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# R&D for Safety, Codes and Standards: Hydrogen Behavior

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Project End Date: Project continuation and direction determined annually by DOE

## Overall Objectives

- Perform R&D to provide the science and engineering basis for the release, ignition, and combustion behavior of hydrogen across its range of use (including high pressure and cryogenic).
- Develop models and tools to facilitate the assessment of the safety (risk) of hydrogen systems and enable use of that information for revising regulations, codes and standards and permitting stations.
- Deliver validated scientific analyses of critical scenarios and provide the science to enable revisions to the 2022 edition of NFPA 2, the National Fire Protection Association Hydrogen Technologies Code.

## Fiscal Year (FY) 2019 Objectives

- Determine whether a round nozzle or non-circular (representative of a crack or slit) yields a larger hazard distance for cryogenic hydrogen.
- Finalize large-scale diagnostic development and measure plumes characteristic of a liquid hydrogen truck depressurization.

## Technical Barriers

This project addresses the following technical barriers from the Hydrogen Safety, Codes and Standards section of the Fuel Cell Technologies

Office Multi-Year Research, Development, and Demonstration Plan<sup>1</sup>:

- Safety Data and Information: Limited Access and Availability
- Insufficient Technical Data to Revise Standards.

## Contribution to Achievement of DOE Milestones

This project will contribute to achievement of the following DOE milestones from Hydrogen Safety, Codes and Standards section of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan:

- Milestone 2.13: Develop and validate simplified predictive engineering models of hydrogen dispersion and ignition. (4Q, 2015)
- Milestone 2.19: Validate inherently safe design for hydrogen fueling infrastructure. (4Q, 2019)
- Milestone 4.8: Revision of NFPA 2 to incorporate advanced fueling and storage systems and specific requirements for infrastructure elements such as garages and vehicle maintenance facilities. (3Q, 2016)

## FY 2019 Accomplishments

- Demonstrated through two experimental campaigns that cryogenic hydrogen released from small (nominally 1 mm) rectangular nozzles has nearly equivalent dispersion and flame characteristics to cryogenic hydrogen released through circular nozzles; the round nozzle is the worst-case scenario for a risk calculation.
- Developed and demonstrated in the lab a novel laser diagnostic that can measure cryogenic hydrogen concentrations from a standoff distance of 40 ft, which can be applied to vent stack releases and large pooling and vaporization experiments.

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<sup>1</sup> <https://www.energy.gov/eere/fuelcells/downloads/fuel-cell-technologies-office-multi-year-research-development-and-22>

## INTRODUCTION

Fire codes govern the required distances between hydrogen sources (e.g., a liquid hydrogen tank at a fueling station) and hazards (e.g., ignition sources). Revisions to the fire code distances require justification, which is facilitated by analysis that includes physical models. These models must be validated by carefully controlled experiments, under relevant conditions, which can include high pressures (10,000 psi) or cryogenic temperatures (20 K). Over the course of this project, a range of experiments have been designed, developed, and executed to provide validation data for models. Models have been developed and exercised to inform the fire codes. This work has enabled quantitative risk assessments of hydrogen systems and subsequent reduction of setback distances from high-pressure hydrogen sources. More recently, efforts have focused on developing a scientific basis for modeling dispersion and flames from cryogenic (liquid) hydrogen sources. The fire codes currently require large distances around liquid hydrogen tanks, hindering the development and construction of hydrogen fueling stations with liquid hydrogen on site, an economically viable station design for large-capacity stations needed in urban areas. Validated models and targeted experiments from this project will be exercised to provide a technical basis for the revision of fire codes related to liquid hydrogen.

