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

Project ID: SCS010

PI: Ethan S. Hecht

Team: Bikram Roy Chowdhury

Sandia National Laboratories

May 1, 2019

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2019-2415 C

Overview

Timeline

- Project start date: Oct. 2003
- Project end date: Sept. 2019*
  - * Project continuation and direction determined by DOE annually

Budget

- FY18 DOE Funding: $500 k
- Planned FY19 DOE Funding: $750 k
- Planned FY19 H2@Scale CRADA funding: $300 k ($150 k from Air Liquide and partners, $150 k from DOE)

Barriers

A. Safety Data and Information: Limited Access and Availability

G. Insufficient technical data to revise standards

Partners

- **Stakeholder CRADA**
  - Frontier Energy (contractor for CaFCP)
  - Fire Protection Research Foundation (research affiliate of NFPA)
- **H2@Scale CRADA**
  - Air Liquide
- **Industry & Research**
  - LLNL
  - CGA 5.5 testing task force
  - Fuel Cells and Hydrogen Joint Undertaking (EU)
  - NFPA 2 code committee
  - Shandong University

Relevance

Objectives:

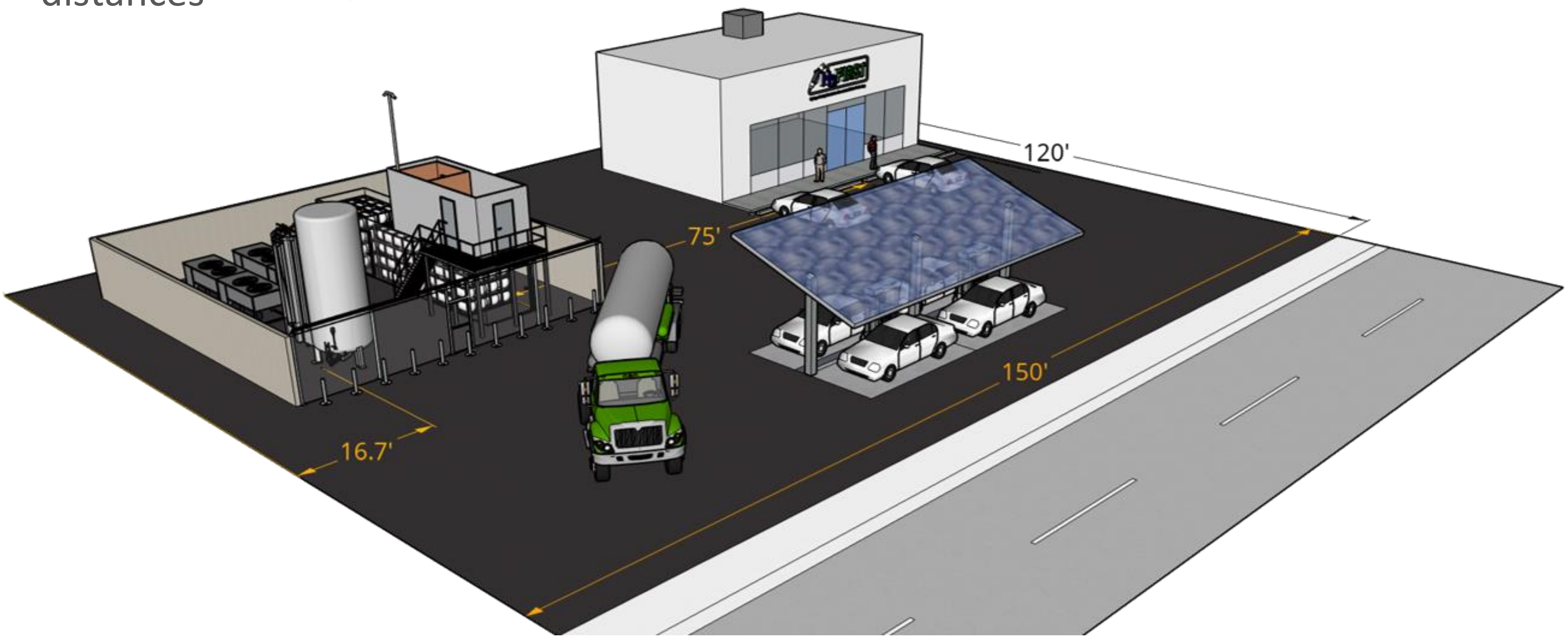
- Perform R&D to provide the science & engineering basis for the release, ignition, and combustion behavior of hydrogen across its range of use (including high pressure and cryogenic)
- Develop models and tools to facilitate the assessment of the safety (risk) of H_2 systems and enable use of that information for revising RCS and permitting stations

Barrier from 2015 SCS MYRDD	Previous year impact
A. Safety Data and Information: Limited Access and Availability	Incorporated validated cryogenic hydrogen dispersion model into HyRAM modeling toolkit
G. Insufficient technical data to revise standards	Performed and planned additional cryogenic hydrogen physics experiments

DOE goal: By September 30, 2022, identify ways to reduce the siting burdens that prohibit expansion of hydrogen fueling stations, through hydrogen research and development that enables a 40% reduction in station footprint, compared to the 2016 baseline of 18,000 square feet

