

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

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DOE Hydrogen and Fuel Cells Program Annual Merit Review

June 7, 2016

Project ID: SCS010

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Overview

Timeline

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

Budget

- FY15 DOE Funding: \$415k
- Planned FY16 DOE Funding: \$600k
- Partner funding:
 - \$100k in kind from Linde
 - \$175k committed stakeholder funds (CaFCP Auto OEM Group, Linde, Shell)
- Total DOE Project Value: \$23M (includes funding for SCS010, SCS011, and SCS025 since 2003)

Barriers

- A. Safety Data and Information:
Limited Access and Availability
- G. Insufficient technical data to revise standards

Partners

- **Stakeholder CRADA**
 - BKi
 - Fire Protection Research Foundation
- **Industry & Research**
 - Linde
 - Tsinghua University
 - NFPA 2 code committee

Relevance

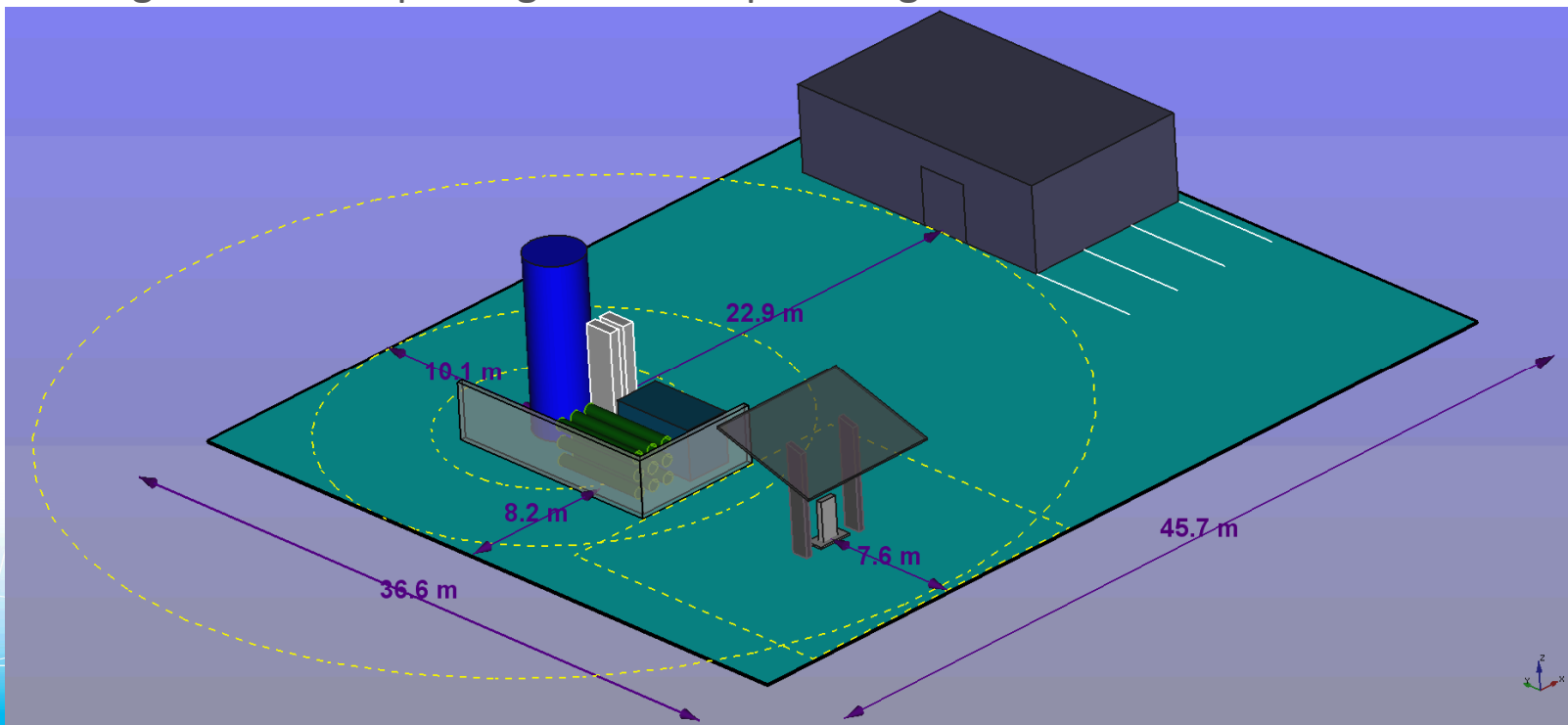
Objectives:

- Develop a science & engineering basis for the release, ignition, and combustion behavior of hydrogen across its range of use (including high pressure and cryogenic)
- Facilitate the assessment of the safety (risk) of H₂ 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

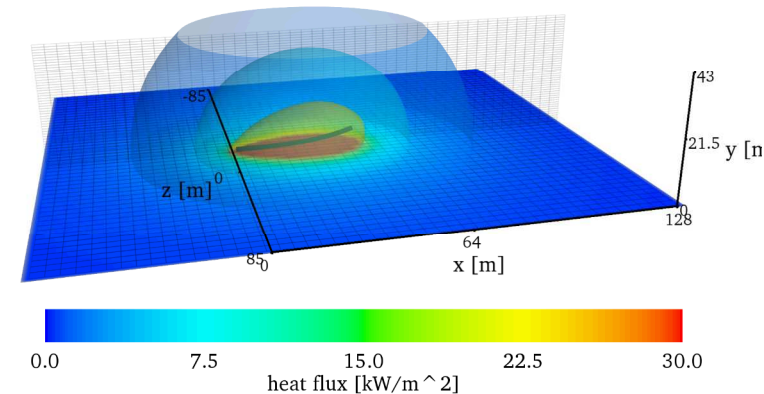
Relevance: Current separation distances for liquid hydrogen are based on consensus, not science

- Previous work by this group led to science-based, reduced, gaseous H₂ separation distances
- Higher energy density of liquid hydrogen over compressed H₂ makes it more economically favorable for larger fueling stations
- Even with credits for insulation and fire-rated barrier wall 75 ft (22.9 m) offset to building intakes and parking make footprint large



Project Approach: Coordinated activities that facilitate deployment of hydrogen technologies

