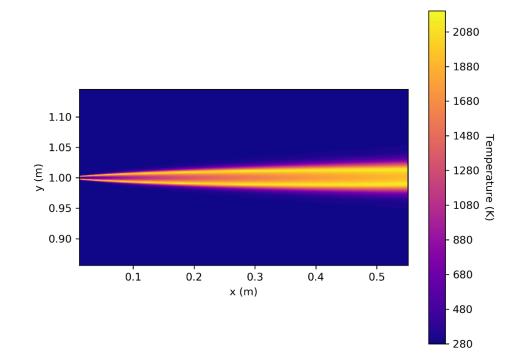
**Figure 3A8:** Diameter = 0.0032m; 1 meter from boat



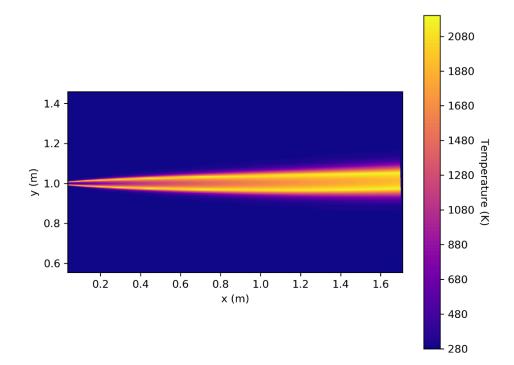
**Figure 3A9:** Diameter = 0.005m; 1 meter from boat

## 3.12: Chapter 3 Appendix 3B: Temperature Plots

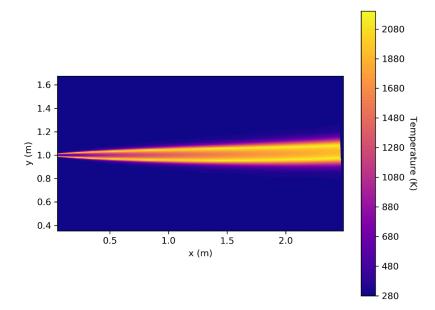
Assuming ignition of the plume, the flame temperature plots are presented here. The filling tank initial pressure is 350 bar. The empty tank on the boat has a pressure of 1.1 bar. The initial temperature of the hydrogen and the ambient temperature are 297 K (75 °F). The time that the leak occurs is 2 seconds after the fueling has started.



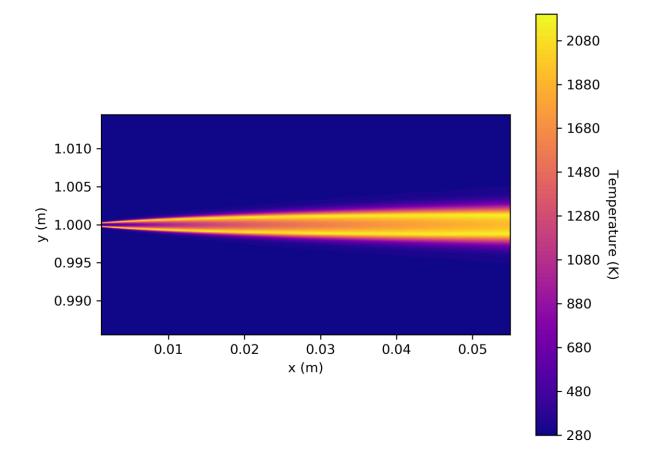
**Figure 3B1:** Diameter = 0.001m; 1 meter from truck



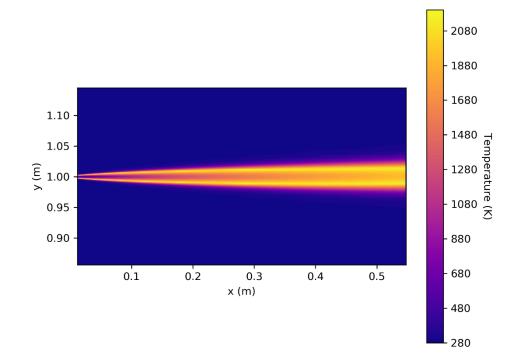
**Figure 3B2:** Diameter = 0.0032m; 1 meter from truck



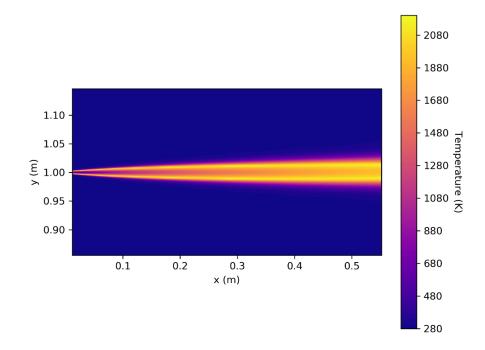
**Figure 3B3:** Diameter = 0.005m; 1 meter from truck