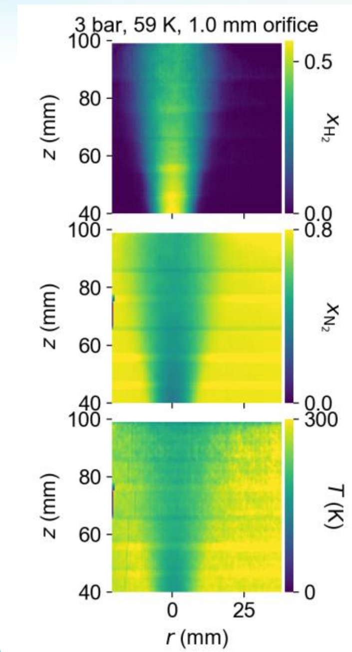
Relevance: Current separation distances for liquid hydrogen are based on consensus, not science

- Higher energy density of liquid hydrogen over compressed H_2 (and lack of pipelines) make this technology viable for larger fueling stations (logistically and economically)
- Even with credits for insulation and fire-rated barrier wall 75 ft. offset to building intakes and parking make footprint large
- Previous work by our group led to science-based, reduced, gaseous H_2 separation distances

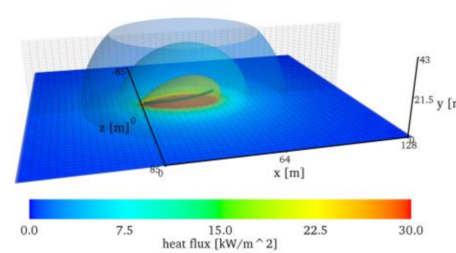


Approach (Sandia H_2 SCS): Coordinated activities that facilitate deployment of hydrogen technologies

- Hydrogen Behavior (this project, SCS010)
  - **Develop and validate scientific models** to accurately predict hazards and harm from liquid releases, flames, etc.
- Quantitative Risk Assessment, tools R&D (SCS011)
  - **Develop integrated methods and algorithms** enabling consistent, traceable, and rigorous QRA (Quantitative Risk Assessment) for H_2 facilities and vehicles
- Enable Hydrogen Infrastructure through Science-based Codes and Standards (SCS025)
  - **Apply QRA and behavior models to real problems** in hydrogen infrastructure and emerging technology



HyRAM
HYDROGEN RISK ASSESSMENT MODELS



Approach: Develop and execute experiments to enable predictive modeling across H_2's range of use

- Issue: Idealized laboratory experiments using circular nozzles may not be the worst-case scenario which is needed to characterize risk
  - Gather data and develop models to characterize non-circular (crack-like) cryogenic hydrogen releases – in progress
- Issue: Larger cryogenic H_2 releases have been outdoors and/or instrumented with low fidelity sensors (space and time), with experimental uncertainty too high for model validation
  - FY19 milestone: Finalize diagnostic development and measure plumes characteristic of a liquid hydrogen truck depressurization – in progress

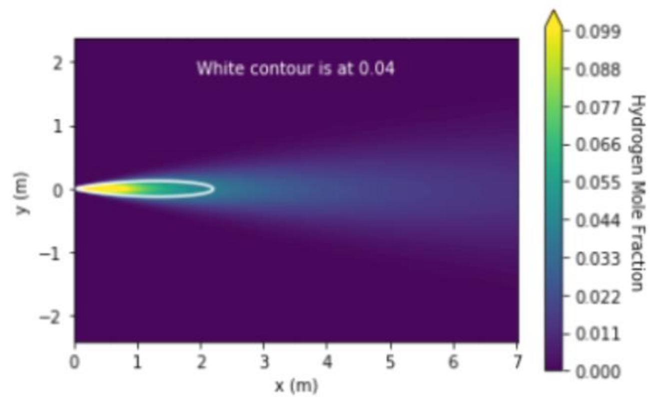
> ➢ Deliver validated scientific analyses of critical scenarios and provide the science to enable revisions to the 2022 edition of NFPA 2

Accomplishment: Updated Python modeling packages (including ColdPLUME) for ease of use

- Exploring the release of HyRAM as open source software (see SCS011)
- Validated version of ColdPLUME included
- Intuitive object oriented structure
- Updated physics and QRA submodules
- Python package implementation with documentation