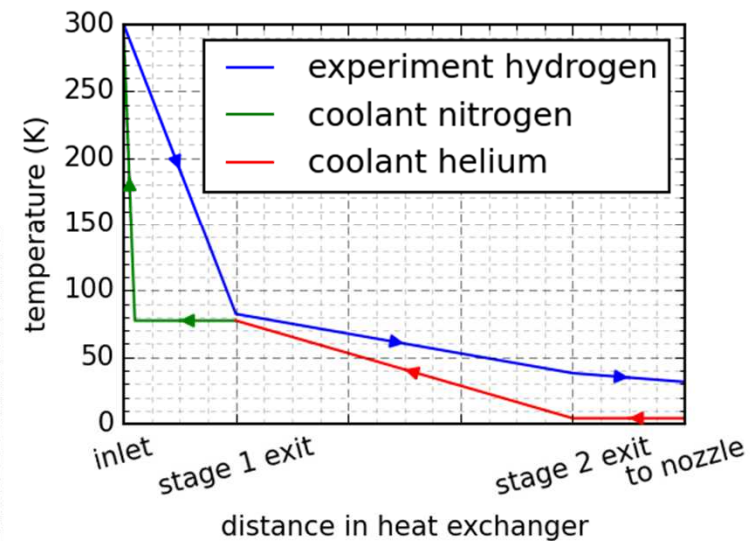
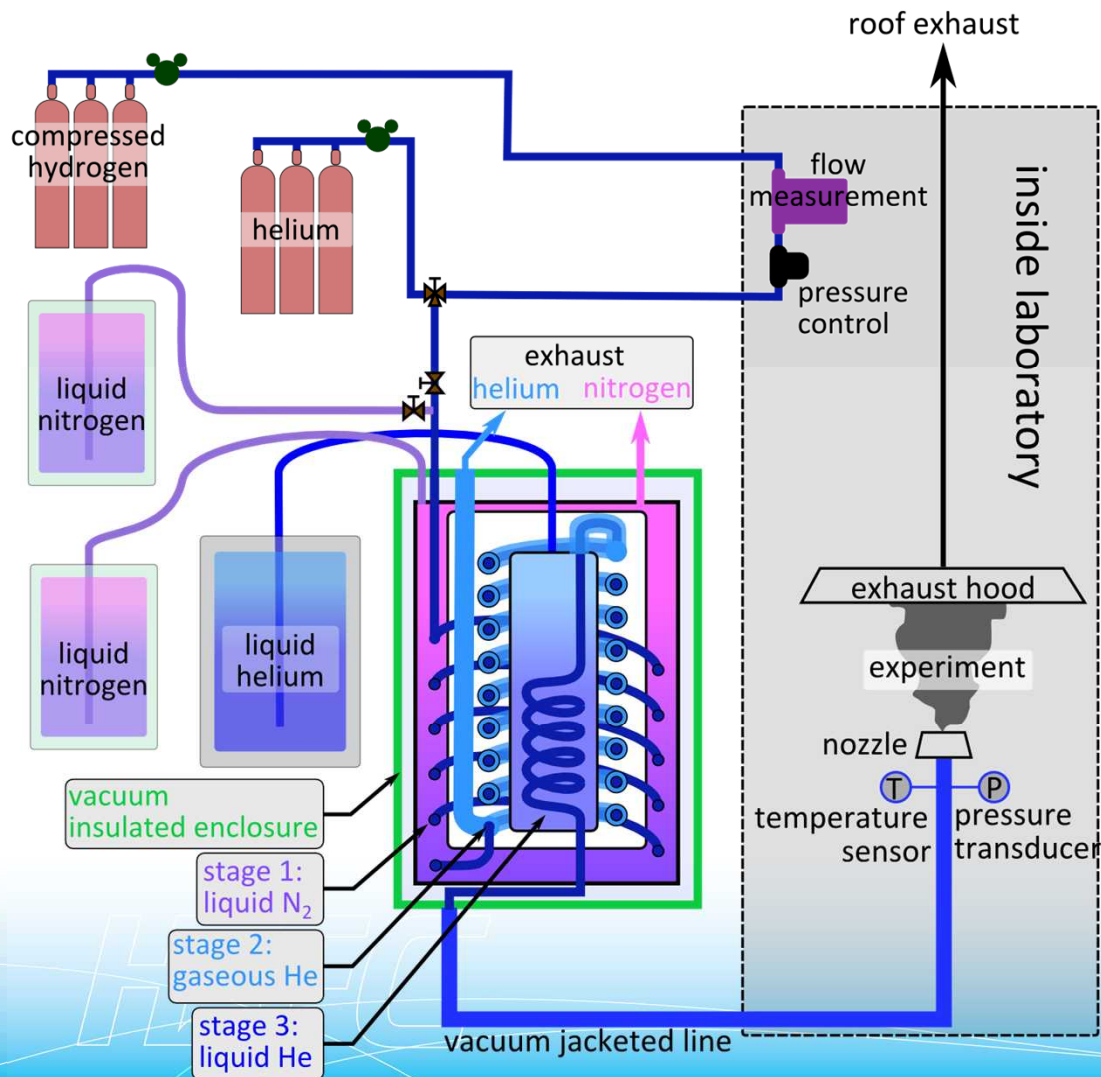
- Hydrogen Behavior (this project, SCS010)
 - **Develop and validate scientific models** to accurately predict hazards and harm from liquid releases, flames, etc.
- Quantitative Risk Assessment, tools R&D (SCS011)
 - **Develop integrated methods and algorithms** enabling consistent, traceable, and rigorous QRA (Quantitative Risk Assessment) for H₂ facilities and vehicles
- Application of R&D in regulations, codes & standards (SCS025)
 - **Apply QRA and behavior models to real problems** in hydrogen infrastructure and emerging technology



Approach: FY15/16 Behavior Milestones

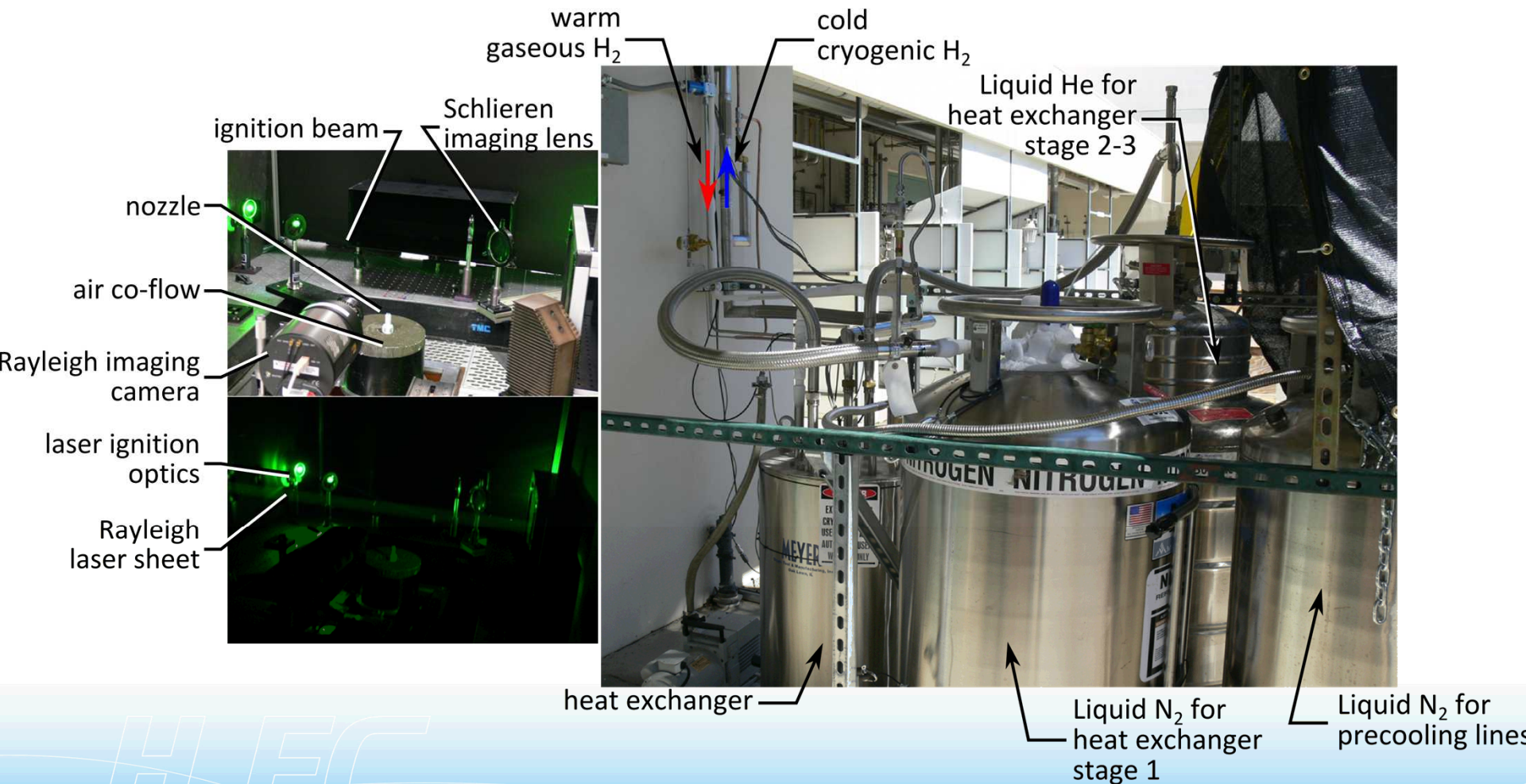
Hydrogen Behavior	Completion date or status
<ul style="list-style-type: none"> • Cryogenic Hydrogen Release Experiment 	
<ul style="list-style-type: none"> • Complete construction of laboratory • Initial experimental campaign • Analyze data in the context of the cold plume model 	Feb. 2016 Ongoing (75%) Ongoing (25%)
<ul style="list-style-type: none"> • Reduced-order physics models and documentation for HyRAM 	
<ul style="list-style-type: none"> • Plume model that includes an energy balance • Additional visualizations for overpressure, plume, and layering behavior • Improved plume model boundary condition implementation • Unvalidated plume/flame wall interaction model <ul style="list-style-type: none"> • Experimental plan for validation data 	Jan 2016 Jan 2016 Jan 2016 Ongoing (50%)
<ul style="list-style-type: none"> • Plume model spreading ratio 	
<ul style="list-style-type: none"> • Experimentally measure concentration to velocity spreading ratio for hydrogen 	Ongoing (50%)

