SAND2021-4482C

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

Project ID: SCS010, AOP #6.2.0.801

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Sandia National Laboratories

2021 Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting

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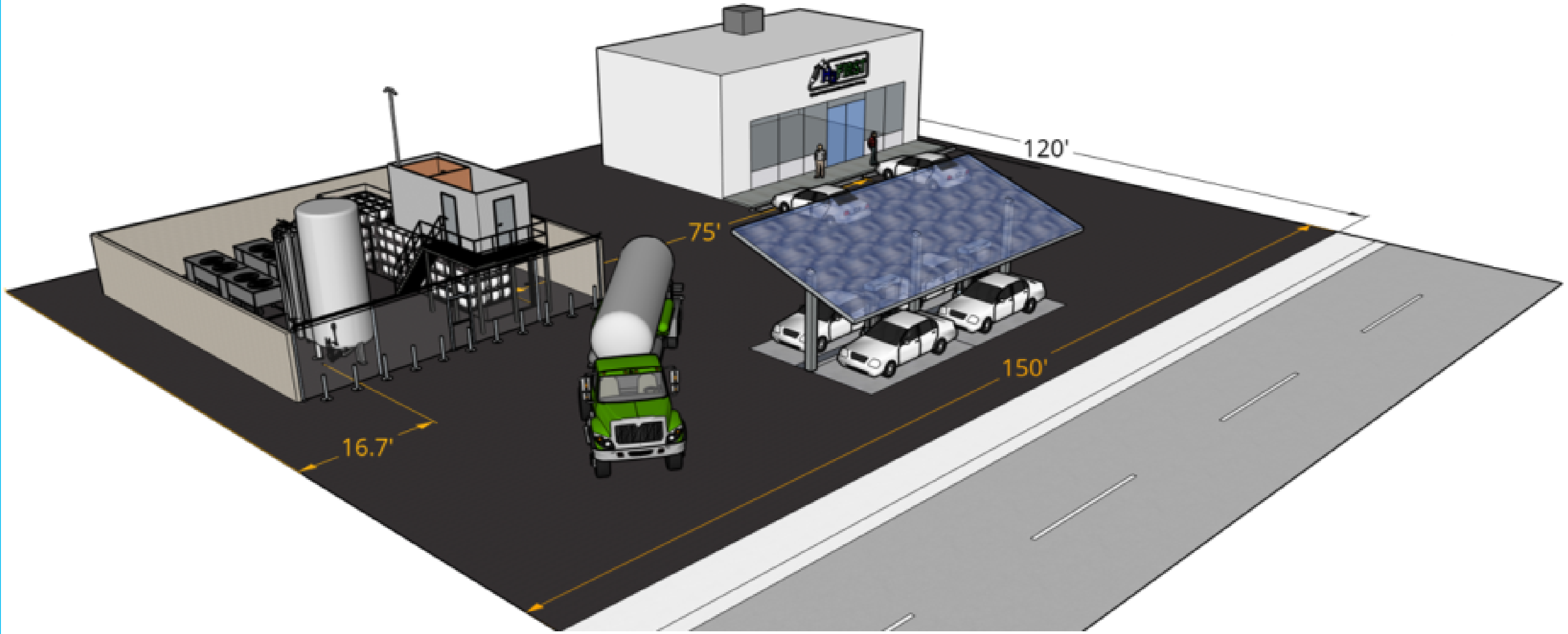
Project Goals

- 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 H2 systems and enable use of that information for revising RCS and permitting stations

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



Overview

Timeline

- Project start date: Oct. 2003
- Project end date: Sept. 2021*

* Project continuation and direction determined by DOE annually

Budget

- FY20 DOE Funding: $400 k
- Planned FY21 DOE Funding: $700 k
- Planned FY21 H2@Scale CRADA funding: $190 k ($75 k from Air Liquide and partners, $115 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