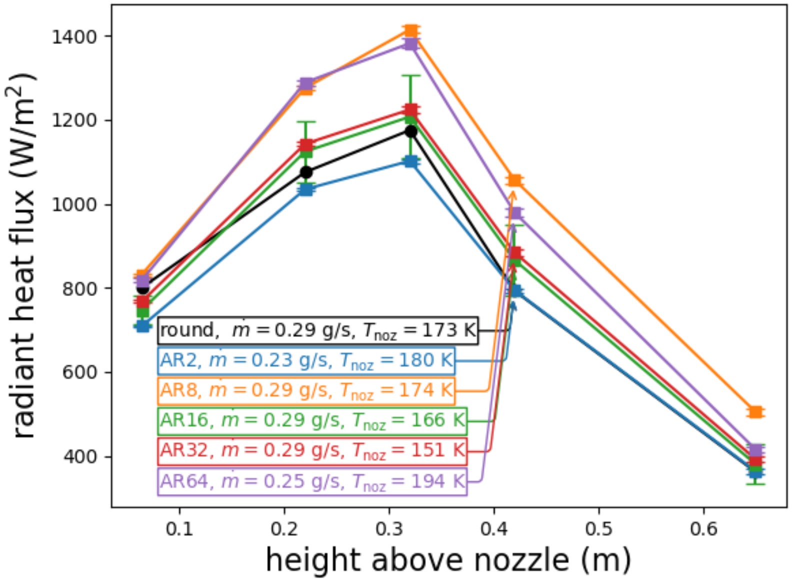
➢ Code organization, ease of use and documentation critical for outside development and use

```
In [1]: from altRAM import phys

In [2]: H2 = phys.Gas(T = 40, P = 5e5);
        air = phys.Gas(T = 295, P = 101325, species =
        ['air']);
        orifice = phys.Orifice(d = 0.001);
        release = phys.Jet(H2, orifice, air);
        release.solve(Ymin = .001);
        release.plot_moleFrac_Contour();

solving for the plume... done.
```



Accomplishment: Measured radiative heat flux for non-circular nozzles

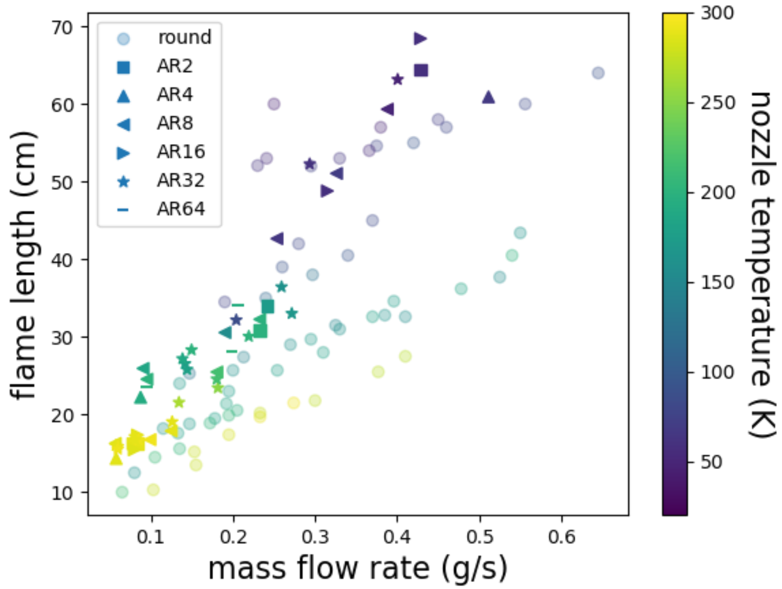
- Aspect Ratios: 2-64
- Nozzle pressures: 1.5-6 bar
- Nozzle temperatures: 48-295K

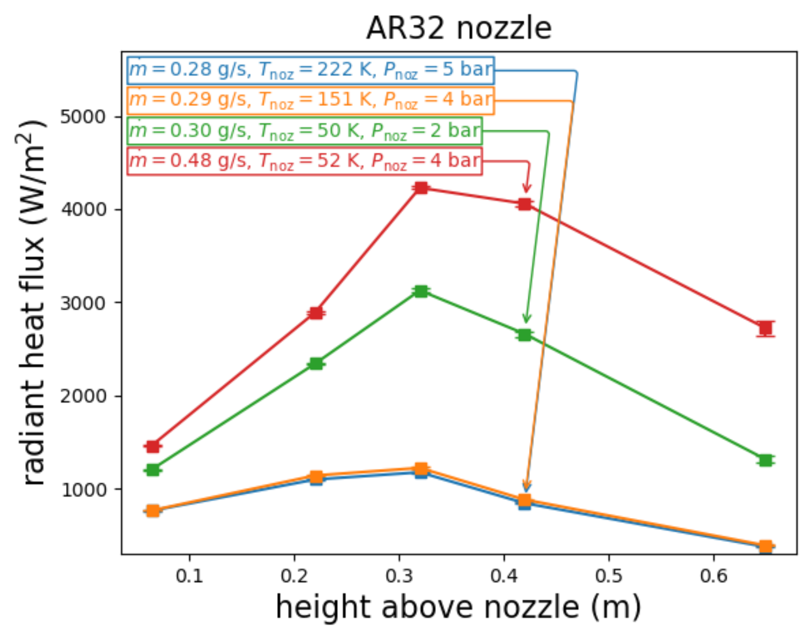


➢ Initial results show no clear heat flux dependency on aspect ratio, therefore circular nozzle assumption is appropriate for QRA calculations

Accomplishment: Measured how flame length and heat flux at scale at cryogenic temperatures

- Aspect ratio does not have a large impact on flame length
- Cryogenic temperatures increase mass flow through nozzles
- For a given mass flux, heat flux *increases* at cryogenic temperatures

