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

2020 Hydrogen and Fuel Cells Program Annual Merit Review

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Overview

Timeline

- Project start date: Oct. 2003
- Project end date: Sept. 2020*
  - * Project continuation and direction determined by DOE annually

Budget

- FY19 DOE Funding: $675 k
- Planned FY20 DOE Funding: $750 k
- Planned FY20 H2@Scale CRADA funding: $280 k ($140 k from Air Liquide and partners, $140 k from DOE)

Barriers

A. Safety Data and Information: Limited Access and Availability

G. Insufficient technical data to revise standards

Partners

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

Relevance

Objectives:

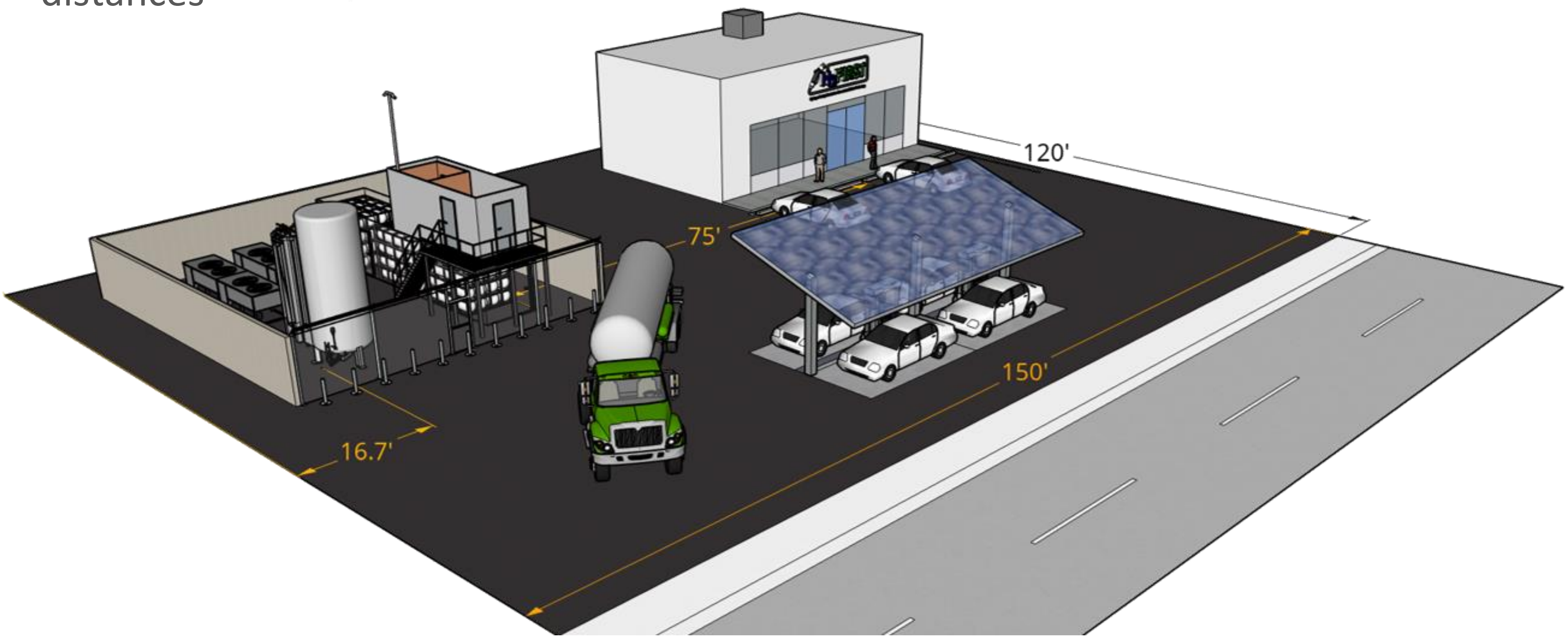
- Perform R&D to provide the science & engineering basis for the release, ignition, and combustion behavior of hydrogen across its range of use (including high pressure and cryogenic)
- Develop models and tools to facilitate the assessment of the safety (risk) of H_2 systems and enable use of that information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

