Sandia National Laboratories

H2FC Hydrogen and Fuel Cells Program

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

Project ID: SCS010

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Sandia National Laboratories

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Overview

Timeline

- Project start date: Oct. 2003
- Project end date: Sept. 2018*
  - * Project continuation and direction determined by DOE annually

Budget

- FY17 DOE Funding: $500 k
- Partner funding (FY17-18): $175k (CaFCP Auto OEM Group, Linde, Shell)
- Planned FY18 DOE Funding: $650 k
- Planned FY18 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**
  - Bki (contractor for California Fuel Cell Partnership)
  - Fire Protection Research Foundation (research affiliate of NFPA)
- **H2@Scale CRADA**
  - Air Liquide
- **Industry & Research**
  - Fuel Cells and Hydrogen Joint Undertaking (EU)
  - NFPA 2 code committee
  - Shandong University

Relevance

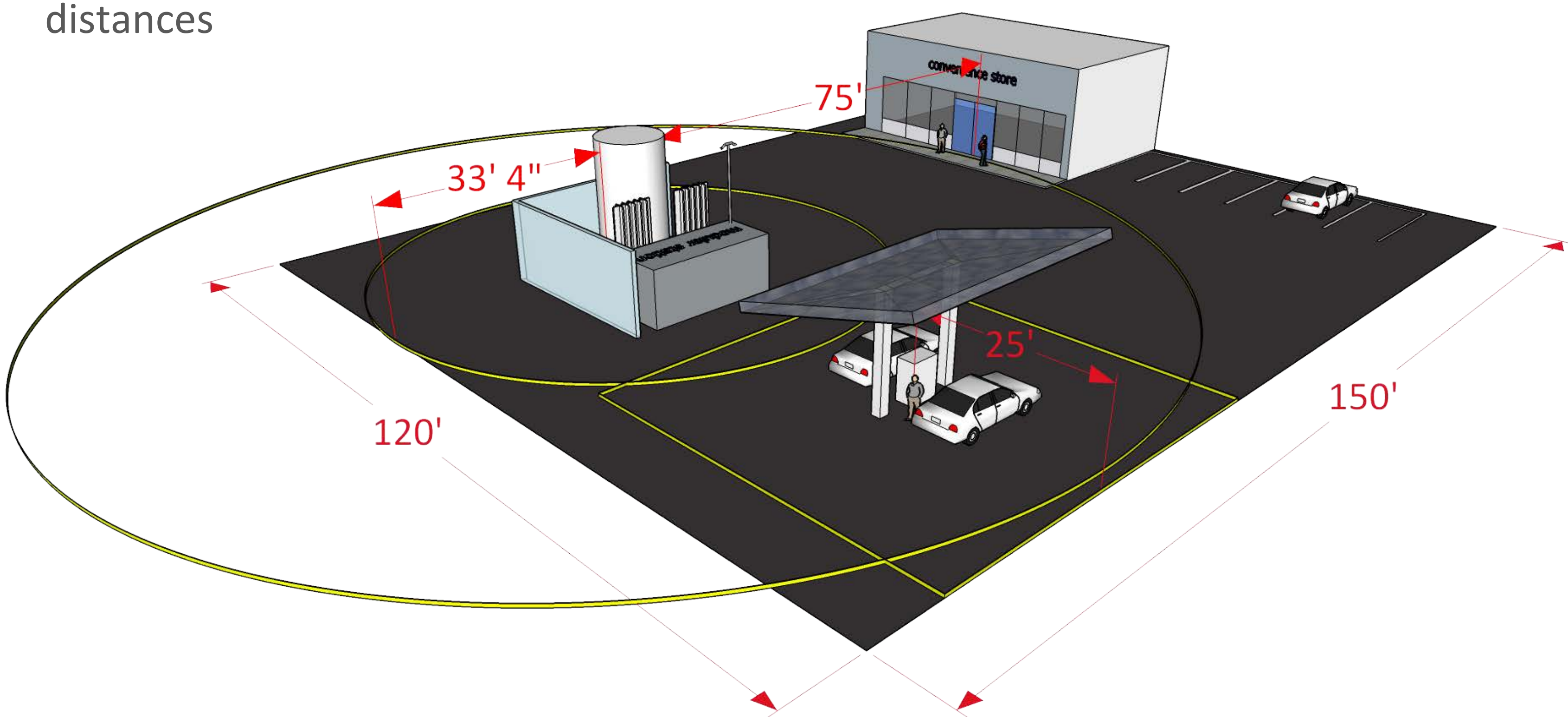
Objectives:

- 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	Goal
A. Safety Data and Information: Limited Access and Availability	Build validated H_2 behavior physics models that enable industry-led C&S revision and Quantitative Risk Assessment
G. Insufficient technical data to revise standards	Perform experiments to address targeted gaps in the understanding of H_2 behavior physics