## APPROACH

The goals of this work are to develop and validate scientific models to accurately predict hazards and consequences from hydrogen releases and combustion/flames. In this project, we previously developed one-dimensional and engineering models of hydrogen dispersion and flames that can run quickly on a PC. While these models are one dimensional, they include enough physics (e.g., the effect of buoyancy) to be accurate under a wide range of scenarios. These models are able to characterize the hazards from hydrogen releases and flames and are fast enough that they can be run multiple times and incorporated into a quantitative risk assessment framework that includes probabilities of leak frequency and size, and probabilistic harm models. While the models in our quantitative risk assessment toolkit (HyRAM) have been validated, carefully controlled experiments are required to validate and develop new models for cryogenic hydrogen to have an impact on liquid hydrogen separation distances. Advanced optical and laser diagnostics are used, along with more conventional diagnostics (e.g., thermocouples), to characterize the dispersion and flame properties of releases at a lab scale. It is important to characterize and understand both ideal (round) releases for modeling purposes as well as more realistic releases such as might develop from a crack or leaking seal. The temperature, pressure, and orifice of the unignited releases and flames are controlled while characteristics are measured (e.g., concentration, flame temperature, radiative heat flux). For liquid hydrogen, some phenomena, such as releases from vent stacks and measurements of vaporization and pooling rates, require larger-scale experiments, and we are currently developing diagnostics and experimental platforms to measure these phenomena.

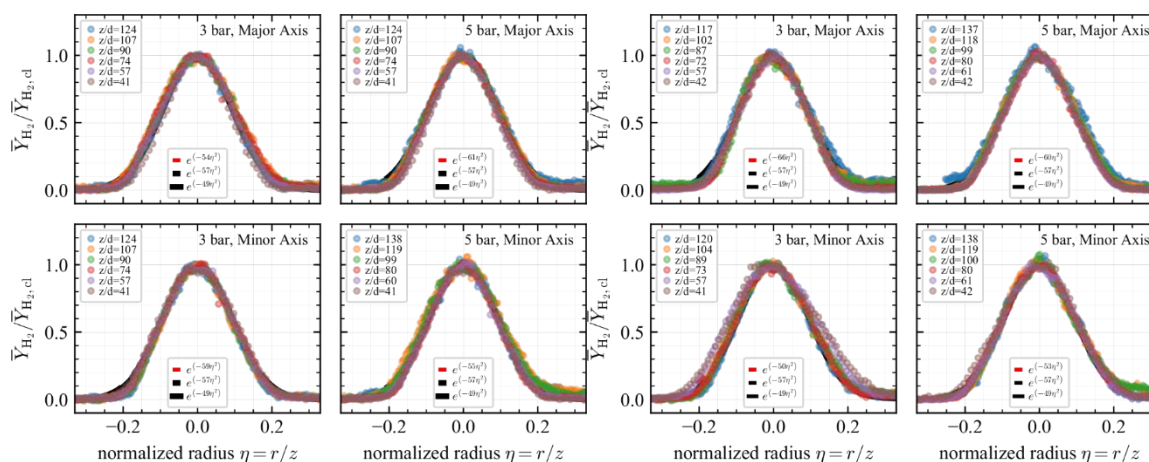
## RESULTS

### Lab-Scale Experiments

In previous years, we characterized the dispersion and flames from cryogenic hydrogen released through round nozzles. Models were validated against these experiments and these models are included in the Hydrogen Risk Assessment Models (HyRAM) toolkit. It is important that risk calculations are accurate or conservative, such that the risk is not underestimated. Realistic leaks from hydrogen infrastructure are far more likely to be through cracks or leaks around seals than through a perfectly round hole. These leaks will have a high aspect ratio (length to width). High-pressure, ambient temperature releases of hydrogen (and other gases) through non-circular orifices often mix faster and have shorter (but wider) flames than releases through their round counterparts. One effort this year focused on understanding the dispersion and flames of cryogenic hydrogen through high-aspect-ratio nozzles.

Spontaneous Raman scattering was used to measure the concentration and temperature field along the major and minor axes of aspect ratio 16 and 32 nozzles for 3 and 5 bar, approximately 55 K, hydrogen. Within the field of interrogation, a self-similar Gaussian-profile flow regime was observed with no significant deviations from releases through round nozzles. Cross-sections of the concentration are shown in Figure 1. The concentration decay rate and half-widths for the high-aspect-ratio cryogenic jets and the temperature fields

were found to be nominally equivalent to that of round nozzle cryogenic hydrogen jets indicating a similar flammable envelope.