Accomplishment: Construction of the cryogenic hydrogen release laboratory was completed



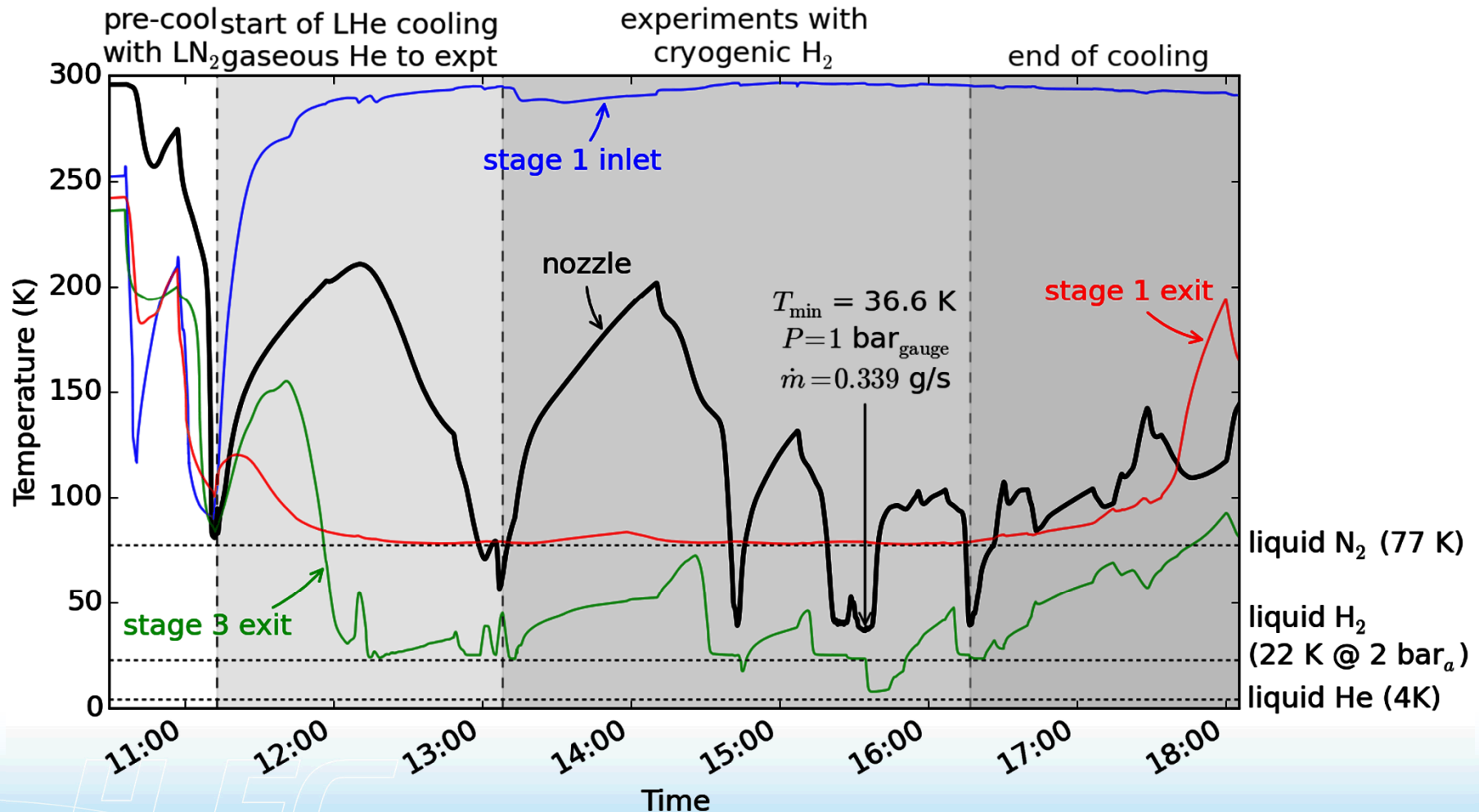
➤ Accurate control/measurement of boundary conditions

Accomplishment: Construction of the cryogenic hydrogen release laboratory was completed



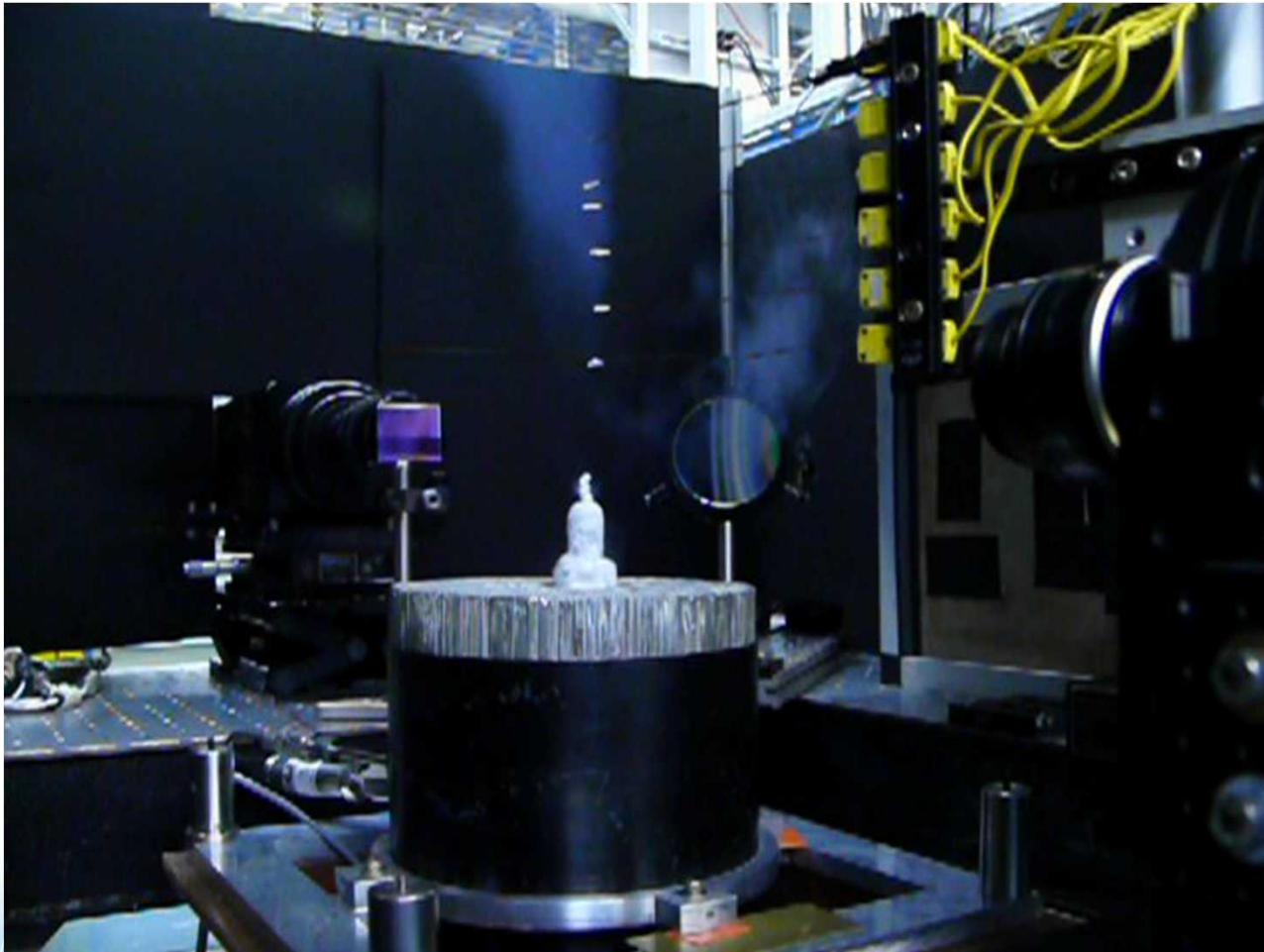
➤ Multiple diagnostics are used to precisely characterize releases