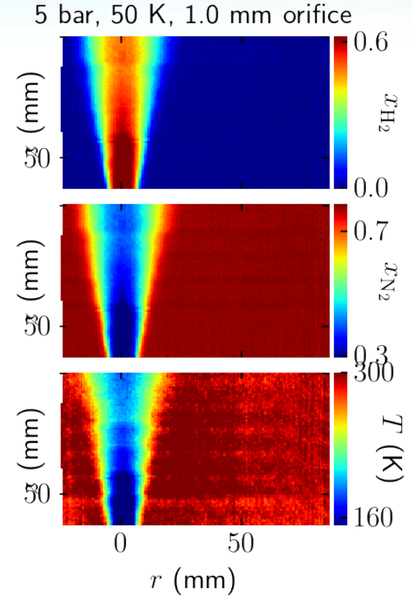
Relevance: Current separation distances for liquid hydrogen are based on consensus, not science

- 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

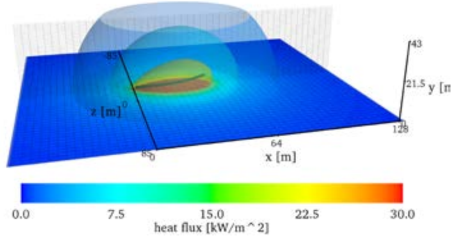


Approach (Sandia H_2 SCS): Coordinated activities that facilitate deployment of hydrogen technologies

- 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: 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

- FY18 goals:
  - Complete analysis of lab-scale experimental data and validation of ColdPLUME model – complete
  - FY18 milestone: Develop a diagnostic and measure the plume from a liquid hydrogen truck depressurization in at least 2 dimensions – in progress

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

Approach: Develop a diagnostic tool for capturing high-fidelity quantitative data for large scale LH_2 experiments

- **Required**: quantitative concentration measurements with < 1 m resolution
- **Desired**: non-intrusive concentration, temperature and velocity measurements in 3-dimensions + time

sensors

Pros:
- Low cost
- Straightforward implementation

Cons:
- Placed in flow, or suction, disturbs flow
- Point measurement (challenging to get spatial resolution)
- Usually slow response time (poor temporal resolution)
- Can be affected by environmental factors (not specific to only H_2)

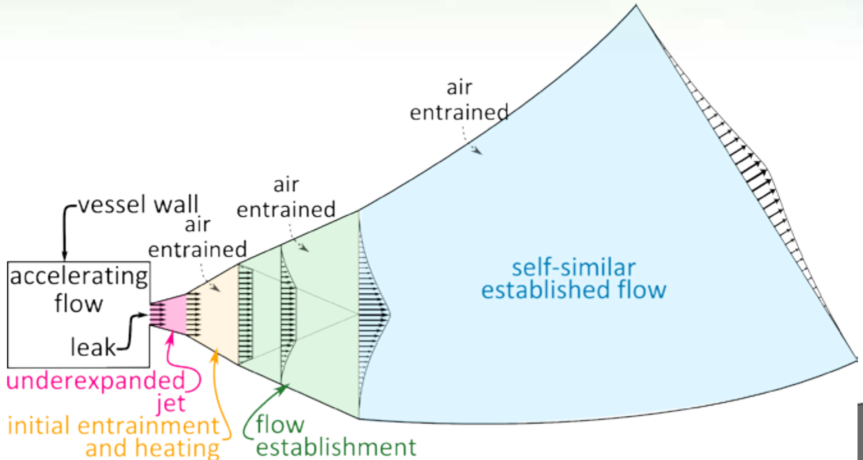
optical diagnostic

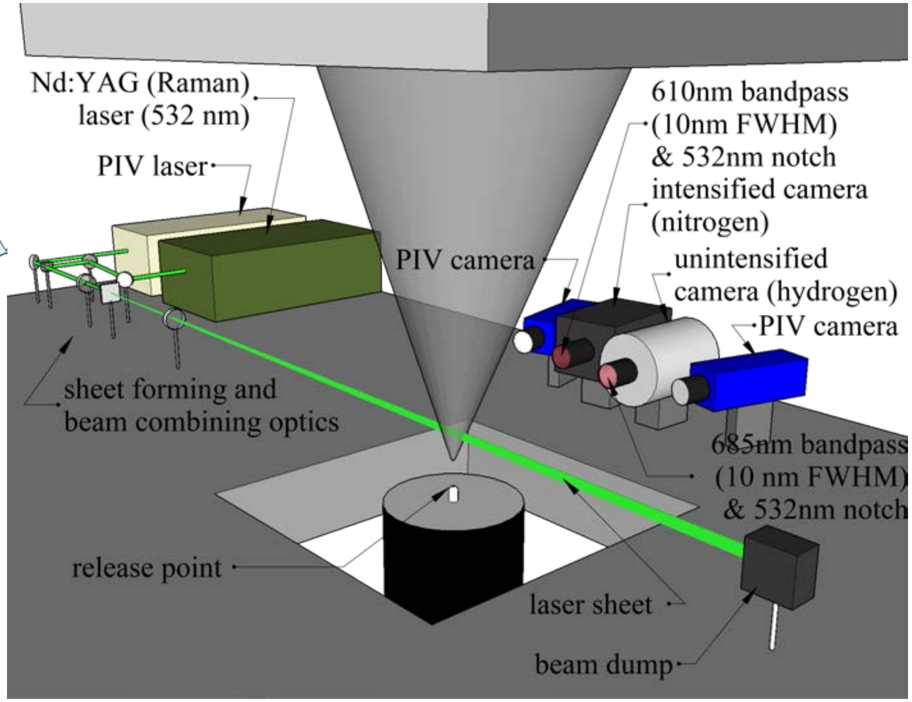
Pros:
- High spatial resolution possible
- High temporal resolution possible
- Non-intrusive