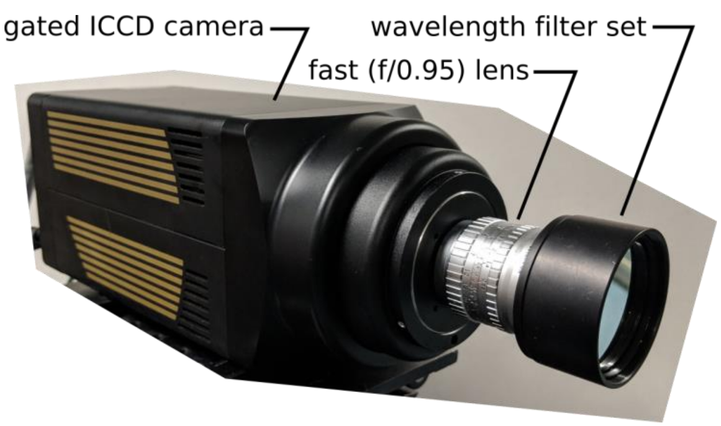




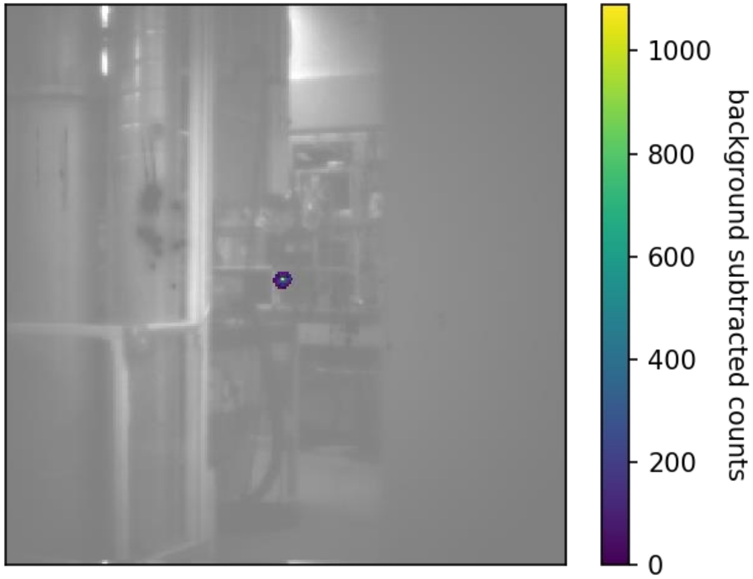
> Critical that model predicts measured heat flux increase at cryogenic temperatures for QRA of liquid hydrogen systems

Accomplishment: Demonstrated acceptable signal to noise for large-scale diagnostic

- Imaged hydrogen from 40 foot standoff distance in the laboratory
- Observed nearly 30 degree field of view (20 ft scene from 40 ft distance)



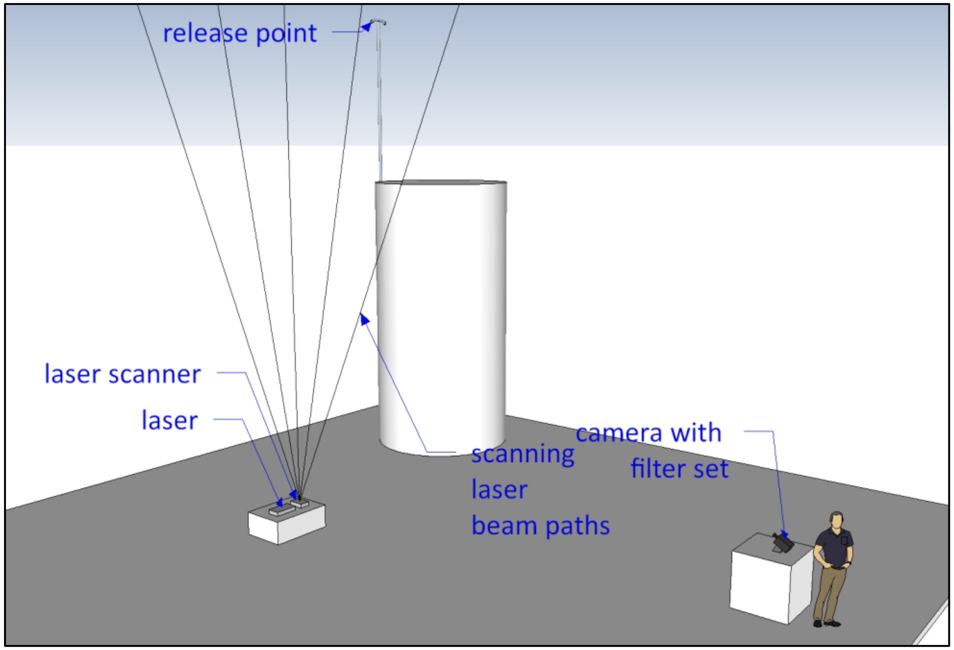
Raman signal overlaid on laboratory scene



➢ Uniquely fast optics enable collection of small Raman signal

Progress: Developed strategies for illumination of large-scale scene

- Effective background light suppression is key (both sunlight and illumination source that reflects off of condensed water vapor)
  - Time gating
  - Spectral gating
- High-powered light source required to excite as many molecules as possible
  - High-power laser scanning in space
  - Concentrations measured along a series of lines
  - 1st generation: low speed galvanometer using 10 Hz laser
  - 2nd generation: high speed polygonal scanning using pulse-burst laser