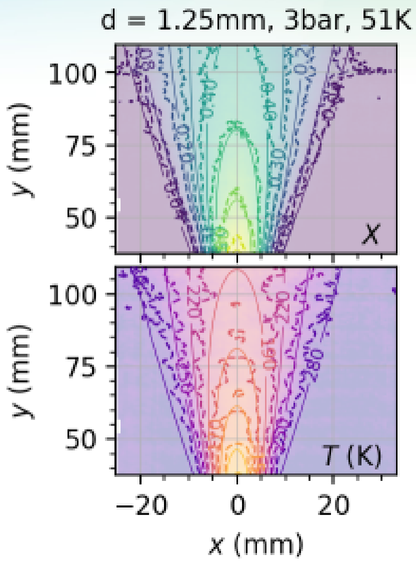
Relevance: Providing data and analyses to support fire code changes

Barrier from 2015 SCS MYRDD	Previous year impact
A. Safety Data and Information: Limited Access and Availability	• Measured the dispersion of cryogenic hydrogen plumes in real-world scenarios
G. Insufficient technical data to revise standards	• Performed analysis justifying smaller liquid hydrogen exposure distances, for certain liquid hydrogen system designs

- 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)
- Current separation distances for liquid hydrogen are based on consensus without documentation of decision basis
- Liquid hydrogen was likely not envisioned for use outside an industrial environment
- 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

➢ Smaller separation distances and footprints can enable construction of hydrogen infrastructure in more locations, increasing zero-emission vehicle (FCEV) use

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.

problems
analysis
models
model needs

HyRAM
HYDROGEN RISK ASSESSMENT MODELS

Enable Hydrogen Infrastructure through Science-based Codes and Standards (SCS025)
Apply QRA and behavior models to real problems in hydrogen infrastructure and emerging technology

problems
analysis

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

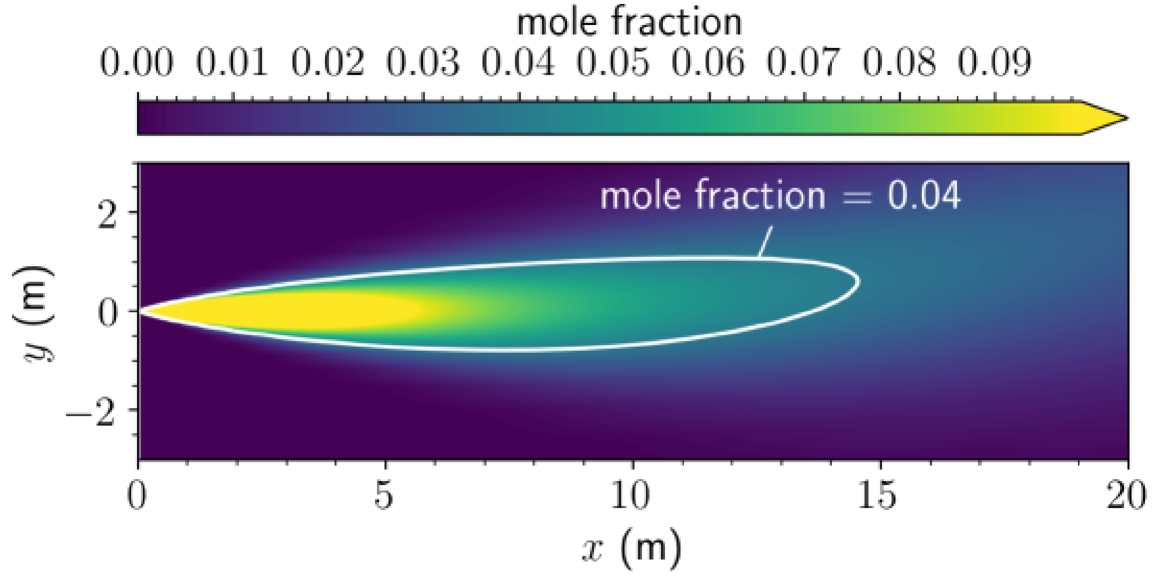
Approach: Develop and execute experiments to enable predictive modeling across H_2's range of use