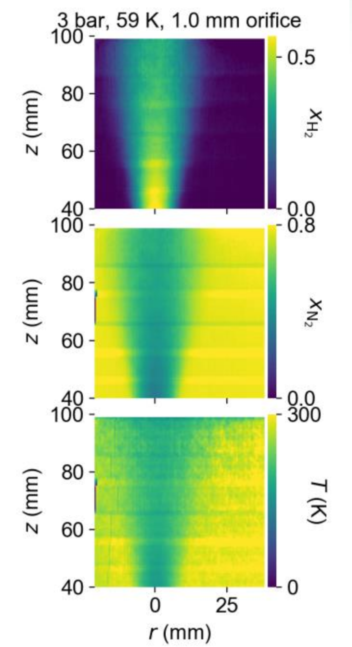
Relevance: Current separation distances for liquid hydrogen are based on consensus, not science

- 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

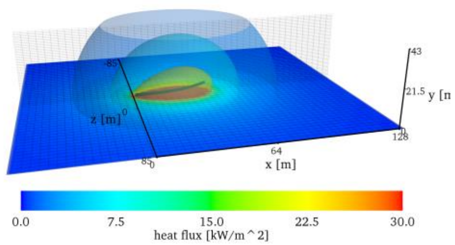


Approach (Sandia H_2 SCS): Coordinated activities that facilitate deployment of hydrogen technologies

- 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

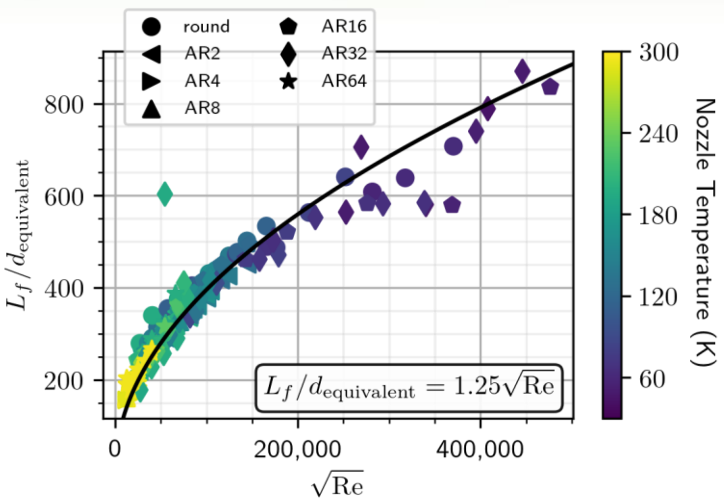


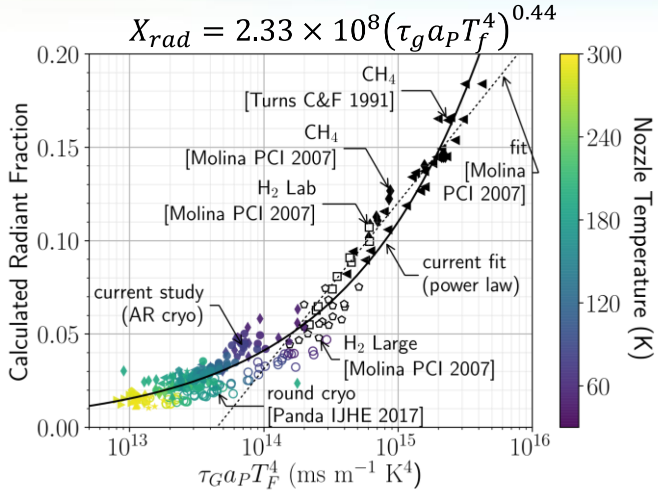
Approach: Develop and execute experiments to enable predictive modeling across H_2's range of use

- 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 – complete
- Issue: Larger cryogenic H2 releases have been outdoors and/or instrumented with low fidelity sensors (space and time), with experimental uncertainty too high for model validation
  - Complete parametric measurements of hydrogen vent stack dispersion using novel laser diagnostic – in progress
  - Support CGA G5.5 testing task force to characterize liquid hydrogen vent stack flames – in progress
  - FY20 milestone: Determine site, perform safety reviews, and commission experimental platform to form a vaporizing liquid hydrogen pool for measuring flames and concentration profiles – in progress

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

Accomplishment: Completed study of cryogenic hydrogen flames from high-aspect ratio nozzles