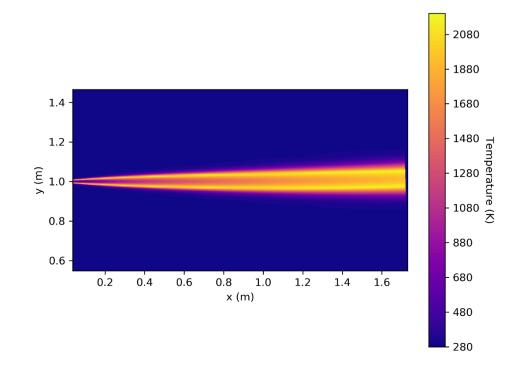
**Figure 3B4:** Diameter = 0.0001m; 25 feet from truck (middle of hose)



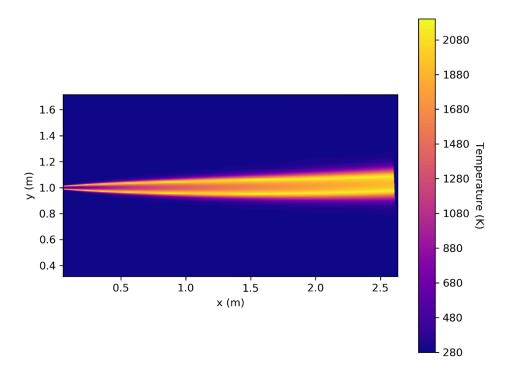
**Figure 3B5:** Diameter = 0.001m; 25 feet from truck (middle of hose)



**Figure 3B6:** Diameter = 0.001m; 1 meter from boat



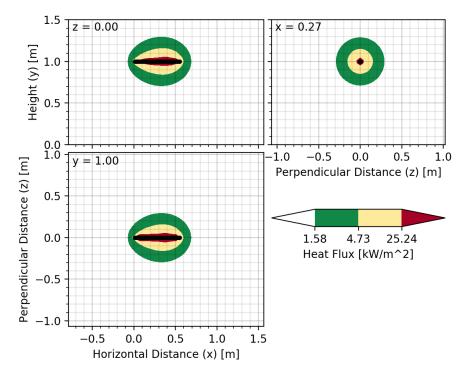
**Figure 3B7:** Diameter = 0.0032m; 1 meter from boat



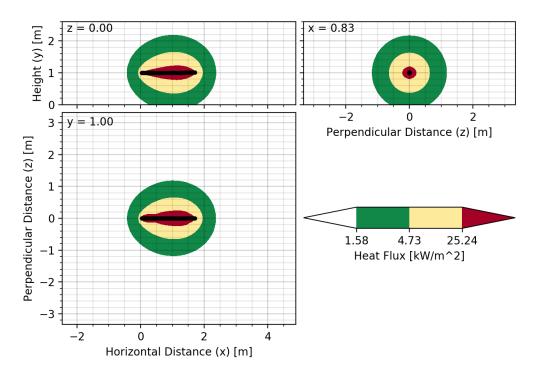
**Figure 3B8:** Diameter = 0.005m; 1 meter from boat

## 3.13: Chapter 3 Appendix 3C: Radiant Heat Flux Plots

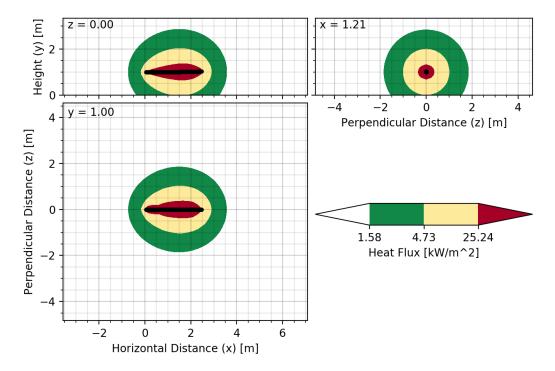
The plots of radiant heat flux are presented here. The filling tank initial pressure is 350 bar. The empty tank on the boat has a pressure of 1.1 bar. The initial temperature of the hydrogen and the ambient temperature are 297 K (23.9 °C, 75 °F). The time that the leak occurs is 2 seconds after the fueling has started.



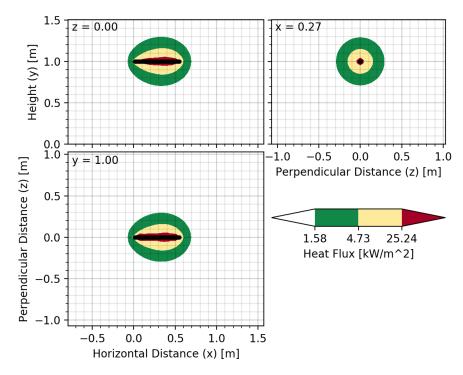
**Figure 3C1:** Diameter = 0.001m; 1 meter from truck.