Accomplishment: Hydrogen was cooled to a liquid and released in the laboratory



➤ Experimental challenges include avoidance of freezing air and hydrogen

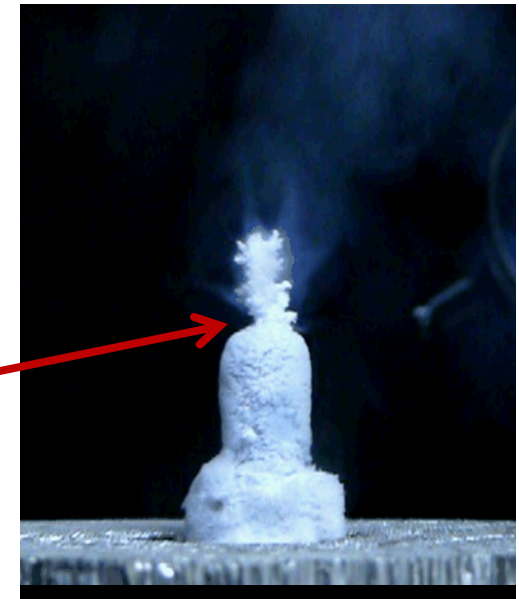
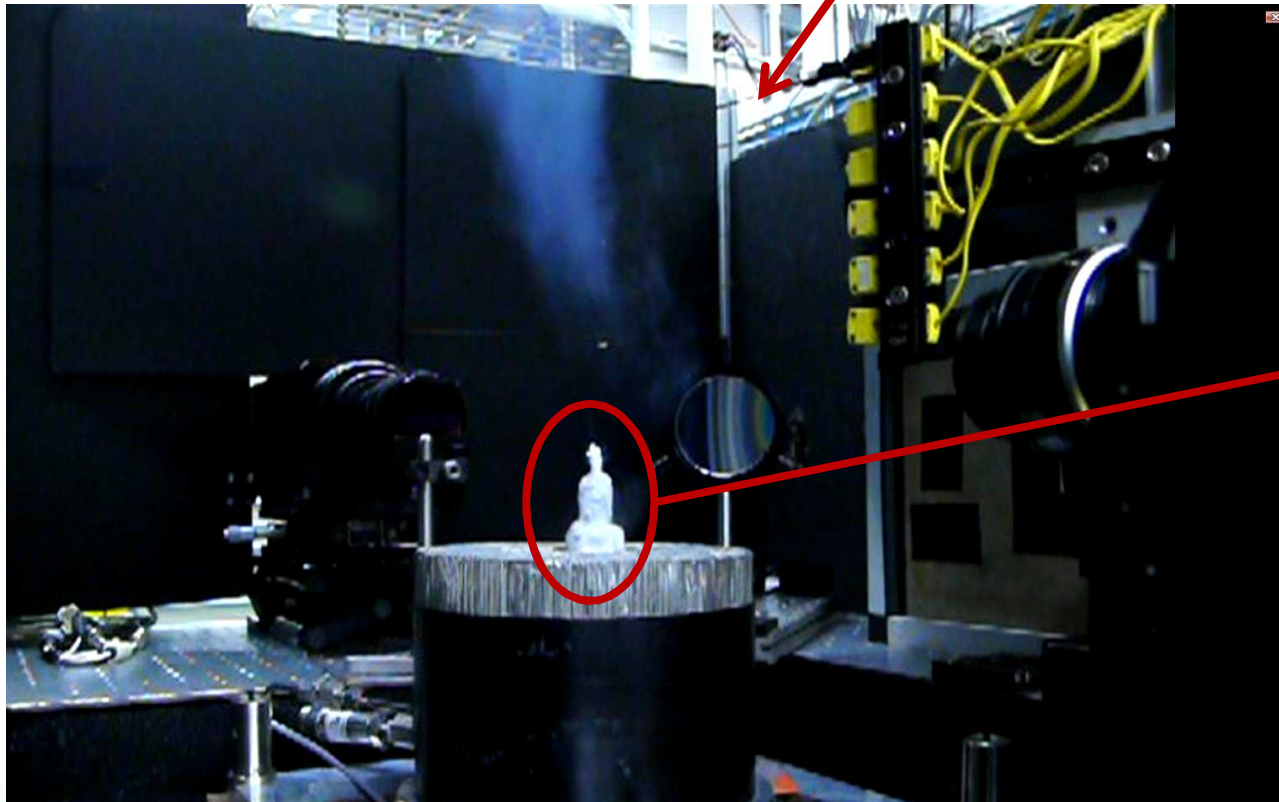
Accomplishment: Hydrogen was cooled to a liquid and released in the laboratory