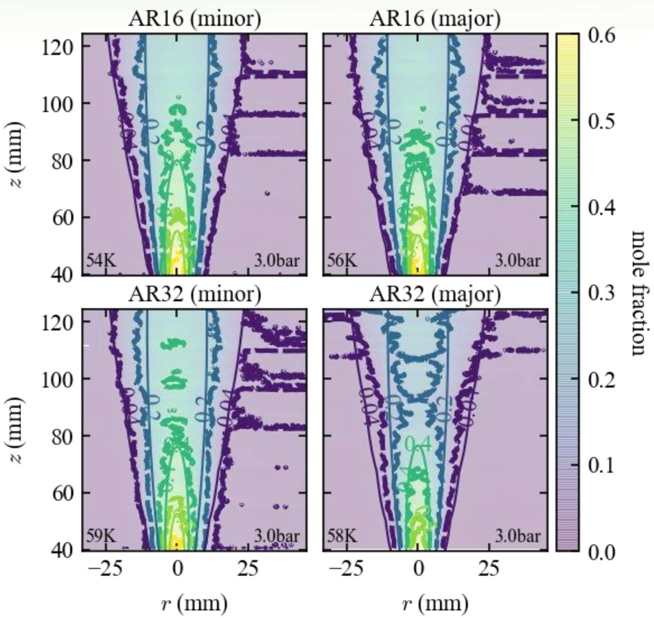


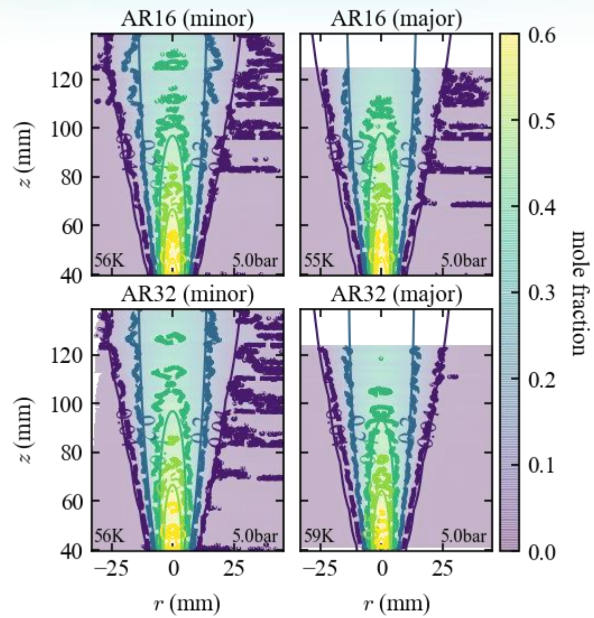


- Leaks from real cryogenic hydrogen system more likely to have a high aspect ratio than a round profile

- Preliminary results suggested that cryogenic hydrogen flames from high-aspect ratio nozzles have the same length and radiative properties as round nozzles in 2019 AMR
- Results here confirm that flame length and radiative fraction from flames through high-aspect ratio nozzles scale the same as for round nozzles
- Correlations shown for flame length and radiant fraction are valid for flames from hydrogen at room temperature all the way down to cryogenic temperatures
- Results give confidence that HyRAM predictions of cryogenic hydrogen flames that assume a round nozzle are accurate regardless of actual release geometry

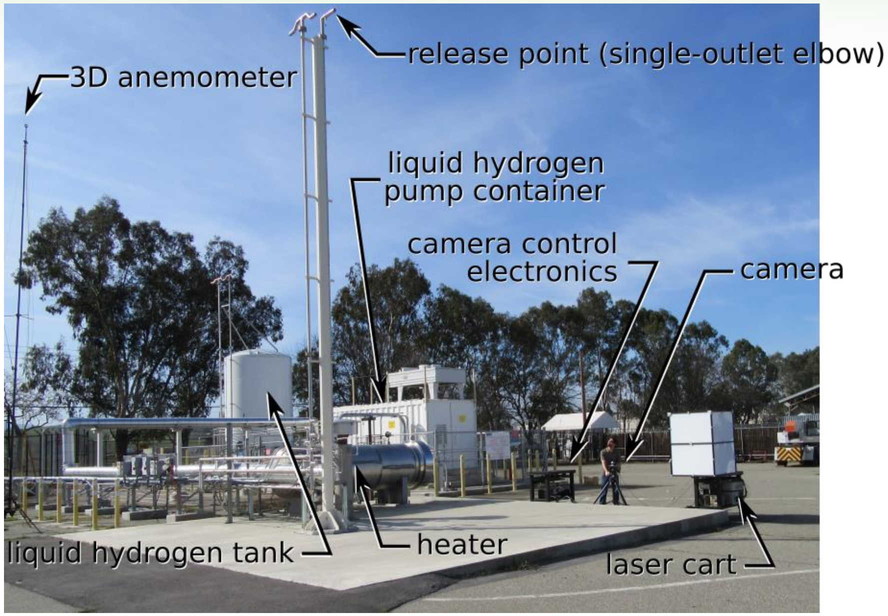
Accomplishment: Cryogenic hydrogen dispersion through high-aspect nozzles is similar to round