Cons:
- H_2 is difficult to measure optically (no strong absorption features, no fluorescence transitions)

➢ Decision: pursue optical techniques

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)

➢ Added diagnostic to measure velocity of cryogenic hydrogen dispersion

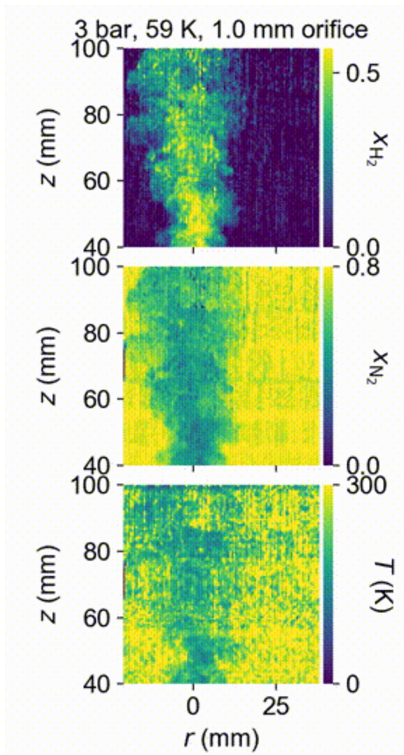
Accomplishment: Experiments with variations in temperature, pressure and nozzle size

Experimental parameters

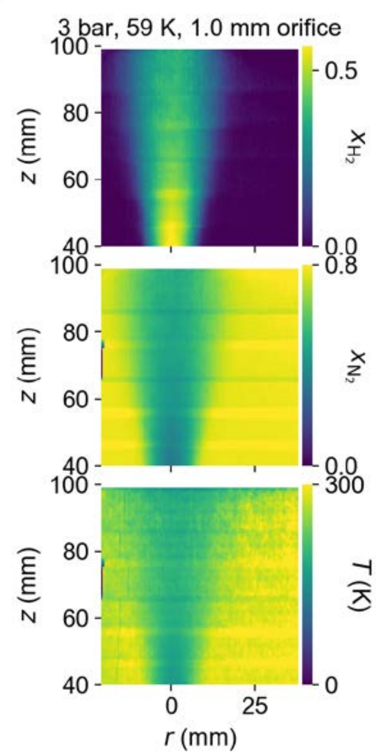
T_{noz} [K]	P_{noz} [bar_{abs}]	d [mm]	T_{throat} [K]	n_{hts}
58	2	1	43.5	4
56	3	1	41.9	4
53	4	1	39.6	4
50	5	1	37.4	5
61	2	1.25	45.7	6
51	2.5	1.25	38.2	2
51	3	1.25	38.2	6
55	3.5	1.25	41.2	3
54	4	1.25	40.4	2
43	4	1	32.1	2
59	3	1	44.2	6
56	3.5	1	41.9	1
80	3	1	60.3	5

With PIV (last four rows)

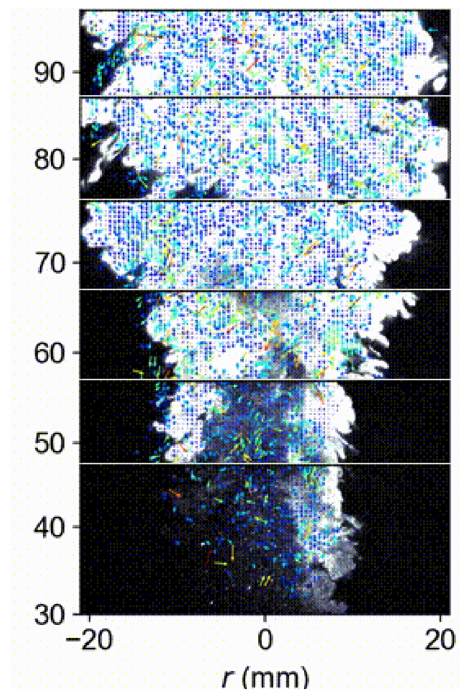
Single image results



Average results



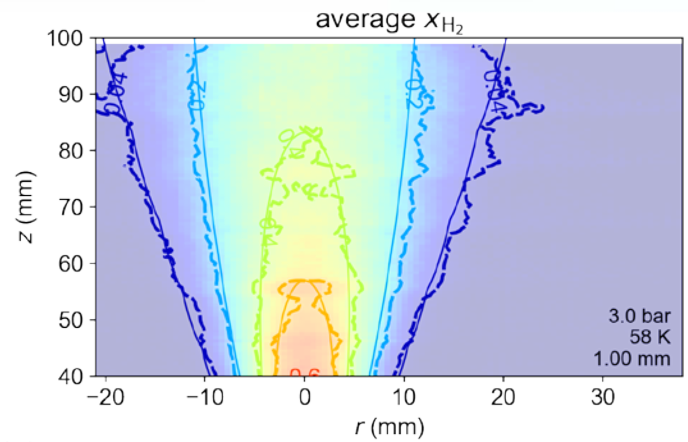
Velocity vectors superimposed on Mie scattering