- Entrained moisture easily condenses, and air may also be condensing

Progress: Icing observed at the nozzle during cryogenic H₂ release

Array of thermocouples measuring the plume temperature

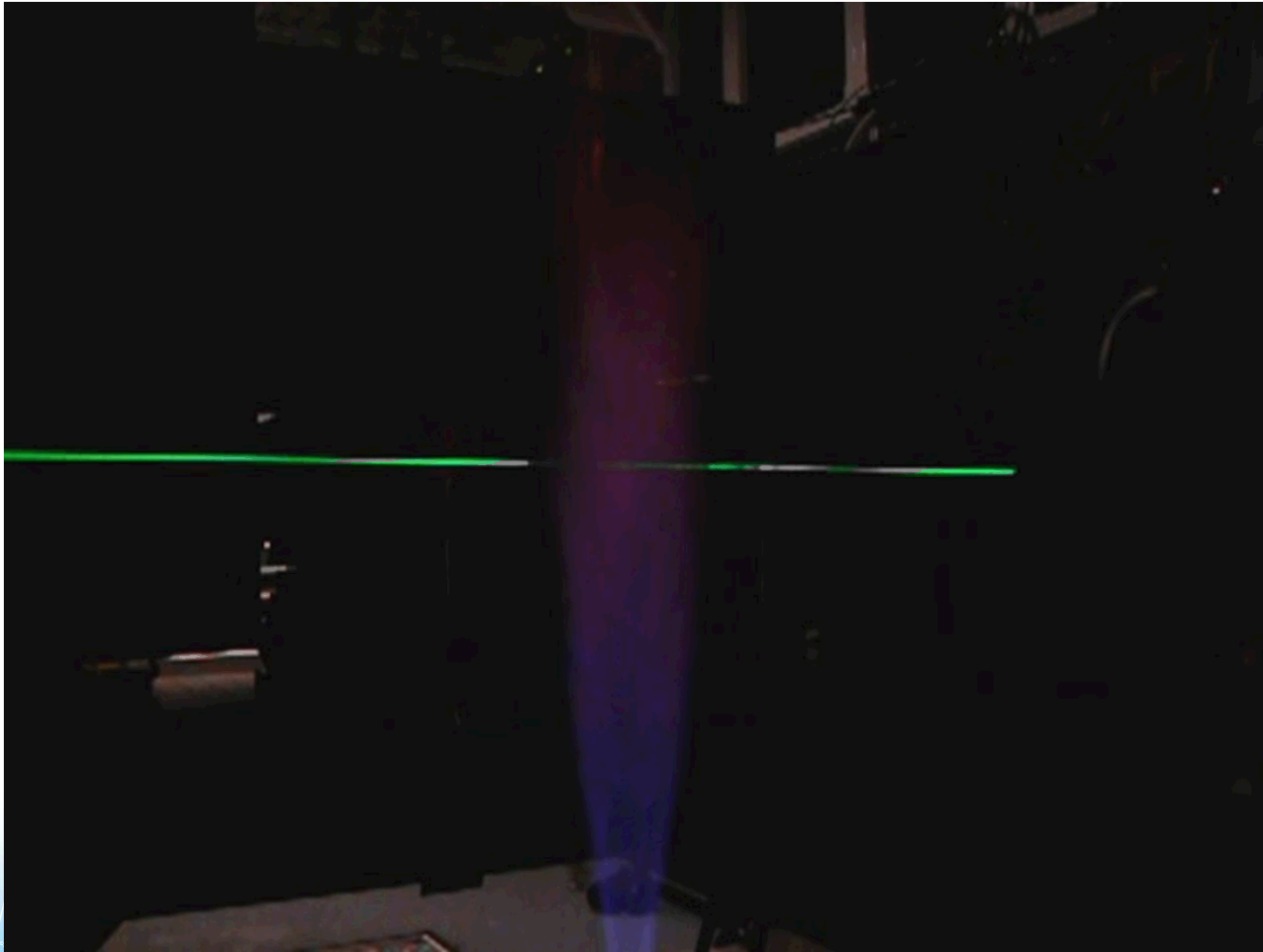


(air, moisture?)
icing around liq.
H₂ jet column

- Challenging to provide sufficiently dried air while maintaining experimental integrity

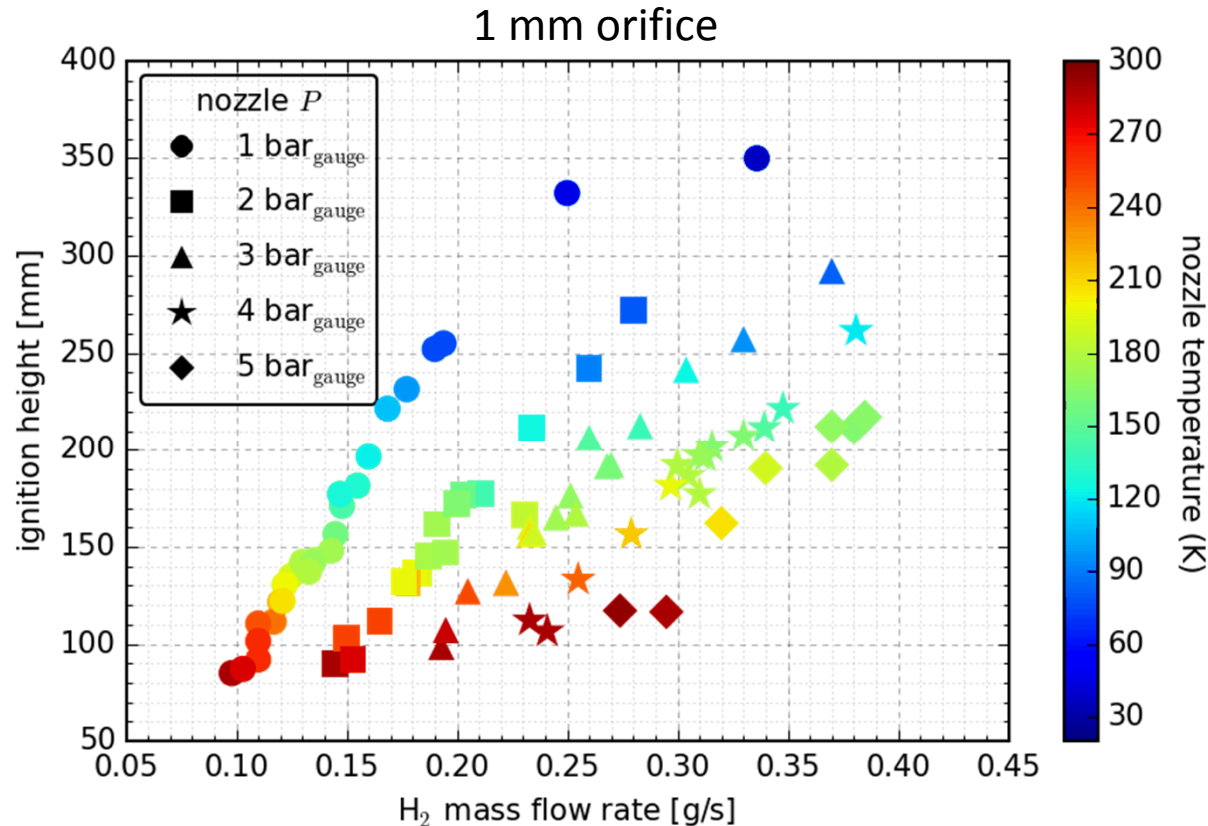
Progress: A laser spark is used to ignite cryogenic hydrogen

P = 1 bar, T = 37 K, Max. Ignition Distance = 325 mm



- Carefully controlled laboratory conditions are ideal for model validation

Progress: The ignition distance for cryogenic hydrogen is being mapped out



- for a given mass flow, ignition of cold H₂ occurs much further from the release point
- mass flow changes from temperature affects ignition distance much more than pressure
- mass flow of H₂ increases significantly as temperature decreases

Response to last year's Reviewer's comments

- More effort should be made to bring portable liquid hydrogen tanks into use in the United States because that would enable release and ignition testing to support model validation and revision of liquid hydrogen setback distances. A facility should be developed to test hydrogen equipment enclosures to validate the sizing models that determine deflagration venting.
 - The cryogenic hydrogen release lab is now operational, despite the lack of liquid hydrogen availability. Ongoing work is aimed at model validation and fire code revision.
- It is recommended that this application [HyRAM] be extended to include effects from liquid spills and overpressures due to confinements.
 - Experimental work on liquid hydrogen will tie directly into HyRAM, extending its functionality. Overpressure models have been implemented in HyRAM this FY (see SCS011 following this presentation).

Note: This effort was not independently reviewed at the 2015 AMR. Portions of this work was communicated in the 2015 SCS-011 presentation: Hydrogen behavior and Quantitative Risk Assessment, and comments were taken from there.