- Issue: Current separation distances for liquid hydrogen are based on consensus without documentation of decision basis
  - Developed analysis for scientifically defensible liquid hydrogen separation distances
  - Proposed changes to NFPA 2
  - Building consensus to get changes accepted
- 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
  - Completed parametric measurements of hydrogen vent stack dispersion using novel laser diagnostic
  - Support CGA G5.5 testing task force to characterize liquid hydrogen vent stack flames – in progress
  - FY21 milestone: Commission new experimental platform to form a vaporizing liquid hydrogen pool for measuring flames and concentration profiles – in progress

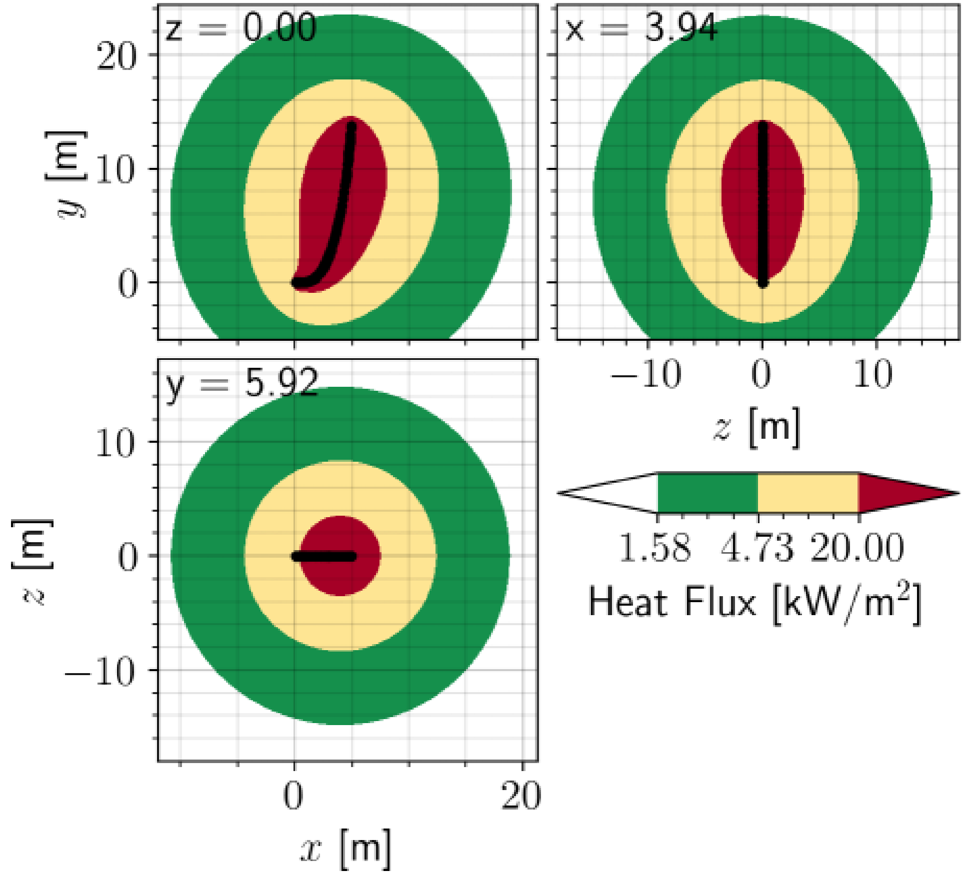
➢ Deliver validated scientific analyses of critical scenarios and provide the science to enable revisions to the 2023 edition of NFPA 2

Accomplishment: Calculated hazards for 1% flow area leaks from a LH2 system

1% leak area jet from 3” pipe at 30 psi (saturated vapor)