**Figure 1. Left: aspect ratio of 16. Right: aspect ratio of 32. Radial mass fraction at selected downstream distances normalized by the centerline mass fraction for both high-aspect-ratio nozzles. Three fits are shown on each graph. The red line corresponds to the fit for each condition (at all heights), the dashed black line is the fit for all four releases conditions (for each nozzle), and the thick black line corresponds to the best fit for round nozzle jets.**

In a separate experimental campaign, we measured the visible flame length and heat-flux characteristics of cryogenic hydrogen flames from high-aspect ratio nozzles ranging from 2 to 64. We varied the temperature from room temperature (295 K) down to 42 K and the pressure from 1.5 to 6 bar. We compared these data to flames of both cryogenic and compressed hydrogen from round nozzles. The aspect ratio of the release does not affect the flame length or heat flux significantly for a given mass flow under the range of conditions studied.

The fact that the geometry of the release did not significantly affect either the dispersion or flame characteristics for cryogenic hydrogen means that the models within HyRAM can be confidently used, even for realistic leak geometries. The pressures studied in these two experimental campaigns (up to 6 bar) are characteristic of liquid hydrogen storage tanks. Some liquid hydrogen systems use a liquid hydrogen pump and achieve much higher pressures. The characteristics of dispersion and flames from cryo-compressed hydrogen systems through high-aspect-ratio nozzles may deviate from their round counterparts and should be investigated before HyRAM is used for cryo-compressed hydrogen infrastructure.

### Diagnostic for Large-Scale Experiments

In the laboratory, we are able to study small leaks of cryogenic (and high-pressure) hydrogen. Questions remain as to whether the same phenomena scale up for larger leaks. For example, the vent stack on a liquid hydrogen tank has the potential to release a large amount of cryogenic hydrogen should the burst disk rupture, and it is common to release significant amounts of gas through the vent stack as a delivery truck depressurizes after transferring hydrogen to the liquid hydrogen tank. There are also physical questions about how ambient conditions (e.g., wind speed, humidity, air temperature) affect large-scale releases through vent stacks. Finally, the physics of pooling and vaporization from liquid hydrogen pools is not very well understood. Having the appropriate diagnostics to measure the hydrogen concentration is critical to gathering validation data for models and answering these questions. For this reason, we have been scaling up our laboratory laser Raman scattering measurements so that we can apply this diagnostic to large-scale releases. This has required innovative laser illumination and light collection strategies.

We completed construction of the large-scale diagnostic this year, which can be seen in Figure 2. For illumination, we have mounted a high-energy Nd-YAG laser on a movable cart. We use the third-harmonic pulses from the laser at the ultraviolet wavelength of 355 nm. Raman scattering is inversely proportional to the wavelength to the fourth power, so using this low wavelength increases the amount of scattered light. In

addition, because the light is in the ultraviolet, it does not pose a startle hazard to any aircraft pilots that might be in the area, facilitating the approval process from the Federal Aviation Administration to use this laser outdoors. A mirror galvanometer is used to raster the laser light around at up to a 20 degree angle such that the concentration of cryogenic hydrogen can be measured throughout the area of interest.