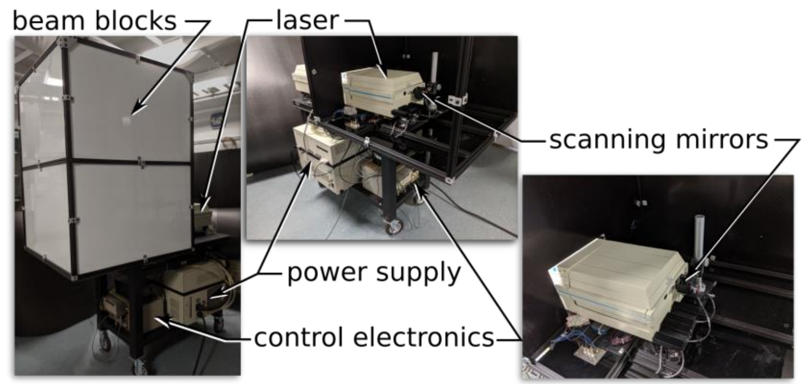




- Figures show that there are little dispersion differences along major and minor axes (left vs right frames) for cryogenic hydrogen dispersion from 3 and 5 bar sources
- Model for dispersion of release through round nozzle (thin solid lines) align well with experimental data (shading and thick dashed lines) for high-aspect ratio nozzles along major and minor axes
- Dispersion predictions using round nozzle are accurate regardless of actual leak geometry

Accomplishment: Large-scale diagnostic construction finalized and delivered to site





- Additional temperature sensors installed along vent stack (at release point and bottom of stack) to validate internal flow model and provide model boundary conditions
- Bull-horn replaced with single outlet to enable model comparisons
- Tank filled and liquid hydrogen pump tested
- Awaiting final safety approvals and return to work from COVID-19 pandemic response – experiments to commence within a few weeks of return to work

Accomplishment: Test plan finalized, representative of a range of operations

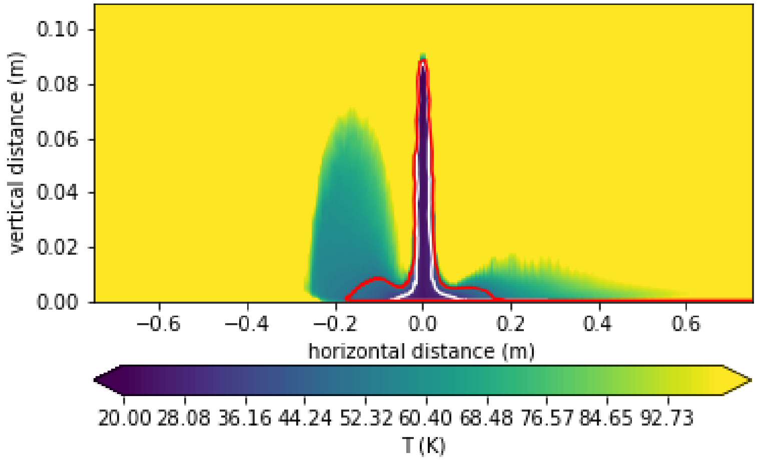
description	flow rate (g/s)	duration (mins)	total H2 (kg)	Wind	Humidity	Purpose	Note
high-flow warm plume dispersion	16.67	30	30	low (< 5 MPH)	any	validate diagnostic (high flow-rate/concentration, no condensation)	Use heater to warm H2 to as high a T as possible, repeat until diagnostic deemed ready
high flow cold dispersion	16.67	30	30	low (< 5 MPH)	low	simulate vent release during transfer	Possibly repeat with high and low ambient temperatures
high flow cold dispersion	16.67	30	30	high (> 5 MPH)	low	simulate vent release during transfer	
high flow cold dispersion	16.67	30	30	low (< 5 MPH)	high	simulate vent release during transfer	
high flow cold dispersion	16.67	30	30	high (> 5 MPH)	high	simulate vent release during transfer	
simulated high-boiloff	0.56	30	1	low (< 5 MPH)	low	simulate high level of boiloff	Possibly repeat with high and low ambient temperatures. May need to precool vent lines with higher flows before reducing flow rate.
simulated high-boiloff	0.56	30	1	high (> 5 MPH)	low	simulate high level of boiloff	
simulated high-boiloff	0.56	30	1	low (< 5 MPH)	high	simulate high level of boiloff	
simulated high-boiloff	0.56	30	1	high (> 5 MPH)	high	simulate high level of boiloff	
normal boiloff	0.07	30	0.125	low (< 5 MPH)	any	normal boilff measured by meter	May need to scrap if diagnostic not sensitive enough.
normal boiloff	0.07	30	0.125	high (> 5 MPH)	any	normal boilff measured by meter	