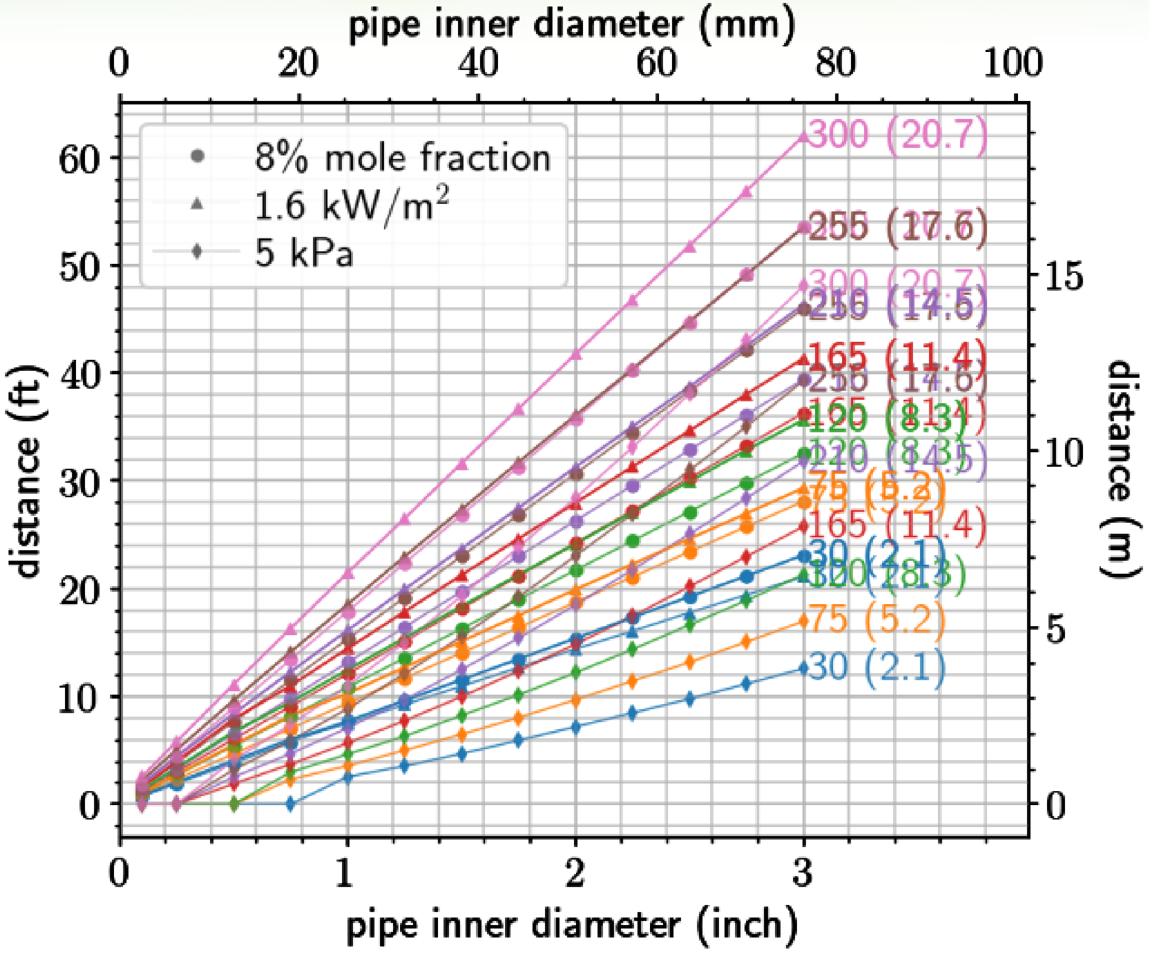


1% leak area flame from 3” pipe at 300 psi (critical temperature)



- Low momentum plumes have little buoyancy
  - Separation distance based on streamline distance to given concentration
- High momentum flames highly buoyant
  - Separation distance based on projected distance to flame length or heat flux level

Accomplishment: Analyzed hazards to develop separation distances for different exposure groups