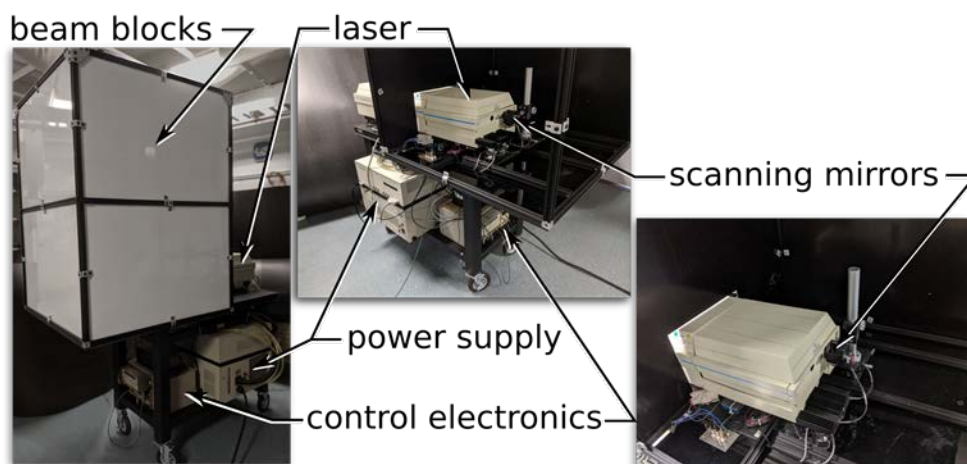


Figure 2. Illumination system for large-scale diagnostic

Light collection for this diagnostic was also a challenge. We investigated many configurations of custom optical systems with large apertures but were limited by the desired field of view and sensor size. We concluded that a Princeton Instruments ICCD with a Howell-Angenieux 25-mm f/0.95 lens gave the best results. We were able to demonstrate acceptable signal to noise using this lens/camera setup, as shown in Figure 3. Both aspects (illumination and light collection) of the large-scale diagnostic are synchronized such that the spatial location of the illumination beam is matched to a camera frame, and a three-dimensional reconstruction of the cryogenic hydrogen releases can be formed.

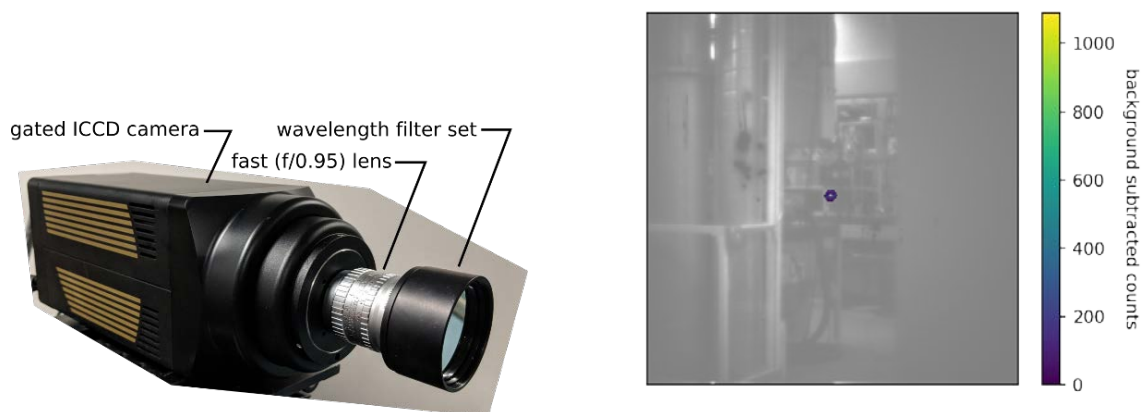


Figure 3. Light collection system (left) and image of Raman scattering signal overlaid on an image of the lab (right). There is only a small amount of hydrogen in the central part of the figure. The figure also shows that we achieve a 20 ft field of view from 40 ft distance.

## CONCLUSIONS AND UPCOMING ACTIVITIES

The goal of this work is to enable revision of the fire code for liquid hydrogen based on validated scientific analyses. At the lab scale, we completed two experimental campaigns to investigate the dispersion and flame characteristics of hydrogen released through high-aspect-ratio nozzles, which are more characteristic of leaks through cracks or faulty seals. We found no significant correlation for the dependence of mixing, warming,

flame length, or radiative heat transfer on the geometry of the release. In essence, the unignited and ignited releases of cryogenic hydrogen through high-aspect-ratio nozzles behaved the same as releases of cryogenic hydrogen through round nozzles. This means that the models in HyRAM, which assume a round nozzle, can be confidently used to calculate the risk for realistic release geometries. Building toward future work, we also completed the construction of a laser Raman scattering diagnostic that can be used on larger-scale releases. Novel illumination and light collection systems were assembled that can quantitatively measure the cryogenic hydrogen concentration in three dimensions. The diagnostic will be used to measure large hydrogen plumes from liquid hydrogen vent stacks or vaporizing pools.