Key questions to be answered by this experimental campaign:

- Does wind cause channeling and increase the distance to the LFL, or improve mixing to decrease the distance to the LFL?
- Does high humidity cause increased buoyancy due to the energy transfer from the condensation of moisture, or does the condensed moisture drag the hydrogen down so it's less buoyant?
- Is the hydrogen concurrent with the condensed moisture? Does concurrency depend on the humidity?
- Is our model accurate enough for risk calculations for larger releases?

Progress: Successfully modeled pooling and vaporization using Ansys Fluent

Temperature contours of liquid hydrogen release – red line is at 50K, white line is at 30K



- Reynolds-Averaged Navier-Stokes turbulence closure
- Includes:
  - Oxygen and nitrogen (and hydrogen) phase change
  - 1-D conduction in the ground
  - 2-phase release
- Simplifications:
  - Dry air
  - Steady horizontal wind (logarithmic profile)

- Initial simulation validation using UK's Health and Safety Lab liquid hydrogen release data
- Simulation capabilities enable calculation of flammable mass for planning unignited pooling and vaporization experiments
- Long-term goal of model validation with experiments

Response to last year's Reviewer's comments

- The timeline continues to slide, and it is critical not to miss important submission deadlines for NFPA documents. The lack of large-scale release testing is being addressed with the development of a project to perform these tests, but the schedule is vague and needs to be accelerated.
- We continue to progress along several fronts simultaneously. While the experimental schedule has slipped a bit, we are working with the NFPA 2 storage task group closely to have placeholder revisions in place for the next code-cycle, with the intention of completing the experimental and modeling work by the time the changes are voted on. We are also attempting to accelerate the experimental schedule by planning the next round of experiments (pooling and vaporization) before the vent stack release experiments are completed, enabling faster transition to the next round of experiments.
- The project should do testing to determine what configurations of barrier walls might be effective and safe (four barrier walls for gaseous hydrogen and three to four barrier walls for LH_2) and the separation distance reduction enabled by these different configurations.
- We agree that there continues to be a gap in the effectiveness of walls and how different levels of confinement (wall configurations) vs. consequence abatement (flame heat flux reduction) affect the risk. Additional testing with barrier walls are included in the future work section.

Collaborations enable this research and expand impact

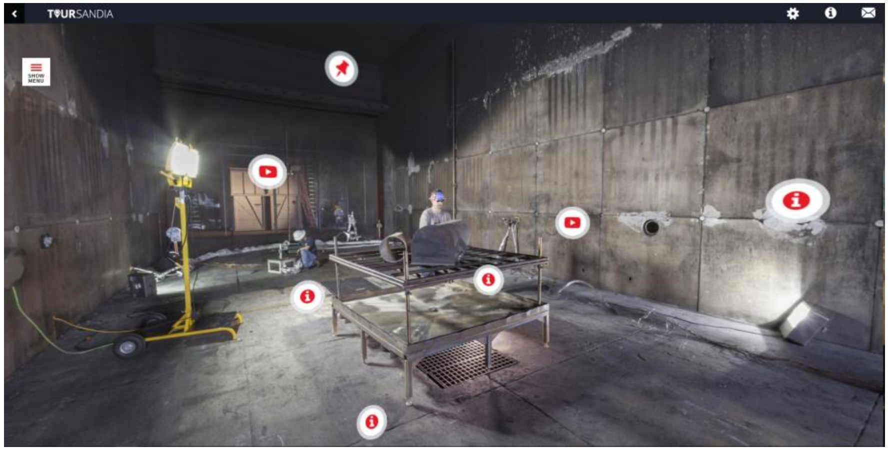
- Experiments at LLNL facility with NREL participating in experimental campaign
- H2@Scale CRADA with Air Liquide ($150 k from Air Liquide and partners, $150 k from DOE)
- Previous CRADA with BKi to fund experiments ($175k received from CaFCP Auto OEM Group, Linde, Shell)
  - Data exchange with contributing members
- 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
- CGA G-5.5 testing task force
  - Providing hardware for and analysis support of measurements of LH_2 vent stack flames

Remaining challenges: Executing vent-stack experiments and planning additional large-scale experiments