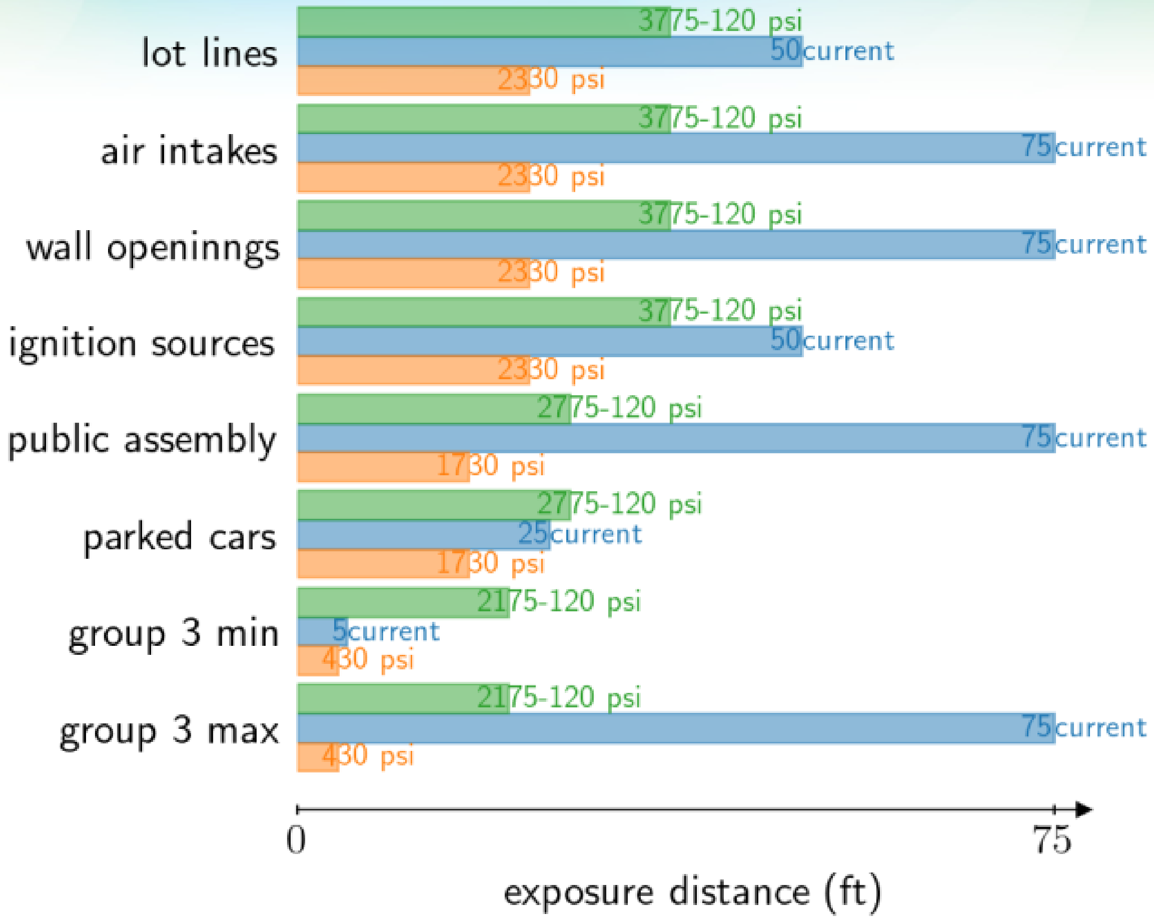
Line labels denote system pressure in psi (bar)

- Example: Group 1, largest of:
  - Mole fraction of 8%
  - Heat flux of 1.6 kW/m2
  - Overpressure of 5 kPa
- Heat flux highest for all but 30psi system pressure
- 8% mole fraction highest for 30psi system pressure

➢ Even at maximum system pressure and diameter, distance (62 ft) is less than current air intake/parking distance (75 ft)
  - ➢ Most systems have smaller pipes (≤ 1.5”) and lower relief pressures (≤ 75 psi)
  - ➢ Safety factor increases for actual exposure distance