➢ On-camera accumulation will provide a complete snapshot of the plume with reasonable resolution

Progress: Working with our colleagues at LLNL to perform LH_2 vent stack releases

- Additional temperature sensors along vent stack to validate internal flow model
- May require additional plumbing changes
- Replacing bull-horn with single outlet to enable model comparisons
- Variations in temperature, flow-rate, and external conditions (e.g. wind) in experiments
- Comparison to NREL sensor approach for some tests

Petitpas & Aceves, IJHE 43: 18403-18420: https://doi.org/10.1016/j.ijhydene.2018.08.097

- ➢ Heaters and pump enable a wide range of flow rates and temperatures at vent stack
- ➢ Proximity to SNL enables experiments to be run on short notice (when weather is right)

Response to last year's Reviewer's comments

- Project weaknesses include lack of practical knowledge in regard to the operating conditions of LH_2 facilities. This lack is reflected by potentially non-representative scaling of laboratory experiments.
- We are continually working with industrial partners to ensure that our simulations are based on practical LH2 operating conditions. By performing the large-scale experiments, we will ensure that our models can scale to practical sizes (vent stacks).
- Vent experiments with larger orifices (at least 10 mm) and lower pressures (less than 1 barg) should be benchmarked against the ColdPlume model predictions based on the current momentum-driven data. The investigators can determine whether the model can adequately predict buoyancy-driven plume behavior.
- The vent stack release experiments this FY will be used to benchmark the model. Low release-rate experiments are planned which will show whether the model is accurate for buoyancy-driven flows.
- The project should work to understand whether there are worst-case conditions for a release, for example, windy, rainy, cold, snowy, humid, hot, or dry weather. If so, perhaps experimentation and model work could focus on these conditions as priority.
- We agree that understanding the worst-case scenario is important for risk calculations. We will strive to measure plume dispersion under as wide of a range of weather conditions as possible. We will at least study dispersion under high and low-wind conditions to understand the effect of wind. Planning for a different ambient temperatures may require experiments in the summer and winter. With the initial tests taking place at LLNL, the proximity enables experiments to be run on short notice (when weather is right).

Collaborations enable this research and expand impact

- CRADA with BKi to fund experiments ($175k received from CaFCP Auto OEM Group, Linde, Shell)
  - Data exchange with contributing members
- H2@Scale CRADA with Air Liquide signed (awaiting funds: $150 k from Air Liquide and partners, $150 k from DOE)
- NFPA 2 Technical Code Committee
  - Regular attendance with expert advisory role
- Fuel Cells and Hydrogen Joint Undertaking (FCH-JU, European Union)
  - Advisory board member for Prenormative Research for Safe Use of Liquid Hydrogen (PreSLHy) project
- Shandong University (China)
  - Hosted visiting professor with expertise on hydrogen behavior
- CGA G-5.5 testing task force
  - Providing hardware for and analysis support of measurements of LH_2 vent stack flames

Remaining challenges: Executing outdoor experiments and planning additional large-scale experiments

Ensure safety when operating laser outdoors

- follow ANSI Z136 standard
- Non-visible (UV light) helps

Perform experiments during a range of weather conditions

- High- and low-wind conditions
- Humidity differences (potentially with precipitation)

Need experiments to characterize:

- Pooling
- Evaporation from LH_2 pools
- Interactions of plumes with ambient

Solution:

- Well-controlled experiments at Sandia facilities
- Partner with others, applying diagnostic at remote locations (European colleagues)

Proposed future work

- Remainder of FY19
  - Complete analysis of non-circular release cryogenic hydrogen flame behavior
  - Experimentally measure non-circular release cryogenic hydrogen dispersion
  - Perform experiments using large-scale diagnostic at LLNL LH_2 pad
  - Develop R&D plans for pooling/vaporization experiments
  - Perform initial simulations of scenarios driving separation distances in NFPA 2
- FY20
  - Refine largescale diagnostic design
  - Conduct large-scale release experiments to characterize hydrogen pooling, evaporation, and interaction with atmosphere
  - Develop validated models of hydrogen pooling and evaporation
- Out years
  - Finalize simulations and analyses of scenarios driving separation distances in NFPA 2 and enable the science-based revision of the liquid hydrogen separation distances in the 2022 version of NFPA 2