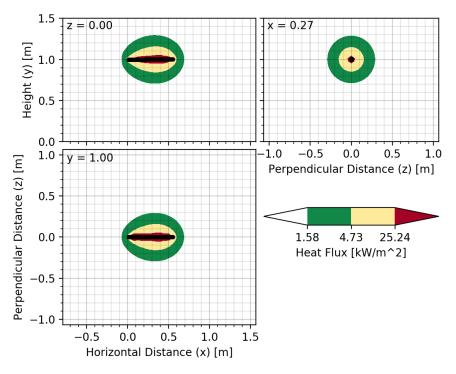
**Figure 3C2:** Diameter = 0.0032m; 1 meter from truck



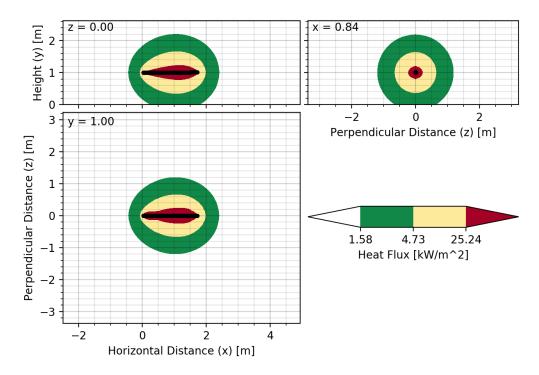
**Figure 3C3:** Diameter = 0.005m; 1 meter from truck.



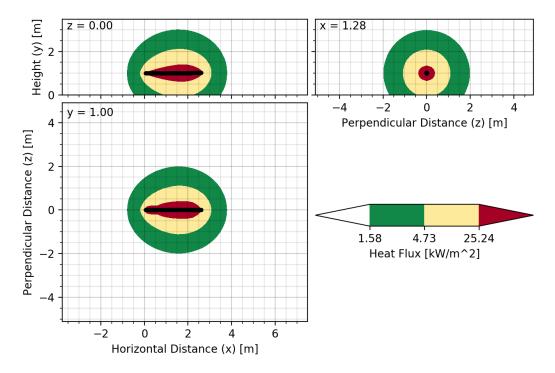
**Figure 3C4:** Diameter = 0.001m; 25 feet from truck (middle of hose)



**Figure 3C5:** Diameter = 0.001m; 1 meter from boat



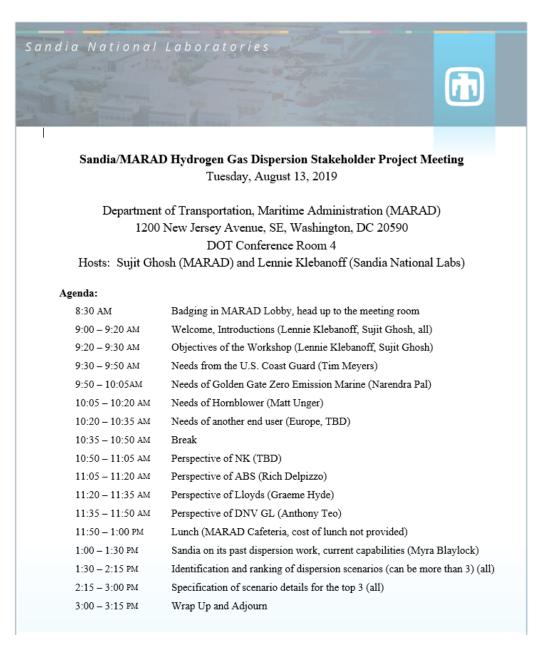
**Figure 3C6:** Diameter = 0.0032m; 1 meter from boat



**Figure 3C7:** Diameter = 0.005m; 1 meter from boat

# **Appendix:**

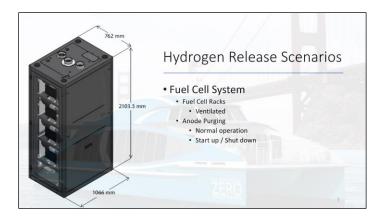
Agenda for Gas Dispersion Stakeholder Project Meeting and Participant Presentations