Collaborations have enabled this research and expanded impact

H₂ behavior (SCS010) collaborations

- CRADA with **Linde** to develop cryogenic release laboratory
 - In-kind support, data exchange to get lab up and running
- CRADA with **BKi** to fund future experiments
 - Commitments from **Shell, Linde, CaFCP Auto OEM group**
 - inquires out to other industry organizations and local government agencies
- **NFPA 2** Technical Code Committee
 - Regular attendance with expert advisory role
- **Tsinghua University**
 - Student visit to study expansion zone of underexpanded jets

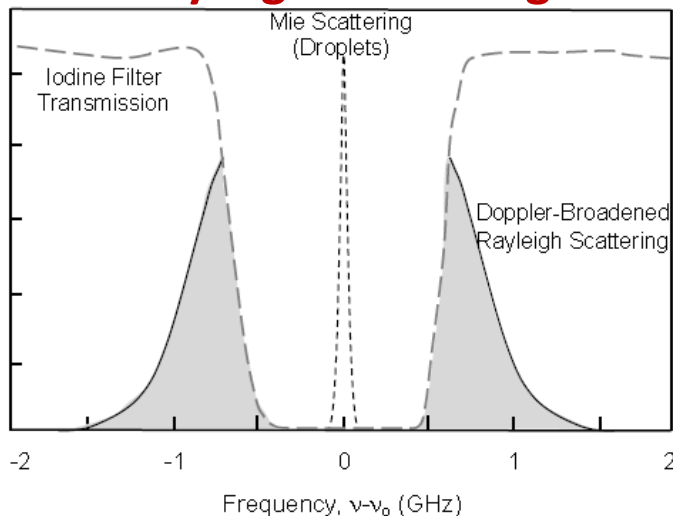
Expanded impact through HyRAM (SCS011) and C&S participation (SCS025)

- HyRAM users – including **ITM Power, Paul Scherrer Inst., ZCES, AVT, ...**
- **Gexcon** - Technical exchanges on validation activities for physics models, integration of safety methodology approaches; In-kind support - provided FLACS research license
- **PNNL** - Technical exchanges on PBD;QRA; Hydrogen Safety Panel
- **NREL** - Technical exchanges on PBD; QRA
- **HySafe** - Technical exchanges on safety methodology; QRA toolkits
- **ISO TC197 WG24**- SNL co-leads sub-team on safety methodology
- **IEA HIA Task 37** -SNL leads sub-task on Safety Integration Toolkits;
- **H2USA** - Various working groups

Remaining challenges: Filtered Rayleigh scattering will allow concentration and temperature measurements

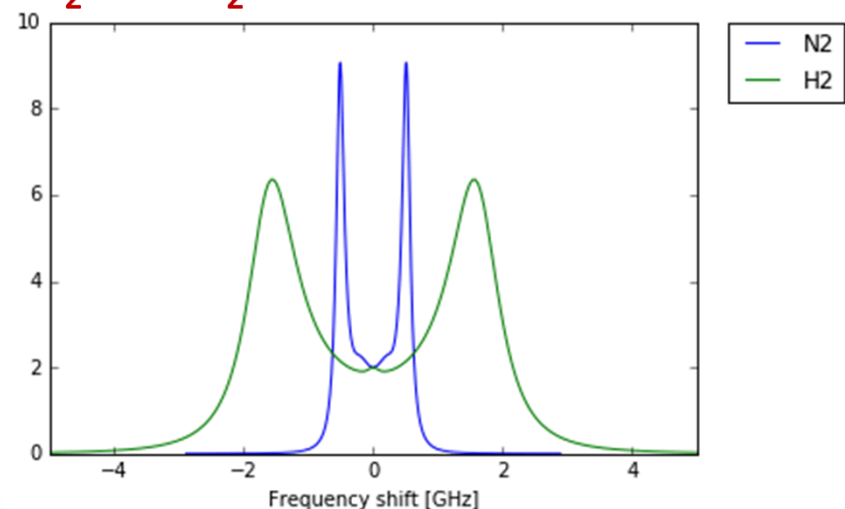
- At temperature below 200 K, water vapor from entrained air condenses
- Mie scattering from condensed water overwhelms Rayleigh signal
 - Filtered Rayleigh takes advantage of Rayleigh scattering line broadening

Filtered Rayleigh Scattering Concept



Using a narrow band-width ($\Delta\nu < 0.003 \text{ cm}^{-1}$) laser and a molecular I₂ filter tuned to center wavelength of the laser beam, it possible to filter out the Mie scattered light

Rayleigh Scattering Spectra for H₂ and N₂ at T = 80 K



Doppler broadened H₂ spectra is promising for filtered Rayleigh scattering measurements

Proposed future work

- Remainder of FY16
 - Complete ignition study
 - Implement filtered Rayleigh scattering diagnostic on cold releases
 - Measure atmospheric temperature velocity to concentration spreading ratio
 - Continued support of HyRAM toolkit (SCS011) with behavior model integration, development, and documentation
- FY17
 - Complete validation/development of cold jet/plume model
 - Simulate high-priority scenarios defined by NFPA 2 code committee
 - Design and begin laboratory experiments with vertical walls
 - Continue validation/development of jet/flame wall model
 - Addition of cryogenic jet/plume model into HyRAM toolkit (SCS011)

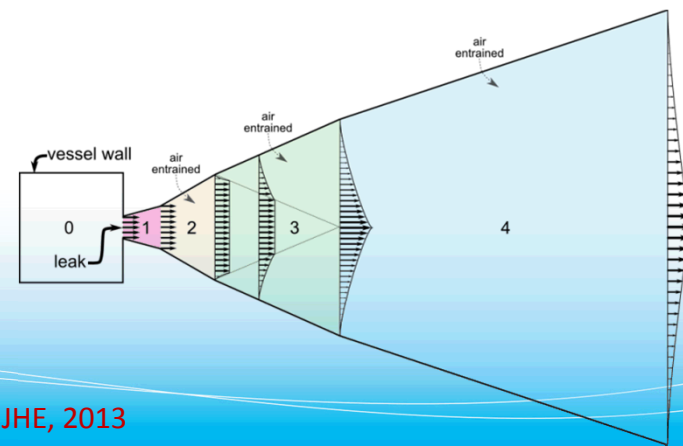
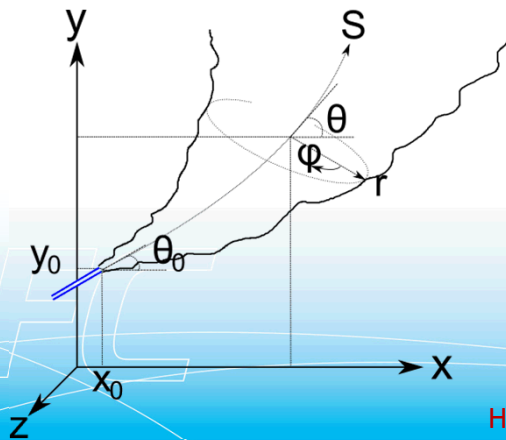
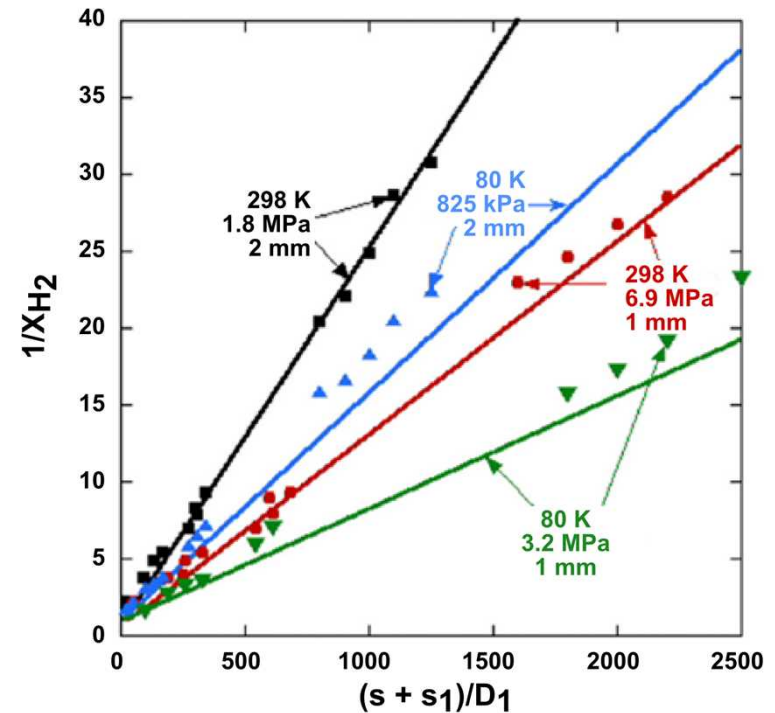
Summary