We are working with our colleagues at Lawrence Livermore National Laboratory, where there is a liquid hydrogen tank on site, to perform liquid hydrogen vent stack dispersion experiments early next year. We will study the effect of ambient conditions (e.g., wind speed, humidity, air temperature) on the dispersion properties (e.g., does high wind channel the hydrogen or improve the mixing), and validate our cryogenic plume model at higher flowrates than are achievable in the lab. We will also plan pooling and vaporization experiments to which our large-scale diagnostic can be applied. From this data, we hope to develop validated models for these phenomena. These models will be integrated into the HyRAM toolkit, enabling a full risk calculation to be performed for liquid hydrogen fueling stations, reducing the footprint for stations with liquid hydrogen.

### FY 2019 PUBLICATIONS/PRESENTATIONS

1. X. Li, Q. Chen, M. Chen, Q. He, D.M. Christopher, X. Cheng, B. Roy Chowdhury, and E.S. Hecht, “Modeling of Underexpanded Hydrogen Jets through Square and Rectangular Slot Nozzles,” *International Journal of Hydrogen Energy* 44 (2019): 6353–6365.
2. E.S. Hecht and P.P. Panda, “Mixing and Warming of Cryogenic Hydrogen Releases,” *International Journal of Hydrogen Energy* 44 (2019): 8960–8970.
3. E.S. Hecht, “Cryogenic Hydrogen Behavior,” presented to representative from NEDO and Kobe Steel in Albuquerque, NM, April 25, 2019, SAND2019-4925 PE.
4. E.S. Hecht and B. Roy Chowdhury, “Codes & Standards Tech Team Update: Cryogenic Hydrogen Behavior,” presented to the USDRIVE Codes & Standards Tech Team, May 9, 2019, SAND2019-5169 PE.
5. E.S. Hecht and B. Roy Chowdhury, “Hydrogen Behavior Research as a Foundation for Codes & Standards,” presented at the KGS Executives meeting in Livermore, CA, June 18, 2019, SAND2019-6857 PE.
6. E.S. Hecht and B. Roy Chowdhury, “Characteristic of Cryogenic Hydrogen Flames from High-Aspect Ratio Nozzles,” *Proceedings of the International Conference on Hydrogen Safety*, Adelaide, Australia, September 24–26, 2019, SAND2019-7883 C.
7. B. Roy Chowdhury and E.S. Hecht, “Dispersion of Cryogenic Hydrogen through High-Aspect Ratio Nozzles,” *Proceedings of the International Conference on Hydrogen Safety*, Adelaide, Australia, September 24–26, 2019, SAND2019-7892 C.
8. E.S. Hecht, P.P. Panda, B. Roy Chowdhury, and D. Ye, *Characteristics of Cryogenic Hydrogen Releases Under Unignited and Ignited Conditions*, SAND2019-9998.  
[https://cafcp.org/sites/default/files/LH2\\_ColdPLUME\\_SAND\\_REPORT.pdf](https://cafcp.org/sites/default/files/LH2_ColdPLUME_SAND_REPORT.pdf).
9. E.S. Hecht and B. Roy Chowdhury, “Characteristic of Cryogenic Hydrogen Flames from High-Aspect Ratio Nozzles,” presented at the International Conference on Hydrogen Safety, Adelaide, Australia, September 24–26, 2019, SAND2019-10521 C.
10. B. Roy Chowdhury and E.S. Hecht, “Dispersion of Cryogenic Hydrogen through High-Aspect Ratio Nozzles,” presented at the International Conference on Hydrogen Safety, Adelaide, Australia, September 24–26, 2019, SAND2019-10522 C.