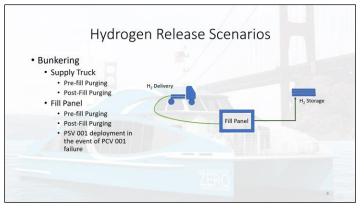


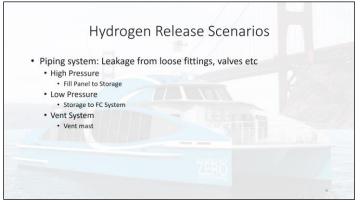
## **Presentation from GGZEM**











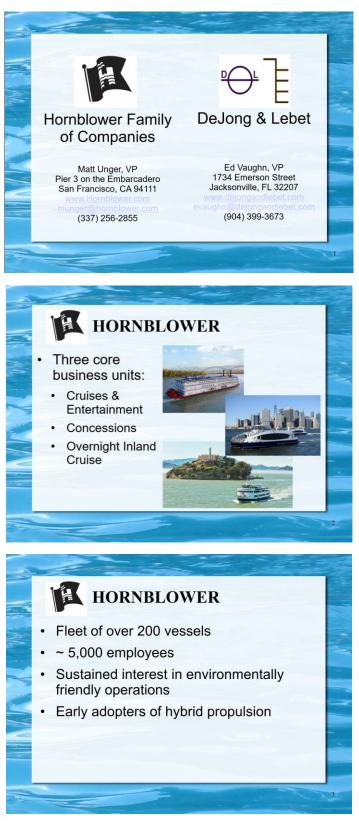


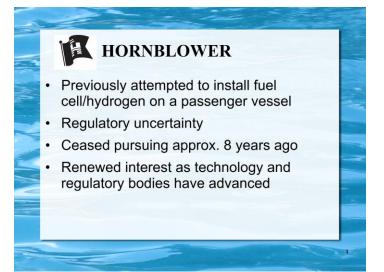
About Presenter

NAME OF TAXABLE PARTY.	Education:
	Masters (Energy):     Indian Institute of Technology, Delhi     PhD (Materials Science & Engineering):     University of Nevada, Reno (DOE Metal Hydride Cente     for Excellence) - Developed NI-Nb-2r Amorphous Alloy     Membrane for Hydrogen separation from mixed     industrial asses
NARENDRA PAL, PhD DIRECTOR OF HYDROGEN	Experience:
	<ul> <li>Over 22 years of experience working in energy industry out of which 16 years working in hydrogen research, development and deployment areas.</li> </ul>
	<ul> <li>Have successfully executed hydrogen infrastructure and application projects for both the vehicle and material handling markets.</li> </ul>
	<ul> <li>Have been a key contributor in formulating roadmap and safety codes &amp; standards, as well as in establishing initial hydrogen fueling infrastructure in India and North America.</li> </ul>
	<ul> <li>Prior to joining GGZEM, as Engineering Head of United Hydrogen Group, I successfully designed and deployed high pressure hydrogen system for refueling mobile storage for materials handling market apart from setting up of 10 TPD liquid hydrogen plant in Charleston, TN and designing and deployment of hydrogen storage demonstration project based on Liquid Organic Hydrogen</li> </ul>
	Carrier (LOHC) technology .
	Principal Member - NFPA-2: Hydrogen Technologies Code committee.

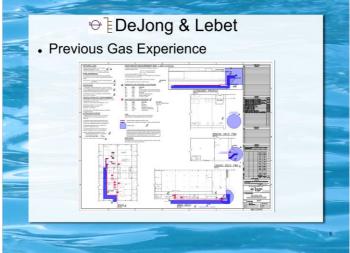
Thank You!	
In case of further questions, please feel free to contact me at; npal@ggzeromarine.com	

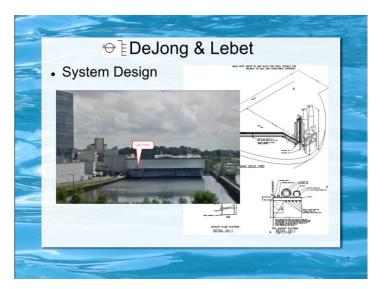
## **Presentation from Hornblower, DeJong & Lebet**

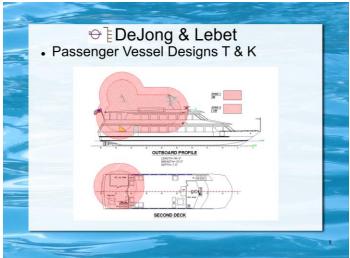










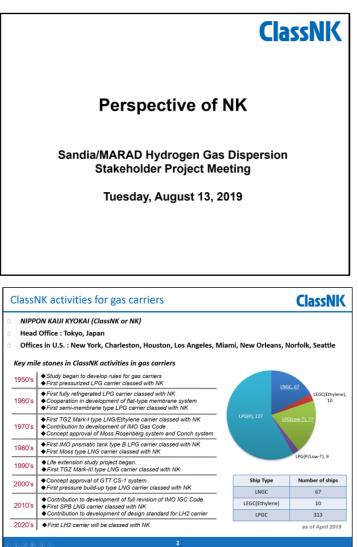


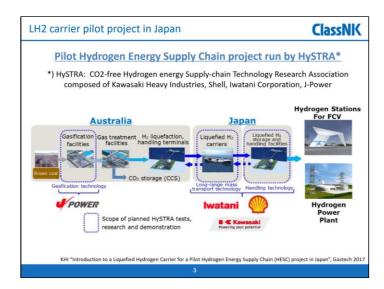
### Summary

- Dispersion analysis is a useful and needed tool
- Unique situations will require modeling an analysis
- A redefined hazardous space shape, using dispersion analysis could help guide new H<sub>2</sub> installation rules and regulations