Vent-stack experiments to commence within a matter of weeks from returning from COVID-19 shutdown

Additional Experiments:

- Controlled experiments at Sandia's Cross-wind test facility to validate models for:
  - Pooling
  - Evaporation from LH_2 pools
- Revisit mitigation from walls, including dispersion and mitigation of liquid hydrogen leaks/flames
  - Effects on unignited dispersion and accumulation
  - Reduction in heat flux/overpressure
- Partner with others, applying diagnostic at remote locations (European colleagues, CGA G-5.5 testing task force) and analyze external data



Proposed future work

- Remainder of FY20
  - Execute experiments using large-scale diagnostic at LLNL LH_2 pad
  - Provide initial proposals to NFPA 2 2022 with reduced separation distances for liquid hydrogen infrastructure
  - Finalize R&D plans for pooling/vaporization experiments
  - Begin planning wall mitigation experiments
- FY21
  - Refine largescale diagnostic design
  - Conduct large-scale release experiments to characterize hydrogen pooling, evaporation, and interaction with atmosphere and develop validated models of these phenomena
- Out years
  - Develop and validate models for risk reduction through the use of barrier walls in different configurations
  - Refine 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

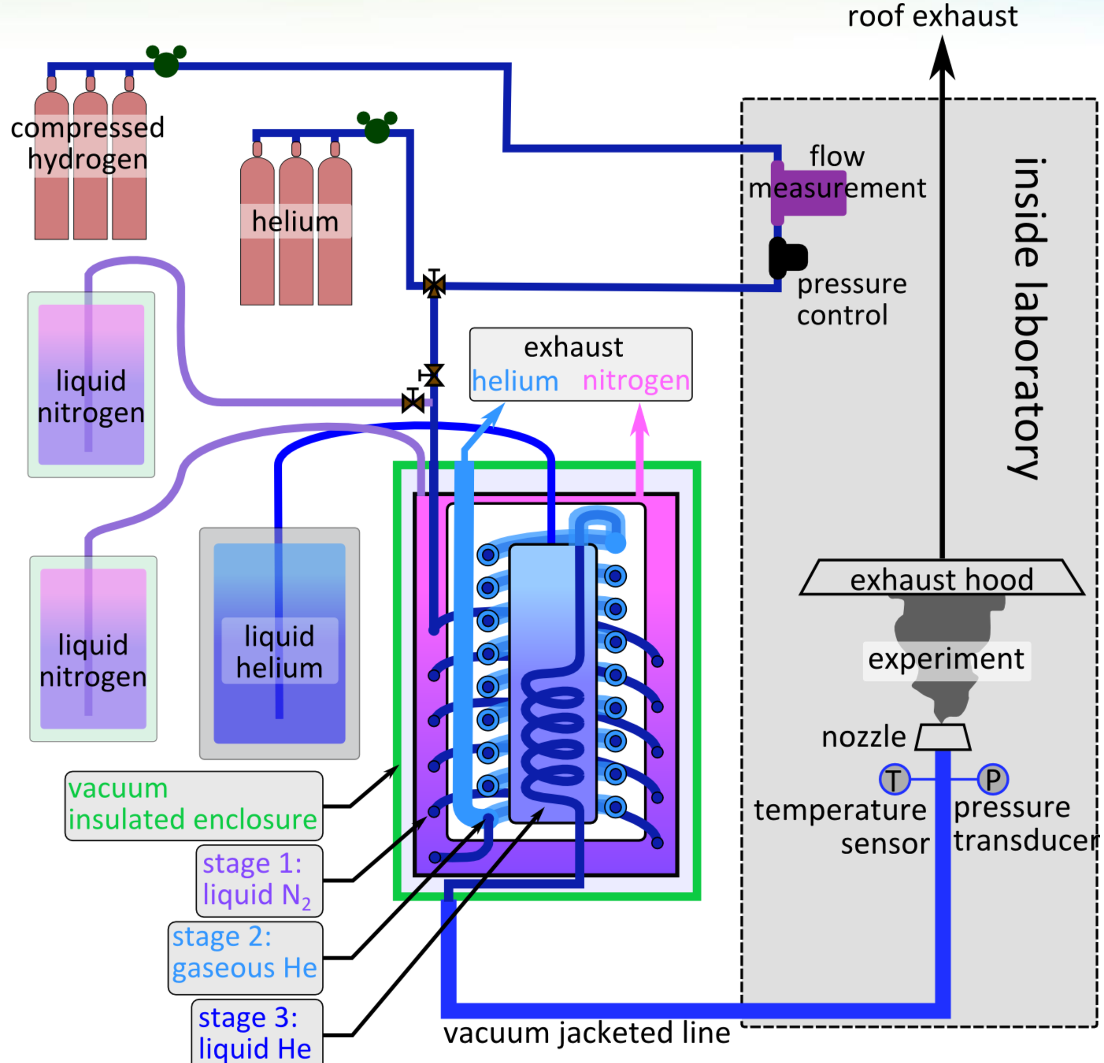
Any proposed future work is subject to change based on funding levels