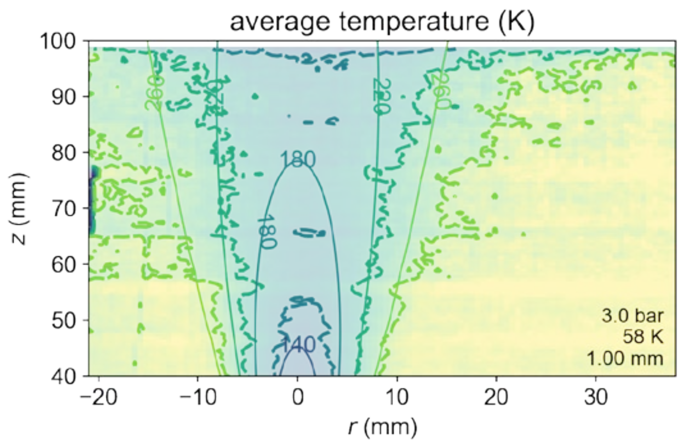


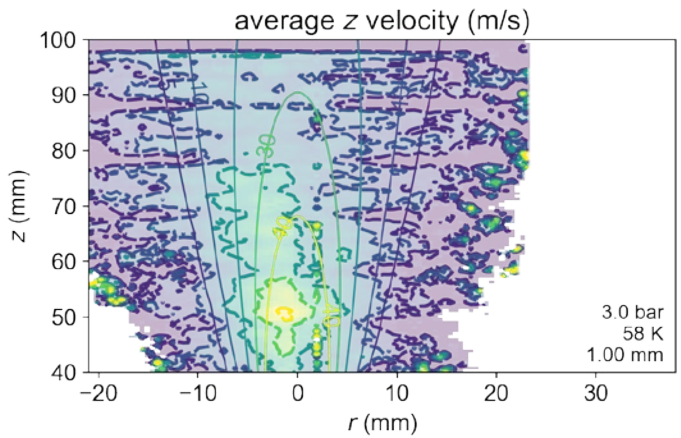
➢ Measuring dispersion in two-dimensions

Accomplishment: The 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, therefore can be used as a predictive tool

Progress: Evaluated the suitability of various optical diagnostics for measuring large-scale LH_2 releases

- Schlieren – cannot distinguish between temperature and concentration caused density variations (not quantitative)
- Fluorescence – no fluorescing species in the flow or species that could be seeded into the flow
- Absorption – no strong absorption features, and complex detector/illumination scheme
- Rayleigh – cannot distinguish between temperature and concentration caused density differences, entrained moisture scatters too much light
- Raman – shown to work in a laboratory setting, enables quantification of temperature and composition in multiple dimensions

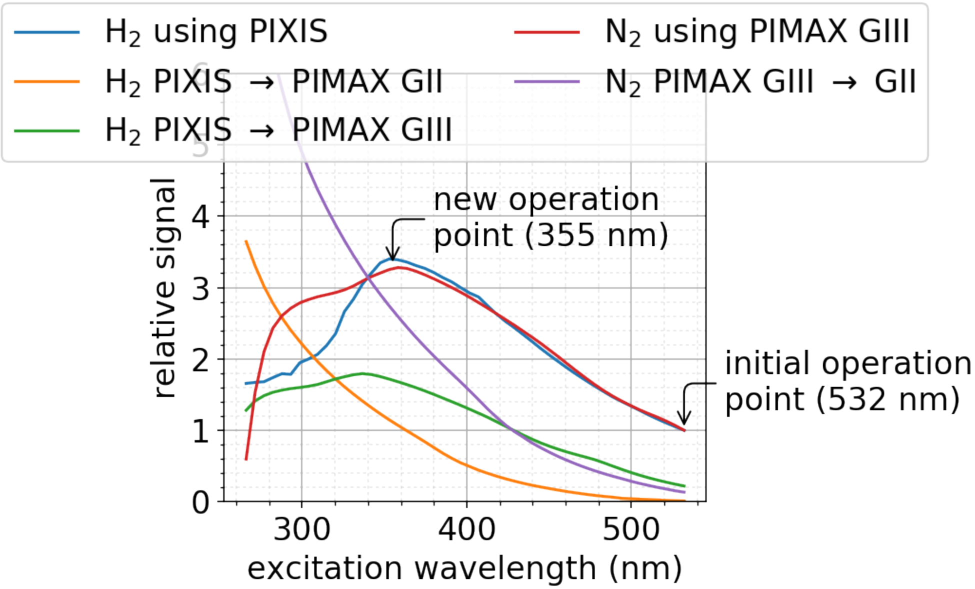
➢ Challenge is how to scale-up laboratory Raman setup for larger releases

Progress: Improvements in the lab-scale approach and tests at lab-scale enable scaling the diagnostic

Shifting Raman excitation from visible (532 nm) to UV (355 nm):