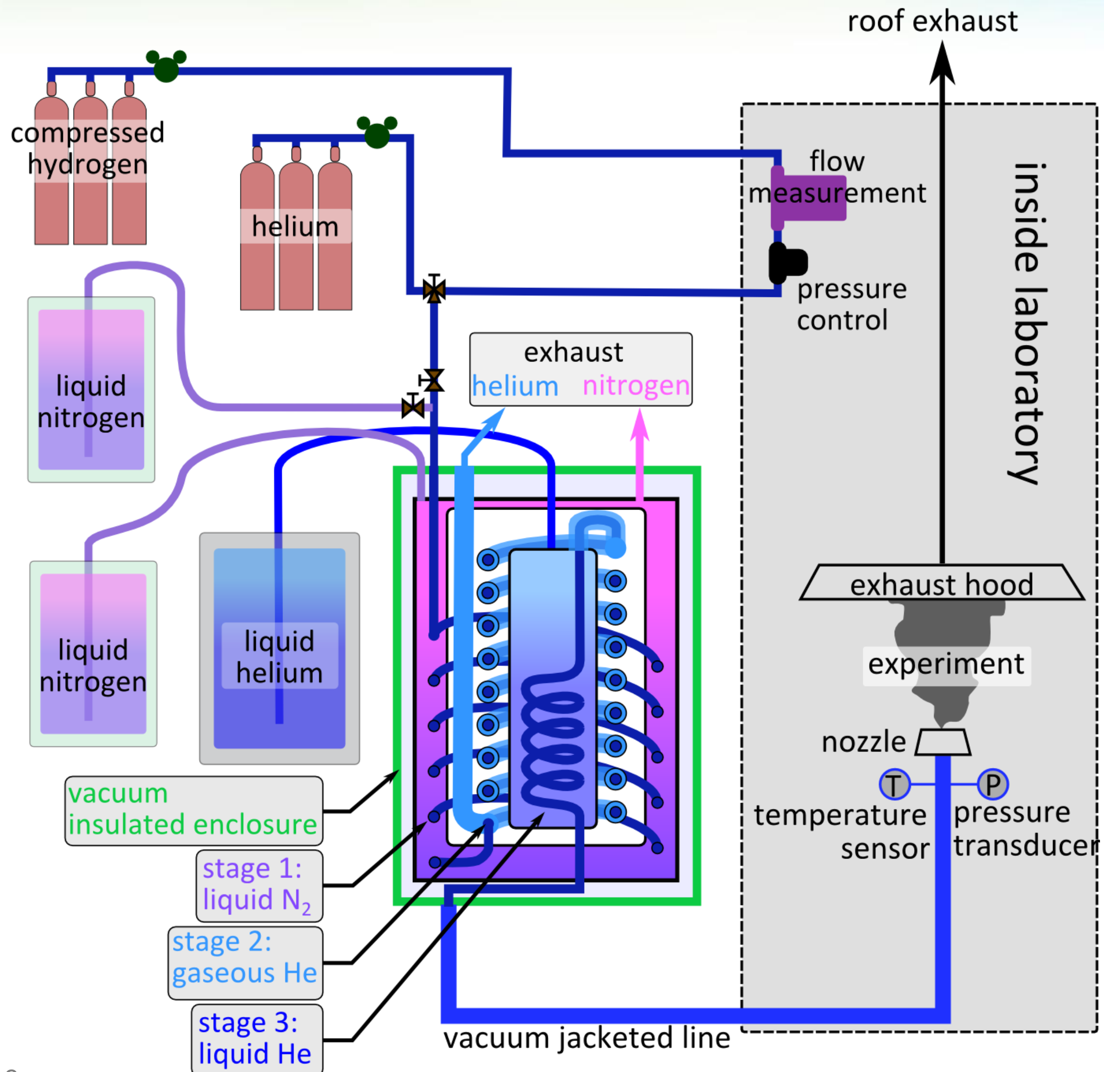
Any proposed future work is subject to change based on funding levels

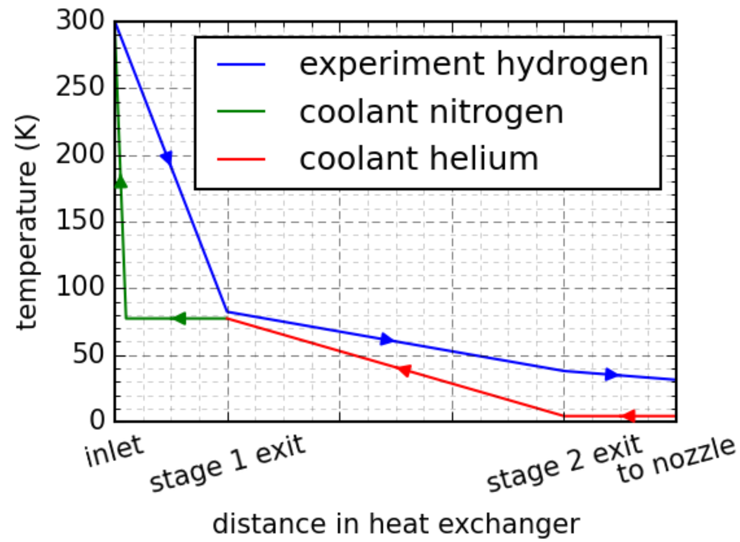
Summary

- **Relevance**: Address lack of safety data, technical information relevant to development of safety codes & standards.
- **Approach**: Develop and validate scientific models to accurately predict hazards and harm from hydrogen (with a focus on liquid hydrogen) releases and subsequent combustion. Generate validation data where it is lacking. Provide a scientific foundation enabling the development/revision of codes & standards.
- **Technical Accomplishments**:
  - Updated Python modeling packages (including ColdPLUME) for ease of use
  - Measured radiative heat flux and flame properties for non-circular nozzles
  - Demonstrated good signal to noise for large-scale diagnostic
  - Planned illumination and data collection strategy for large-scale diagnostic
- **Future work**:
  - Perform vent-stack dispersion experiments at LLNL LH_2 pad
  - Perform large-scale experiments and develop models for pooling and evaporation
  - Use models to advise NFPA 2 code committee on hazards and harm for high priority scenarios (to inform 2022 edition of NFPA 2)