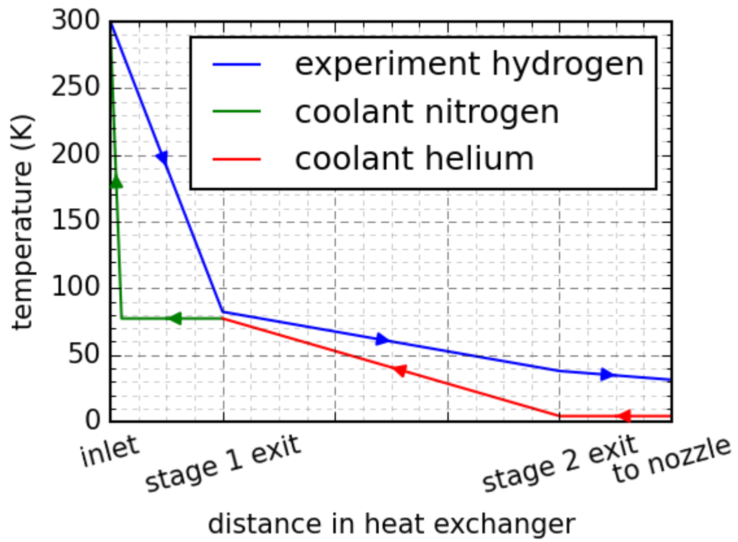
Summary

- **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**:
  - Completed studies of cryogenic hydrogen dispersion and flames through high-aspect ratio nozzles
  - Determined that for typical liquid hydrogen tank pressures (up to 5 bar), the leak geometry does not significantly affect heat flux or dispersion
  - Constructed and deployed large-scale laser Raman diagnoistic at LLNL liquid hydrogen research pad
- **Future work**:
  - Execute vent-stack dispersion experiments for a range of conditions 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 justify LH_2 infrastructure siting reductions in 2022 edition of NFPA 2

TECHNICAL BACKUP SLIDES

The laboratory experiment is used to generate cryogenic hydrogen releases





- Accurate control/measurement of boundary conditions

The NFPA 2 liquid hydrogen setback distance task group has a path for separation distance reduction, but there are gaps for LH_2

Public input for 2023 edition by June 30, 2020

Gaseous

- ✓ Determine list of exposures
- ✓ Conduct hazard analysis
- ✓ Create representative system
- ✓ Acquire leak data
- ✓ Calculate leak frequency (using representative system and leak data)
- ✓ Calculate consequence distances using physics models and representative leak parameters
  - Unignited concentration of 8%
  - Heat flux of 4.7 kW/m^2
- ✓ Determine separation distance using frequency calculations and consequence calculations
  - – Function of size and pressure