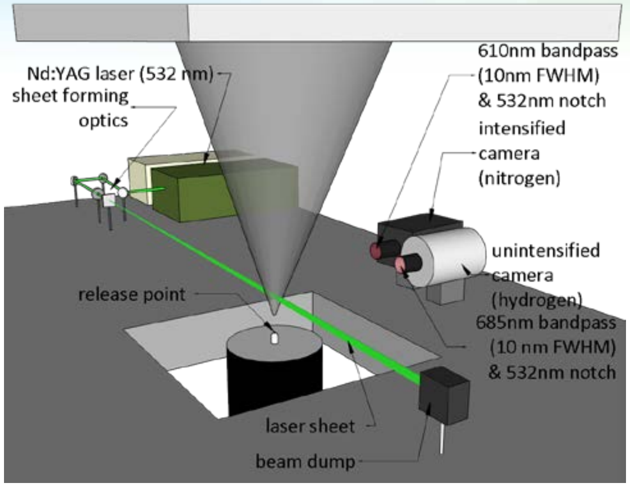
- Improves signal to noise (key for scaling diagnostic)
- Enables truly simultaneous PIV and Raman (PIV pulses can bracket Raman pulse without interference in either diagnostic)

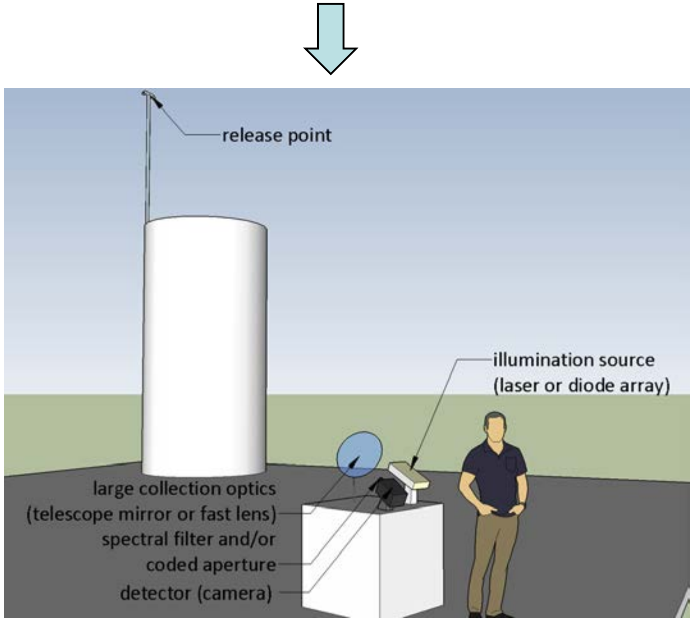
Relative response for different camera/gas detection combinations



Progress: Identifying technical hardware solutions to enable the large-scale diagnostic

- Challenge: need large field of view and large aperture to collect small number of photons emitted
  - Reflective optics (large telescope mirror)
  - Refractive optics (Fresnel lens)
- Challenge: reasonable cost illumination system with high-power, low-wavelength, pulsed system
  - High-power laser with volumetric illumination
  - High-repetition rate laser scanned across the area quickly
  - High-power diodes/diode arrays
- Challenge: Effective background light suppression (both sunlight and reflected illumination light from condensed water vapor)
  - Time gating
  - Spectral gating
- Challenge: Improved temporal, spectral, and/or spatial resolution
  - Coded aperture sensing
  - Tomography





Response to last year's Reviewer's comments

- There could be additional focus on how some of the observed effects—for example, condensation of air gases …— might be an issue in real-world hazards.
- 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 will include experiments to study these environmental effects (e.g. variations in atmospheric humidity) in our test plans and experiments after developing the diagnostic
- The project will need to address a wide array of release scenarios in order to have an impact on setback distances. The investigators should work now to understand the scope of relevant scenarios and incorporate them into future plans (in addition to currently planned baseline work).
  - We agree that there are a wide array of release scenarios. That is why the focus of our work is on model validation so we can perform targeted experiments to make sure the models are predictive and exercise the models rather than experimentally investigating all scenarios of interest.
- The large-scale experiment will be critical. The project needs correct funding through increased contribution from industry
  - We have secured a commitment for additional funding through an H2@Scale CRADA with Air Liquide that will accelerate progress.

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 being negotiated (as of April, 2018: $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)
  - Hosting visiting professor with expertise on hydrogen behavior

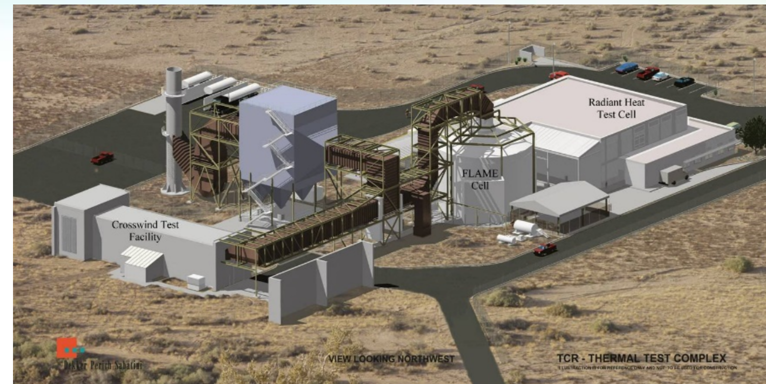
Remaining challenges: Assembling a cost-effective system and designing large-scale release experiments