TECHNICAL BACKUP SLIDES

We are running an experiment, releasing ultra-cold hydrogen in the laboratory





- Accurate control/measurement of boundary conditions

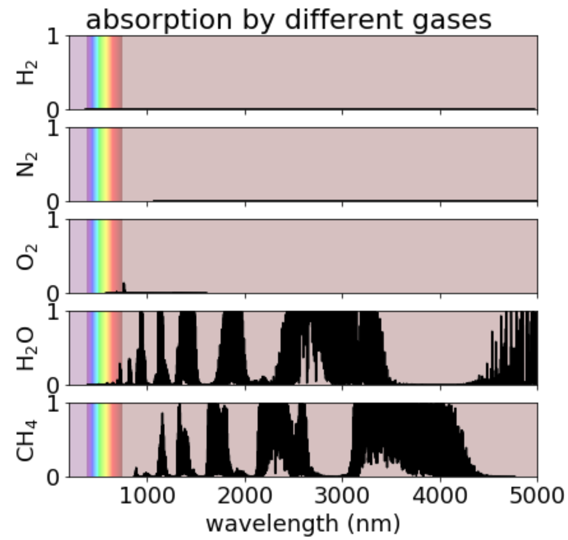
Two high priority scenarios identified by the NFPA 2 code committee are initially targeted for modeling

- ✓ Flow from vent of ultra-cold hydrogen (e.g. trailer venting excess pressure after normal LH_2 delivery or burst disk rupture)
  - Are vent stacks appropriately designed?
  - Separation distance from air intakes and overhead utilities
  - Vertical discharge, 3” diameter pipe, 20-140 psig
- ❑ Release from pipe containing liquid H_2 (e.g. leading from tank to vaporizer or vaporizer itself - caused by thermal cycles or ice falling from vaporizers)
  - Requires ability to model flashing, pooling and evaporation from pools
  - Need to model concentration plume and heat flux from a subsequent fire
  - Horizontal discharge, ¾”-2” diameter pipe, 20-140 psig

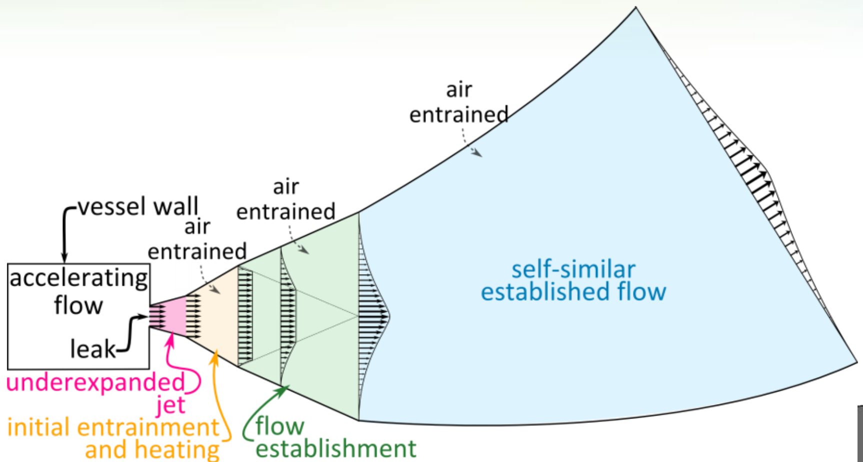
Optical techniques to visualize gas flows