**Presentation from Class NK** 



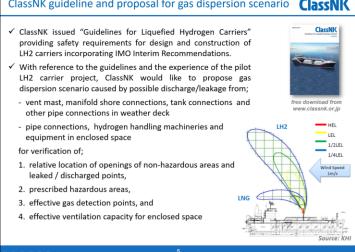




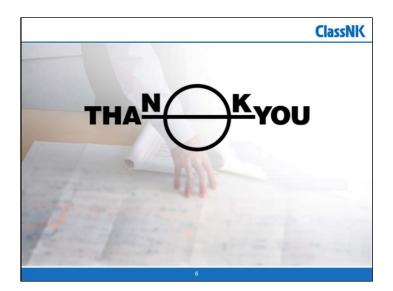
✓ Design and construction in accordance with IGC Code and IMO Res. 420(97) "INTERIM RECOMMENDATIONS FOR CARRIAGE OF LIQUEFIED HYDROGEN IN BULK"

✓ Under construction toward delivery in 2020

✓ ClassNK contributed to development of safety requirements at IMO discussion, various safety assessments (e.g. HAZID, HAZOP, FMEA, QRA, etc.) and technical advise from safety aspects.



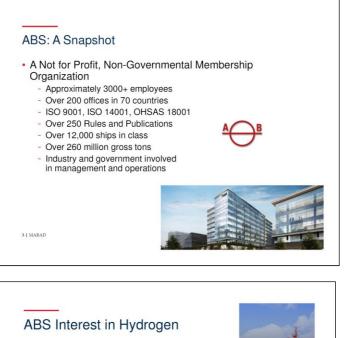
#### ClassNK guideline and proposal for gas dispersion scenario **ClassNK**



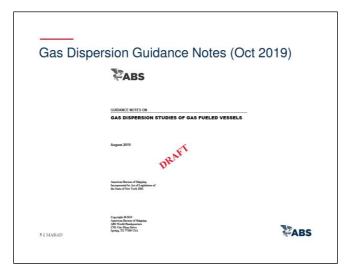
**Presentation from ABS** 





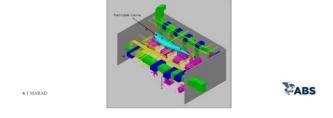


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### ABS Interest in Hydrogen (2010s)

- Evaluated H<sub>2</sub> releases in process plants using both simple and complex (CFD) methods
- Modeling performed for indoor and outdoor releases of both gaseous and liquefied hydrogen
- · Discharge and dispersion modeling performed using commercial tools - Canary, SLAB, and FLACS (CFD)
- Explosion modeling using internal tools implementing vapor cloud explosion models

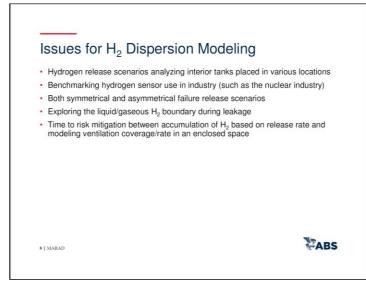


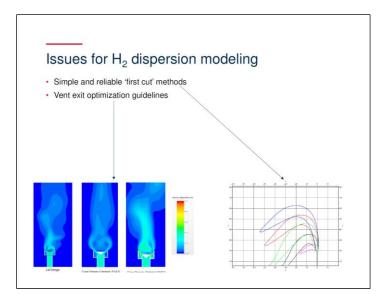
### ABS Acceptance Basis for H<sub>2</sub> Systems

ABS Rule Sets

- Qualifying New Technology/Novel Concept Guides
   5 stage process compatible with API RP 17N/Q and ISO 16290
- Guides on Fuel Cells and Gas Dispersion
- IMO & Industry Standards
  - IGF Code Code for Gases or other Low-FP Fuels - IMO CCC 2/3/1 (IGF Code with Fuel Cell Additions)









## **Presentation from Lloyds Register**



#### **Delivered Vessel - Hydroville**

Project Partners: CMB, BW Seacat and Revolve

Antwerp maritime group Compagnie Maritime Belge (CMB) has launched its hydrogenpowered passenger vessel in 2017, Hydroville, classed by LR. The vessel is a showcase for the use of clean fuels and is primarily a project to test hydrogen technology for applications on larger vessels. The vessel was constructed by builder BW Seacat with the hydrogen bunkered by Air Liquide.

Lloyd's Register's Deliverables:

- Approval services
- Hazard studies



Lloyd's Register

#### Future Vessel - Viareggio Super Yachts VSY LOHC

Project Partners: Viareggio Super Yachts and Siemens

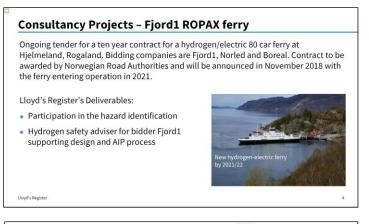
Viareggio Super Yachts (VSY) and Siemens have signed an agreement to develop a project for the application of hydrogen fuel cell technology on a special version of the new VSY 65m WATERECHO project by Espen Øino. The vessel will be fuelled with LOHC, liquid organic hydrogen carrier.