Diagnostic requires optical components with unique characteristics

- Need to work within limited budget
- Time constraints for next edition of NFPA 2

Solution:

- Use off-the-shelf components in unique configurations



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 FY18
  - Complete truly simultaneous Raman/PIV using different laser excitation wavelengths for each diagnostic
  - Incorporate validated ColdPLUME model into HyRAM
  - Prove out largescale diagnostic concepts and lay-out path forward for final diagnostic design
  - Develop R&D plans for large-scale experiments
- FY19
  - Refine largescale diagnostic design and put together final system
  - Conduct large-scale release experiments to characterize hydrogen pooling, evaporation, and interaction with atmosphere
  - Develop validated models of hydrogen pooling and evaporation
- Out years
  - Simulate 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

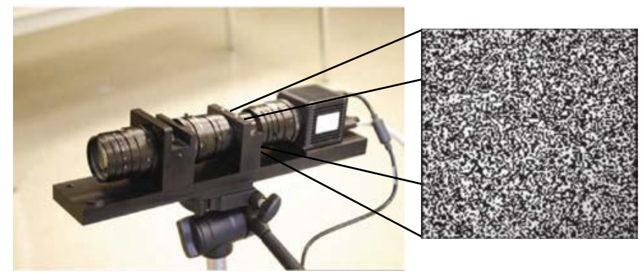
- **Relevance**: Address lack of safety data, technical information relevant to development of safety codes & standards.
- **Approach**: Develop and validate scientific models to accurately predict hazards and harm from hydrogen (with a focus on liquid hydrogen) releases and subsequent combustion. Generate validation data where it is lacking. Provide a scientific foundation enabling the development/revision of codes & standards.
- **Technical Accomplishments**:
  - Simultaneous Raman imaging and particle imaging velocimetry used to characterize concentration, temperature, and velocity profiles of cryogenic hydrogen releases at lab-scale
  - ColdPLUME model proven to be valid for lab-scale cryogenic hydrogen releases
  - Determined Raman scattering to be the most applicable scientific phenomena to quantify large-scale cryogenic hydrogen release physics
- **Future work**:
  - Finalize design and construction of large-scale diagnostic
  - 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

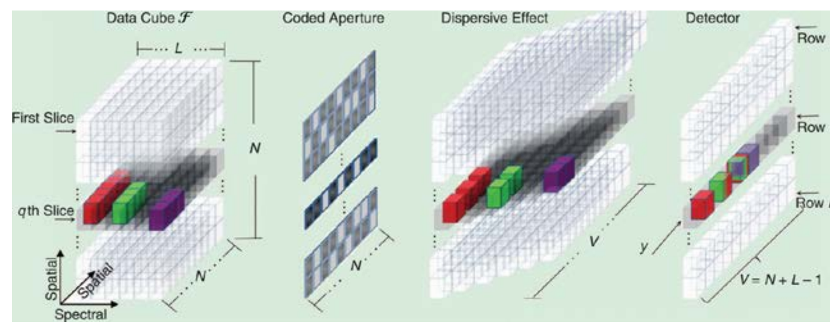
Optical techniques to visualize gas flows

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.