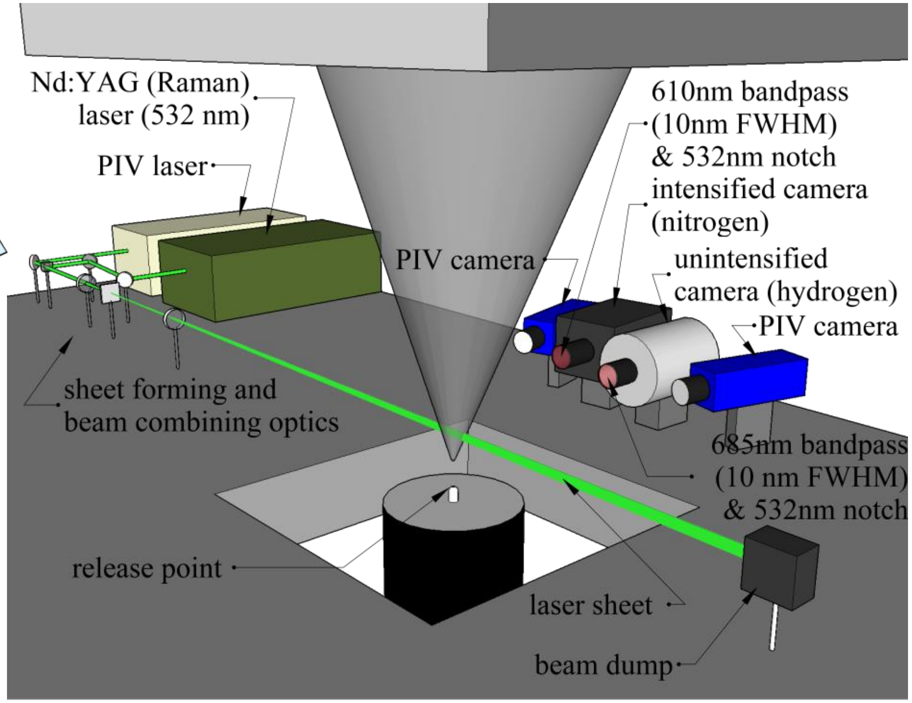
Technique	Principle
Shadowgraphy	Refractive index gradients bend light rays as they pass through density variations.
Schlieren	Same as shadowgraphy. Knife edge enables focused image to form rather than simply shadow.
Fluorescence	Photons are absorbed by molecules at a resonant transition and light is reemitted at a shifted wavelength
Absorption	Gases have absorption features for certain wavelengths of light.
Rayleigh scattering	Elastic scattering off of different molecules is proportional to their cross-sections and number density.
Raman scattering	Inelastic scattering off of different molecules gives each component a spectral fingerprint.

- Why not absorption?
  - H_2 lacks strong absorption features (unlike CH_4)
  - Would require illumination and light collection on opposite sides of plume (or mirror to reflect light)
  - Line-integrated absorption, to quantify, requires multiple angles, tomography



Accomplishment: Completed cryogenic hydrogen dispersion analysis and model validation

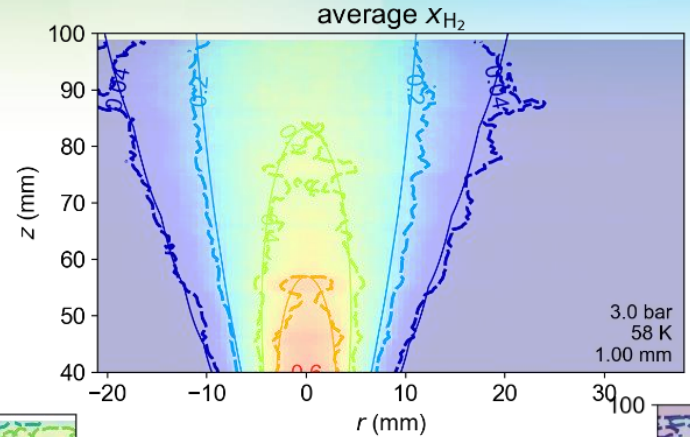


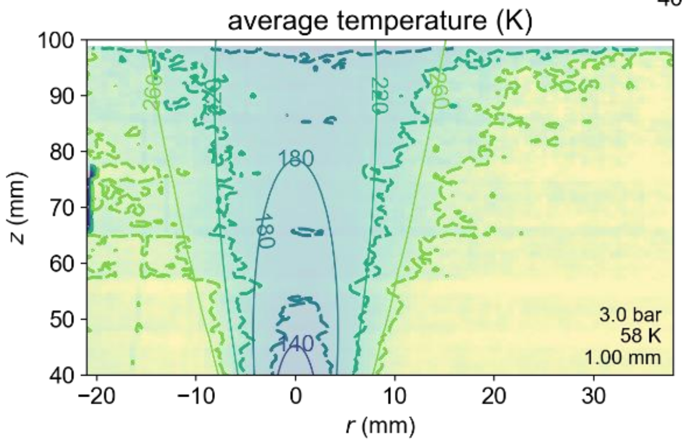


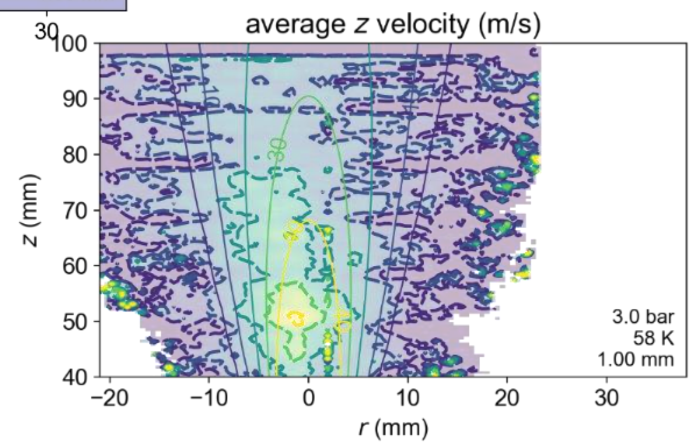
Measuring all independent model parameters:

- ✓ T - temperature
- ✓ x - mole fraction
- ✓ v - velocity
- ✓ B - halfwidth (velocity, concentration, temperature)

ColdPLUME model shows good agreement with the data







- Experimental results shown by shading and thick, dashed lines
- ColdPLUME model results are thin, solid lines

➢ Model accurately simulates mole fraction, temperature, and velocity -- can be used as a predictive tool