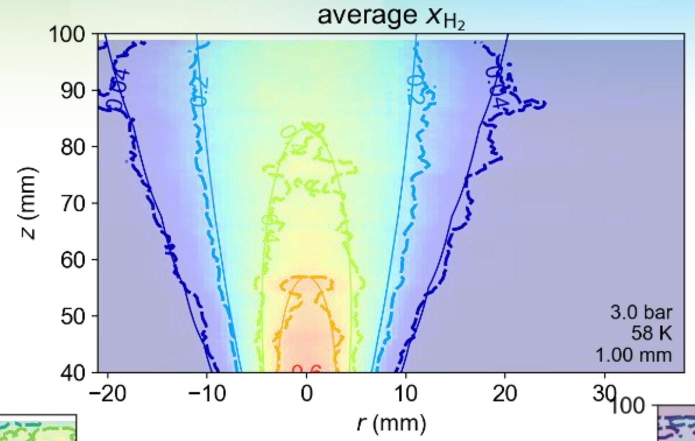
Liquid

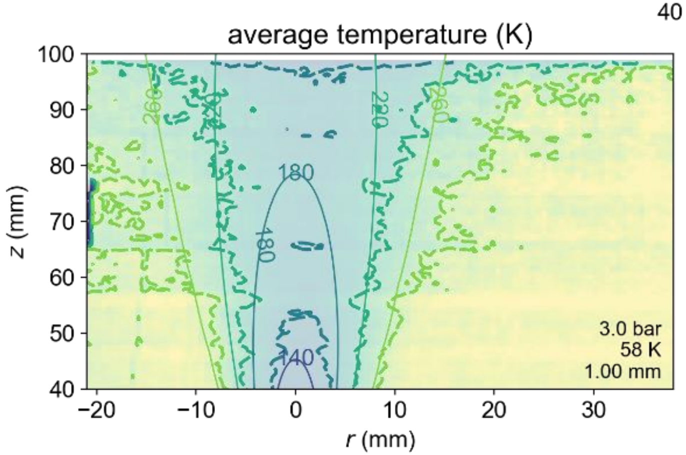
- ✓ Determine list of exposures
- ✓ Conduct hazard analysis
- ✓ Create representative system – additional parameters for LH_2
  - Temperature
  - Phase (liquid or gas)
- ❑ Acquire leak/vent data ✓
  - ❑ Unanticipated leaks
  - ❑ Vent rates
- ❑ Calculate leak/vent frequency
- ❑ Calculate consequence distances using physics models and representative leak/vent parameters
- ❑ Determine separation distance using frequency calculations and consequence calculations
  - – Function of LH_2 volume or something else?

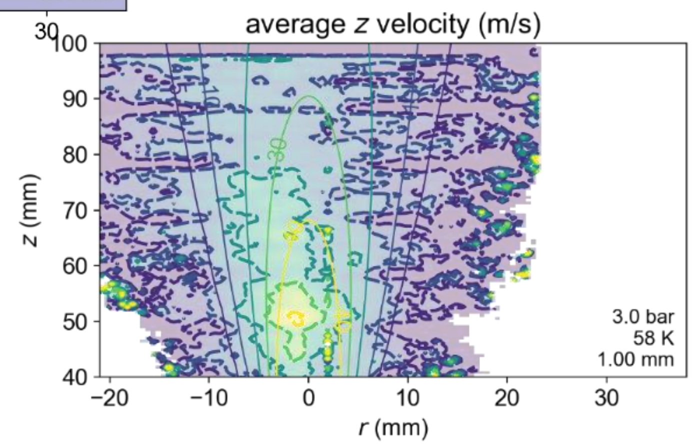
Placeholder data for proposal varied to see if overall risk changes

this work enables

ColdPLUME model shows good agreement with the data





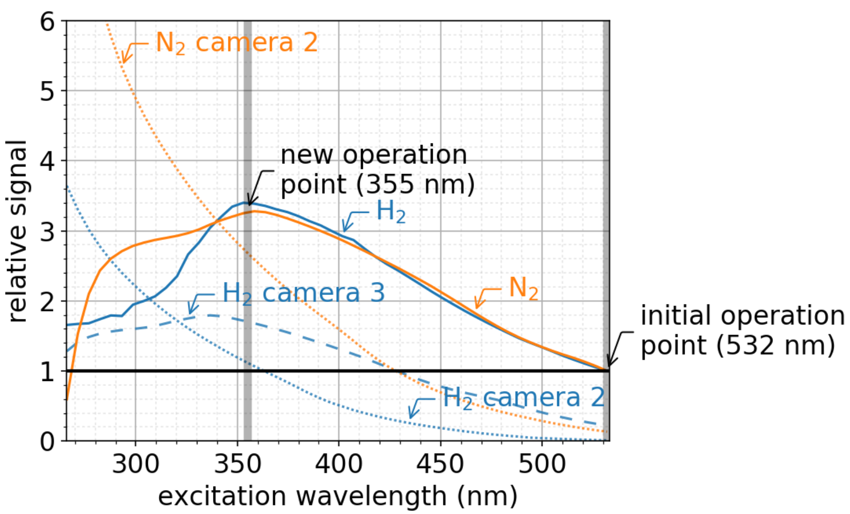


- Experimental results shown by shading and thick, dashed lines
- ColdPLUME model results are thin, solid lines

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

Signal-to-noise ratio for large-scale Raman diagnostic is boosted by using a lower wavelength

- $\text{Raman signal} \propto (incident\ energy)(cross - section)(number\ density)$
- $cross - section \propto (1/\text{wavelength} + \Delta energy)^4$



- Signal scales inversely with wavelength to the 4th power
- Cameras/sensors can have reduced efficiency at low wavelength
- Laser harmonic generation reduces output power
- Net win in signal (>3x) going from 532→355 nm