Lloyd's Register's Deliverables:

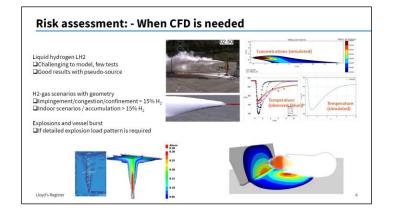
 Approval in Principle for the use of LOHC with associated activities

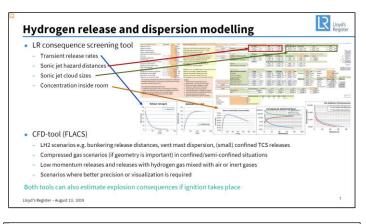
Lloyd's Register

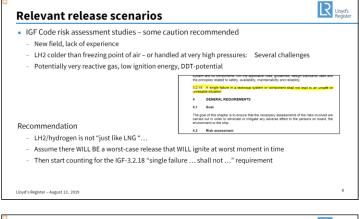


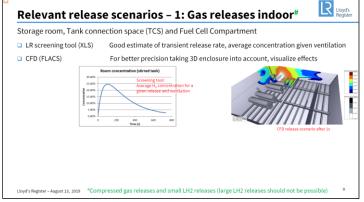


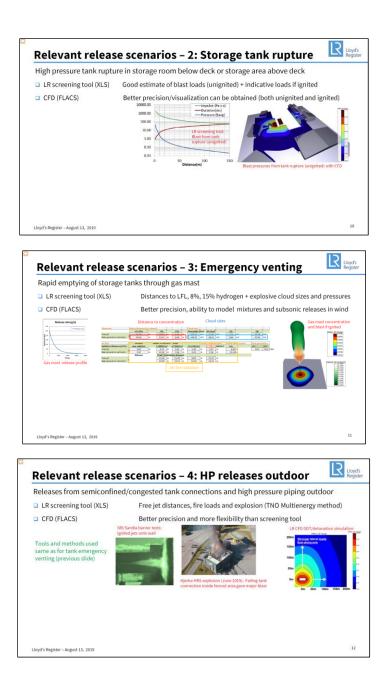


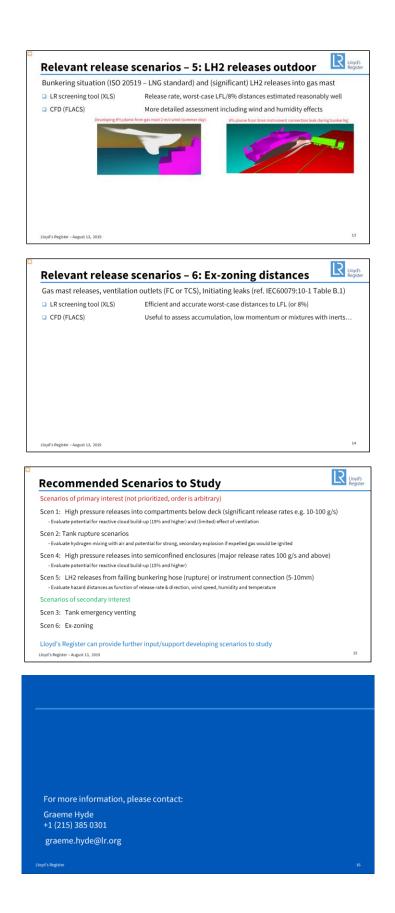




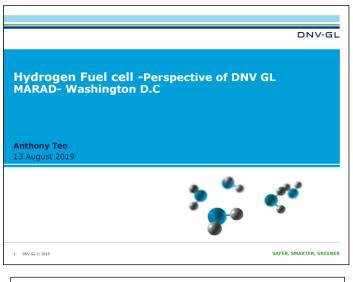


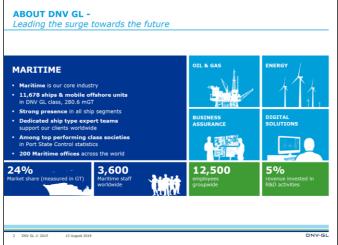






## **Presentation from DNV GL**



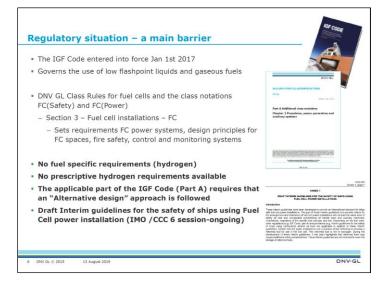


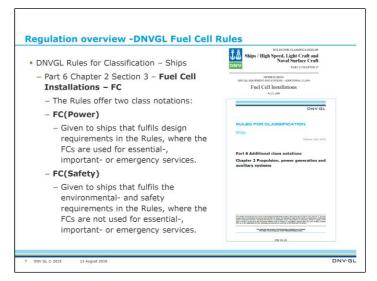


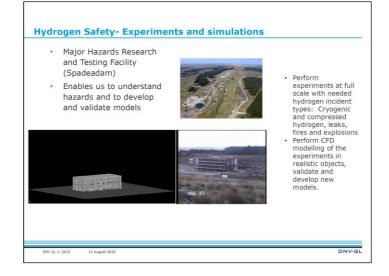
Norwegian Public Roads Administration	H2 Ferry 2020 -Study of technical, regulatory and financial feasibility of hydrogen fuel cell ferry by 2020. Frame agreement supporting NPRA in their process for the hydrogen electric ferry that shall be built from dec 2018 – sept 2020, then tested and start normal operation with passengers in 2021.	2016-202
Green Coastal Shipping Programme – Hydrogen Pilot	Hybrid hydrogen fuel cell powered high speed passenger ferry in Flora. DNV GL contributions are feasibility of concept, cost estimates, emissions savings, regulatory and safety aspects. Launch planned for 2021.	2017
Fiskerstrand. HYBRIDskip	Hybrid hydrogen (700 – 100 kg H2/day)fuel cell ferry with batteries. Ferry to start operation by 2020. DNV GL contribute with safety and classification competence and experience. 2017-2018 activities supported by PLIDT-E.	2017-2020
European Maritime Safety Agency (EMSA)	Study on the use of fuel cells in shipping covering fuel cell technologies, review of applicable standards, regulations and guidelines, regulative gaps, safety assessment (Available on: <u>http://emsa.europa.eu/main/air-pollution/aiternative-fuels.html</u> )	2016-2017
Sogn og Fjordane County Authority	jordane County potential production sites, scenarios for future hydrogen demand, regional	
Eidesvik JIP	FellowSHIP/Viking Lady 330 kW molten carbonate FC for auxilliary power. Hybrid supply yessel with DNV GL class notation - Fuel Cell Safety	2003-2011

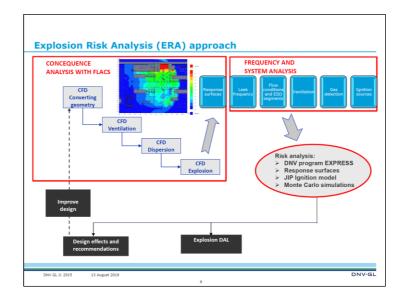