coded apertures can decode additional information from images



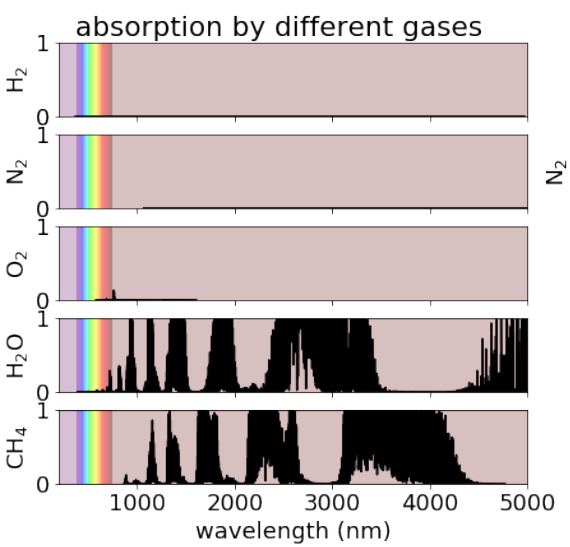
dx.doi.org://10.1117/12.919292

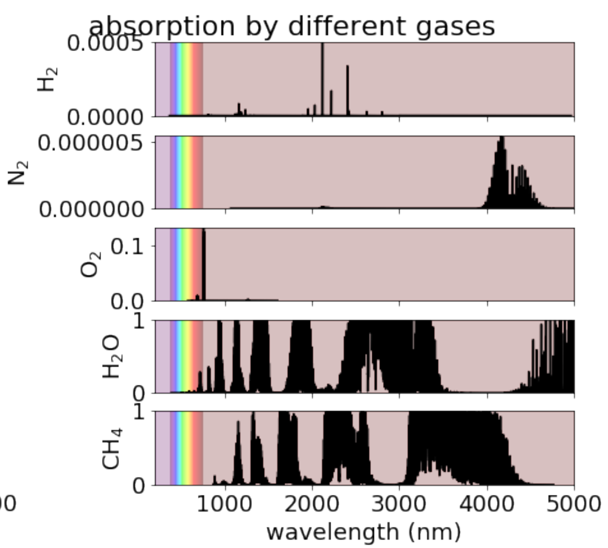


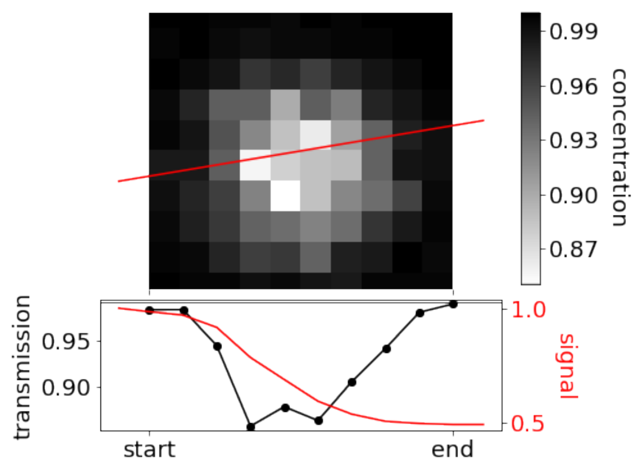
dx.doi.org://10.1109/MSP.2013.2278763

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

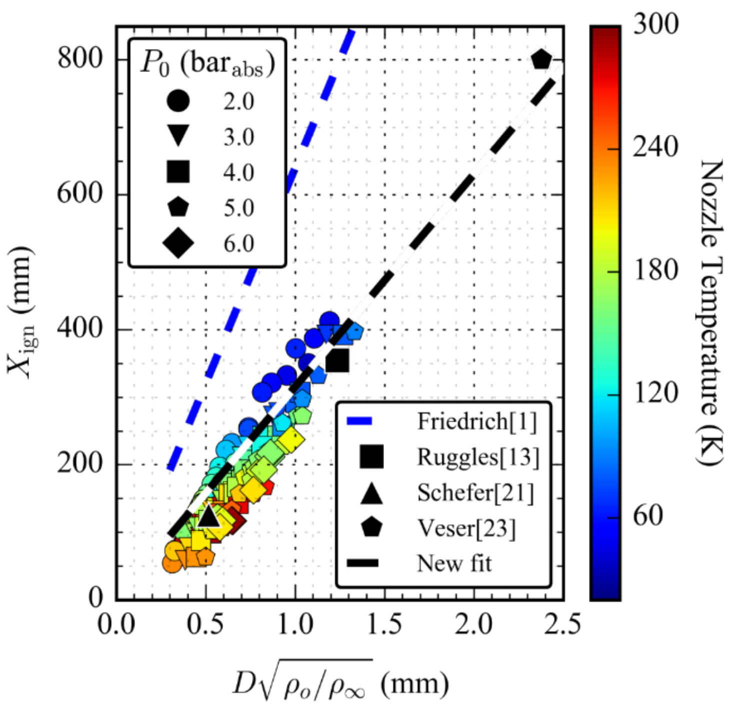


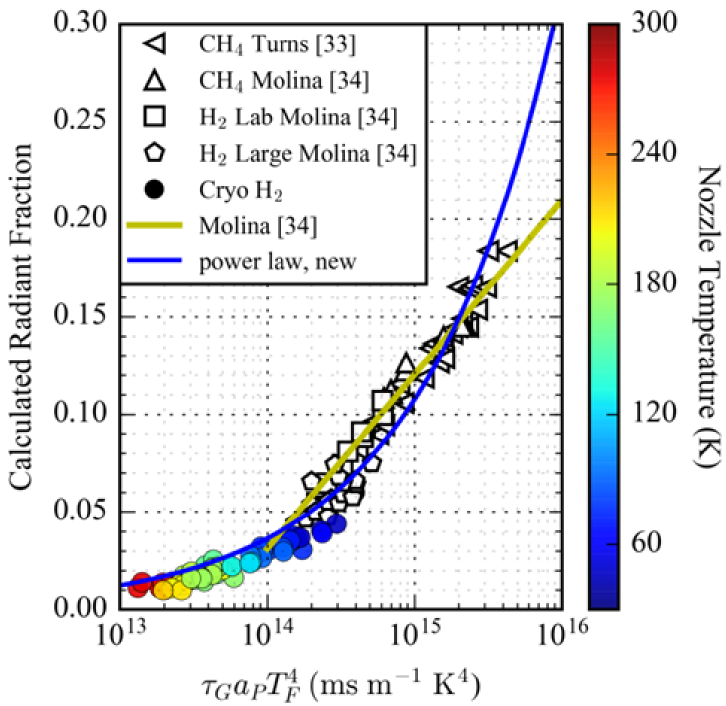




Data from HITRAN Application Programing Interface (HAPI): 10.1016/j.jqsrt.2016.03.005