- **Relevance:** Address lack of safety data, technical information relevant to development of Codes & Standards.
- **Approach:** Develop and validate scientific models to accurately predict hazards and harm from liquid releases, flames, etc. Generate validation data where it is lacking.
- **Technical Accomplishments:**
 - Cryogenic hydrogen release laboratory constructed and commissioned
 - Experiments on-going
 - Schlieren imaging
 - laser spark ignition to find cryogenic hydrogen ignition distance as function of temperature, pressure, nozzle diameter
 - heat flux measurements
- **Future work:**
 - Implement filtered Rayleigh scattering diagnostic necessary for quantitative concentration measurements (laser being repaired)
 - Use data to validate and guide development of models
 - Use models to advise NFPA 2 code committee on hazards and harm for high priority scenarios (results in early 2017)

TECHNICAL BACKUP SLIDES

A conceptual model needs to further validation

- Conservation of mass, momentum, species, **energy**
- 5-zones:
 - Zone 0: accelerating flow
 - Zone 1: underexpanded jet
 - Zone 2: initial entrainment and heating
 - Zone 3: flow establishment
 - Zone 4: self-similar, established flow
- 1-dimensional along streamline, can curve due to buoyancy

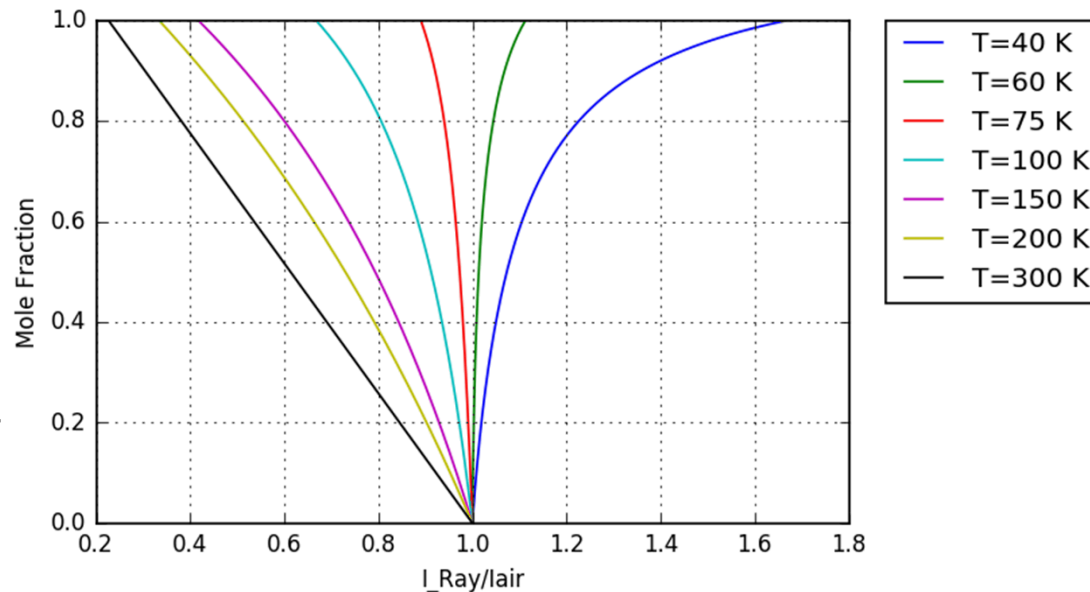


Temperature dependent Rayleigh signal intensity correction

$$I_{ray} = CI_0N[(1 - X_{H2})\sigma_{air} + X_{H2}\sigma_{H2}]$$

Number density (N) depends on temperature, hence, a temperature correction is required to calculate hydrogen mole fraction

$$X_{H2} = \left[\frac{I_{ray}}{I_{air}} \frac{T_{mix}}{T_{air}} - 1 \right] \frac{1}{\sigma_{H2}/\sigma_{air} - 1}$$



Rayleigh signal between air and H₂ is indistinguishable in the temperature range 60 – 75 K

Cold Hydrogen Concentration and Temperature Measurement

Cold Hydrogen Jet Conditions:

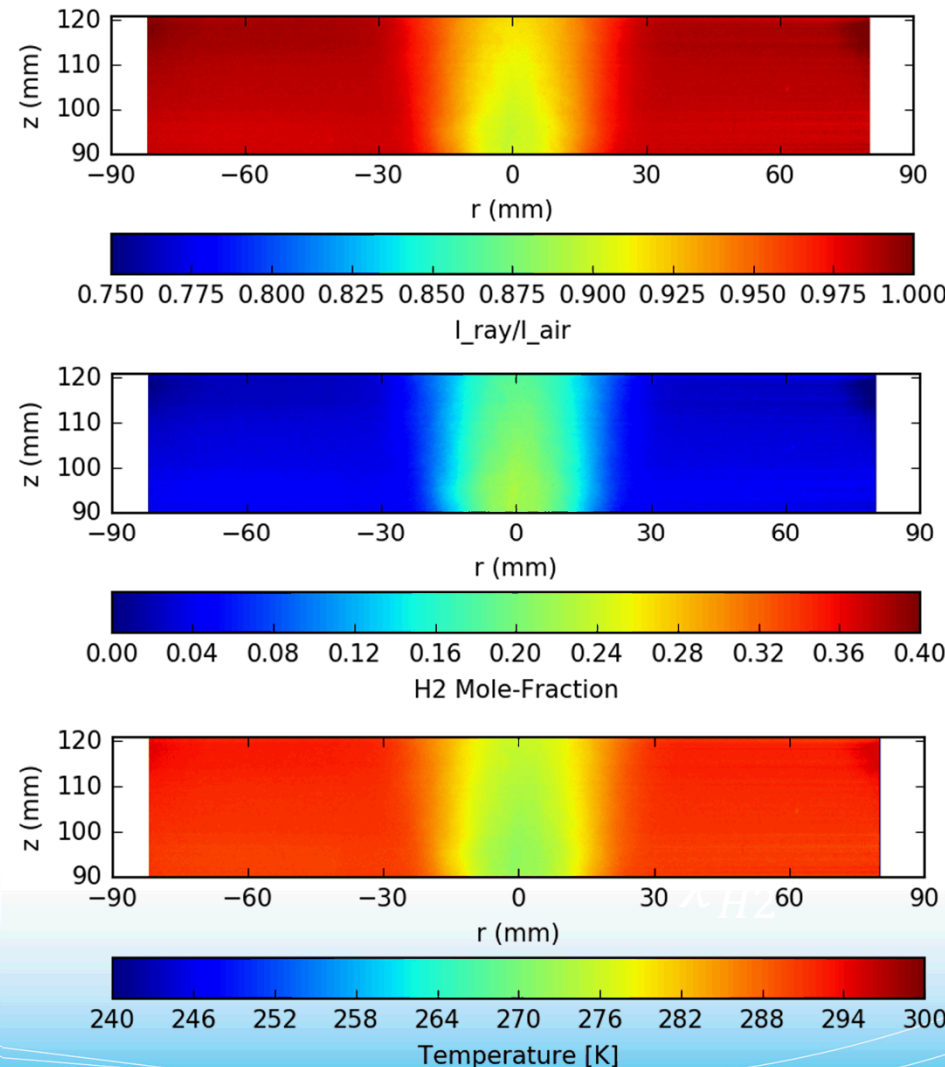
P : **1 bar**

T : **190 K**

Nozzle Diameter : **1 mm**

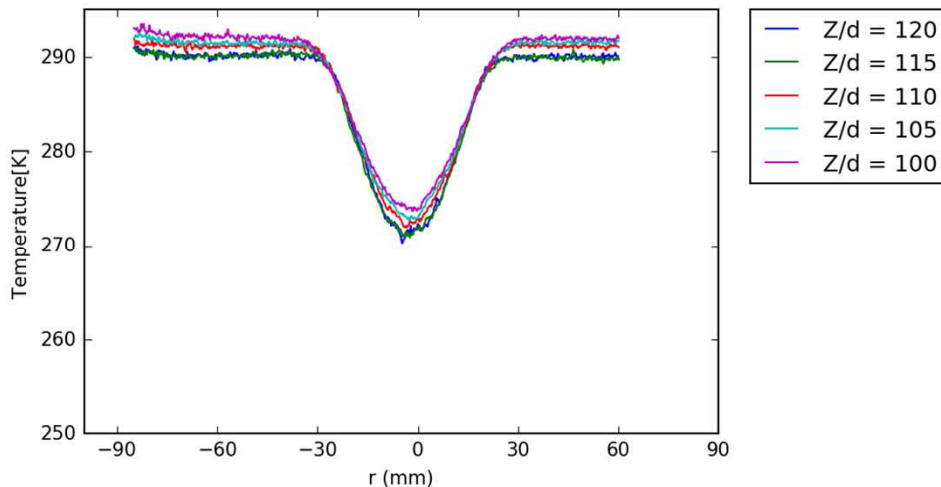
\dot{m} : **0.12 g/s**

- Existing analysis code modified to take in to account temperature variation in the hydrogen plume
- Adiabatic mixing assumed

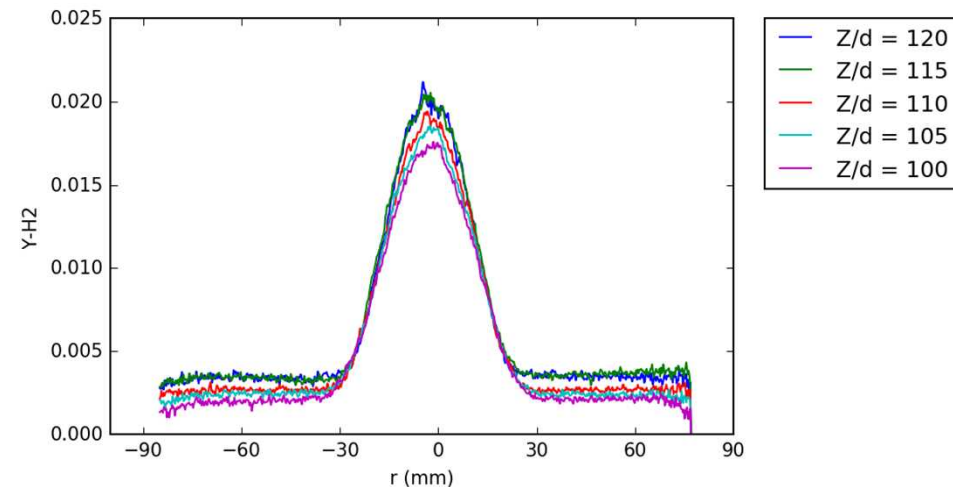


Expected Gaussian profiles for temperature and mass fraction are observed

Temperature



Mass-Fraction



- Thus far, only able to measure profiles in relatively warm regions of the jet where there is not much moisture condensation

High priority scenarios have been identified by the NFPA 2 code committee

- Release from pipe leading from tank to vaporizer or vaporizer itself caused by thermal cycles or ice falling from vaporizers
 - Modeling results of hydrogen concentration plume and heat flux from a subsequent fire will be used for all other separation distance exposures because this is the highest risk priority
 - Horizontal discharge, ¾"-2" diameter pipe, 20-140 psig
- Flow from trailer venting excess pressure after normal LH₂ delivery
 - Modeling results will be used to calculate separation distance from air intakes and overhead utilities
 - Vertical discharge, 3" diameter pipe, 20-140 psig



REVIEWER ONLY SLIDES

Critical Assumptions and Issues

- While the current laboratory low temperature jet/plume testing is a necessary part of advising the C&S community on liquid hydrogen, it may not be sufficient for fire code revision. For example, the effects of hydrogen pooling/evaporation, air condensation also need to be studied. Larger scale tests may also be necessary to justify model scaling.
- Assumption: the science-based approach to setback distances will be smaller than the current expert consensus numbers. It may very well be that the risk-informed, science-based setback distances are not smaller than the current values.

Publications and Presentations

- E.S. Hecht, M.D. Zimmerman, A.C. LaFleur, M. Ciotti. "Design of the Cryogenic Hydrogen Release Laboratory." SAND2015-7521. Sandia National Laboratories, August 2015.
- X. Li, E.S. Hecht, I.W. Ekoto. Validated equivalent source model for an underexpanded hydrogen jet. Presented at the International Conference on Hydrogen Safety, Yokohama, Japan, October 2015.
- E.S. Hecht & P. Panda. Validation data for releases from cryogenic hydrogen sources. SAND2015-9782 PE. Presented at the Codes and Standards Tech Team Meeting. November 2015.
- K.M. Groth, E.S. Hecht and J.T. Reynolds. *Methodology for assessing the safety of Hydrogen Systems: HyRAM 1.0 technical reference manual*. SAND2015-10216, Sandia National Laboratories, Albuquerque, NM, November, 2015.
- X. Li, E.S. Hecht, D.M. Christopher. Validation of a reduced-order jet model for subsonic and underexpanded hydrogen jets. *International Journal of Hydrogen Energy*, 41 (2016) 1348–1358.
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- E.S. Hecht & P. Panda. Liquid Hydrogen Behavior Studies. SAND2016-3269 PE. Presented to the Project Technical Panel Kick-off Meeting for 'Spatial Separation Distances for Liquid Hydrogen Storage.' April, 2016
- C. San Marchi, E. S. Hecht, I. W. Ekoto, K. M. Groth, C. LaFleur, B. P. Somerday, R. Mukundan, T. Rockward, J. Keller & C. W. James. "Overview of the DOE hydrogen safety, codes and standards program, part 3: Advances in Research and Development to Enhance the Scientific Basis for Hydrogen regulations, Codes and Standards." *Submitted for publication in International Journal of Hydrogen Energy*, (Submitted Feb 2016).
- K.M. Groth & E.S. Hecht. "HyRAM: A methodology and toolkit for Quantitative Risk Assessment of hydrogen systems." *Submitted for publication in International Journal of Hydrogen Energy* (Submitted Feb 2016).