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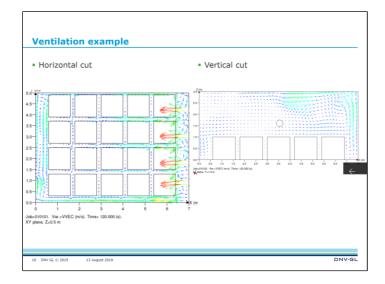
	FellowSHIP	320 kW MCFC system for auxiliary power of Offshore Supply Vessel	Eidesvik Offshore, Wirtsilä, DNV	2003-2011	MCFC	320 kW	LNG
Contraction of the local division of the loc	ZemShip - Alsterwasser	100 kW PEMFC system developed and tested onboard of a small passenger ship in the area of Alster in Hamburg, Germany	Proton Motors, GL, Alster Touristik GmbH, Linde Group etc.	2006-2013	PEM	96 kW	Hydroge
-	E4Ships - SchIBZ MS Forester	100 kW containerized SOFC system de- veloped and tested for the auxiliary power supply of comercial ships. Scalable up to 500 kW units.	Thyssen Krupp Marine Sys- tems, DNVGL, Leibniz Univer- sity Hannover, OWI, Reederei Rörd Braren, Sunfire	Phase 1: 2009-2017 Phase 2: 2017-2022	SOFC	100 EW	Diesel
	E4Ships - Pa-X-ell MS MARI- ELLA	60 kW modularized HT-PEM fuel cell sys- tem developed and tested for the decen- tralized auxiliary power supply onboard passenger vessel MS_MAREFLA.	Mayer Werft, DNVGL, Lürssen Werft, etc	Phase 1: 2009-2017 Phase 2: 2017-2022	HTPEM	60 kW (each stack is 30 kW)	Methanol
AND DESCRIPTION OF	Nemo H2	Small passenger ship in the canals of Amsterdam	Rederij Lovers etc	2012- present	PEM	60 kW	Hydroger
-2-	RiverCell	250 kW modularized HT-PEM fuel cell system developed and to be tested as a part of a hybrid power supply for river cruice vessles	Meyer Werft, DNVGL, Neptun Werft, Viking Cruises	Phase 1: 2015-2017 Phase 2: 2017-2022	HTPEM	250 kW	Methanol
-	SF-BREEZE	Feasibility study of a high-speed hydro- gen fuel cell passonger ferry and hydro- gen refueling station in San Francisco bay area	Sandia National Lab., Red and White Fleet	2015 - present	PEM	120 kW per module. Total power 2.5MW	Hydroge
		Sandi architi techni coasta	V - Hydrogen Fuel-Ct a partnered with the Sc ect firm Glosten and the cal, regulatory and ecoi al research vessel. published on 7 <sup>th</sup> May- ht y/hydrogen/market-trar	tipps Insti class soc nomic feas	tution o iety DN sibility o y.sandi	of Oceanograp IV GL to asses of a hydrogen ia.gov/transpo	s the fuel-cell