Ignition distance and radiant fraction were mapped out in FY16

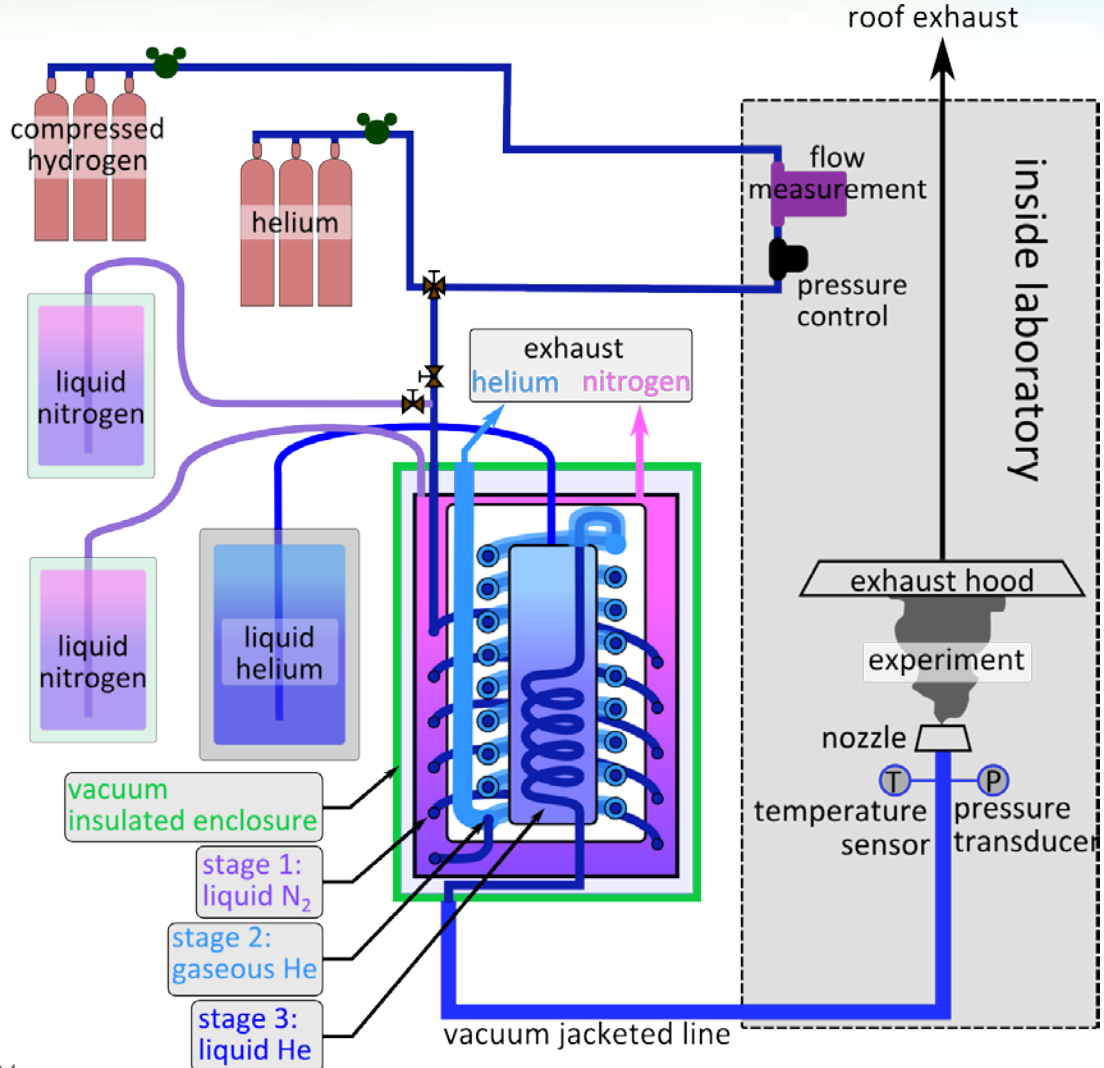


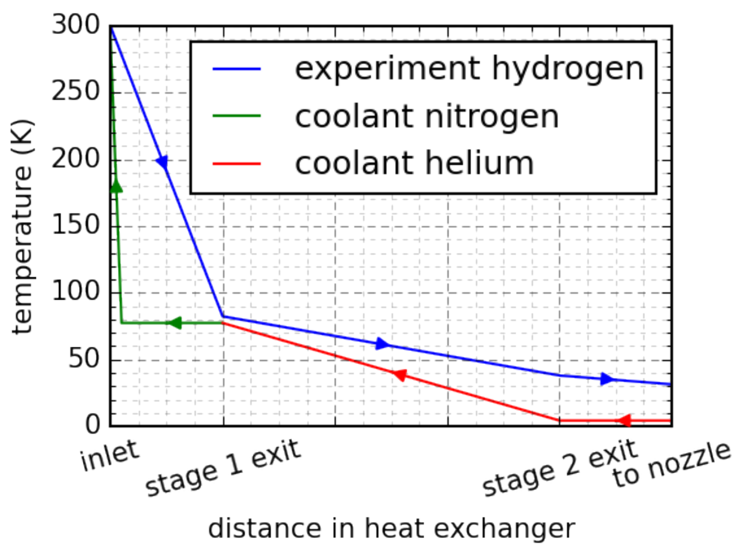


Two high priority scenarios identified by the NFPA 2 code committee are initially targeted for modeling

- ✓ 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

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





- Accurate control/measurement of boundary conditions