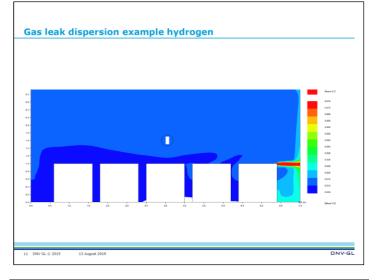


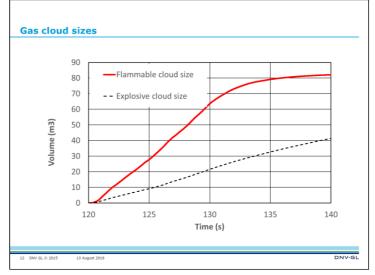


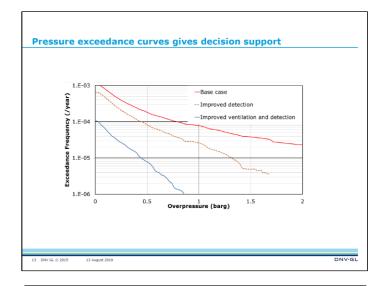










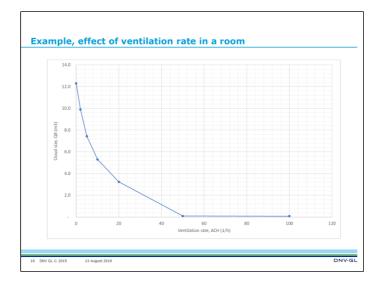


#### Fuelcell room dispersion scenarios

- If volume of gas in ESD segment is large enough to creat explosive cloud
   Can optimize ventilation rate and room design
- Run a matrix of cases with different ventilation rates and leak gas volumes:
- Test with different room and ventilation arrangements
- Run 16 cases for each ventilation and room design according to matrix
- With 4 room designs total 64 cases
- Batch running gives quick trunaround

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Ventilation rates (ACH) \ Leak gas volumes (m3)	10	20	50	100
Small				
Medium				
Large				
Very large				



#### Other scenarios (start up , normal ops, shut down, ESD, Idle time, Safe state)

- Vent stack dispersion Effect of cold gas from cryogenic release
- Effect of rain protection plate/top hat on stack can it direct gas down?
- Bunkering leaks
- Cryogenic hydrogen leak, pool formation and cold gas dispersion
- Explosion in congested areas
- Onboard storage of cryogenic hydrogen & Fuel cell Room
- Leaks in tank connection space
- Ventilation, dispersion and explosion simulations can also be suggested
- Experiments are planned with liquid hydrogen leaks
- Ignited leaks and fire consequences
- High temperature
- High radiation when leak rate is large

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#### Conclusions

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 An Explosion and Fire Risk analysis for maritime rooms /compartment provides good inputs to designers

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- The method can support the process to get approval
- The risk based approach gives optimization of safety systems and design
- Investigate and apply measures that stop the event as early as possible in the accident chain of events until acceptable risk is achieved
- Meaning may need more safety measures as in normal ships to show equivalence
- Risk based approach can be used to reduce number of design cycles

#### DNV GL initiative - MARHYSAFE: Maritime Hydrogen Safety Joint Development Project Goal: Status: - Currently discussing with potential - Remove regulatory and approval barriers partners Develop the knowledge required for safe - Open for more partners and reliable onboard hydrogen storage, bunkering and use of hydrogen in shipping – Planning to start the project soon (2019) Indication of partners: Public: Norwegian Maritime Authority, Norwegian Public Roads Administration, Norwegian Defence Material Agency (Navy, NDMA) - Private: Equinor, Scandlines, RCCL, Air Liquide, HySeas Energy, Redrock (Canada), UMOE, Hexagon, Standards Council of Canada

#### **R&D** partners:

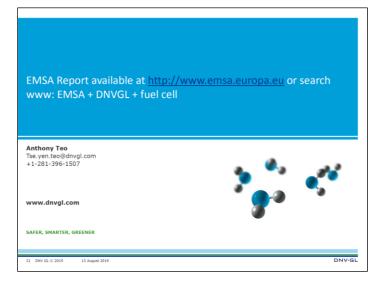
University of South-Eastern Norway (USN)

### MARHYSAFE

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	Applied research and development including experimental setups     Explosion and fire experiments and research
	Realization of demonstration projects     -Techno-economic road mapping for technology or solutions     -System Integration with renewables/electricity/
Implementation support	Technology qualification     Explosion and fire save design analysis     Recommended practice and standards development     Guideline for HRS user Interface Improvement process
Realisation support	Consortium initiation/execution     Safety assessments (HAZOP, HAZID, QRA, RRR, CFD modeling)
	Custody transfer?     Performance validation     Performance validation     Horopointation     H2 Incident and accident database (HIAD)
	Safer, Smarter, Green



## **Presentation from Sandia National Laboratories**