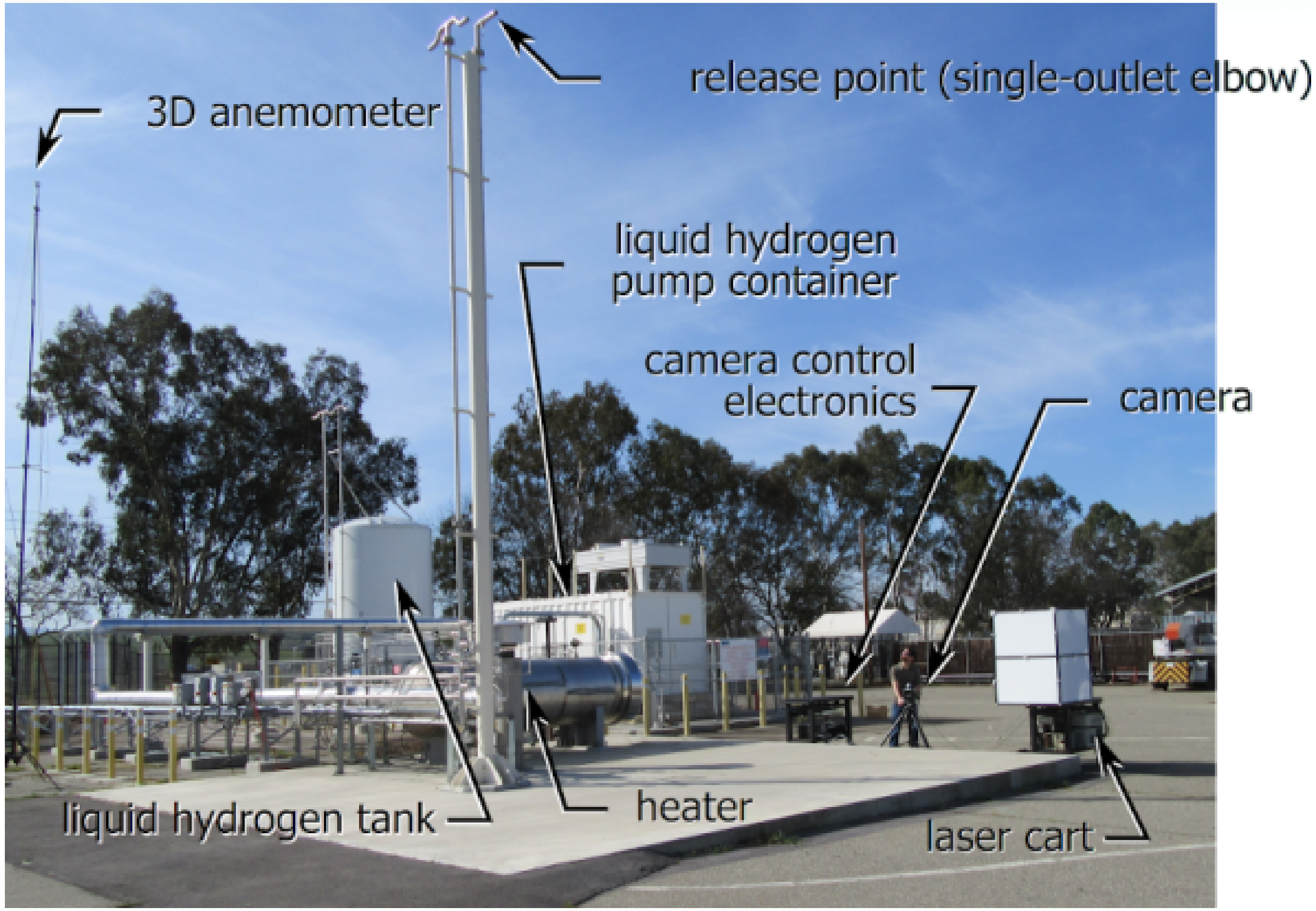
Accomplishment: Developed science-based liquid hydrogen exposure distance tables for NFPA 2

- Proposal submitted to first draft of NFPA 2
- Providing additional justification for subsequent revisions to code
- Separation distances grouped same as gaseous distances
- Distances function of pipe size and system pressure instead of tank volume
- Safety factor of 2 included to account for uncertainty (safety factor of 1.5 used for gaseous distances)



➢ Most distances reduced for typical pipe size (1.5”) and operating pressure (vs typical tank volume); some increase (but mitigations, i.e. walls can be used)

Accomplishment: A series of outdoor cryogenic hydrogen release experiments have been completed for a range of weather conditions



Challenges overcome:

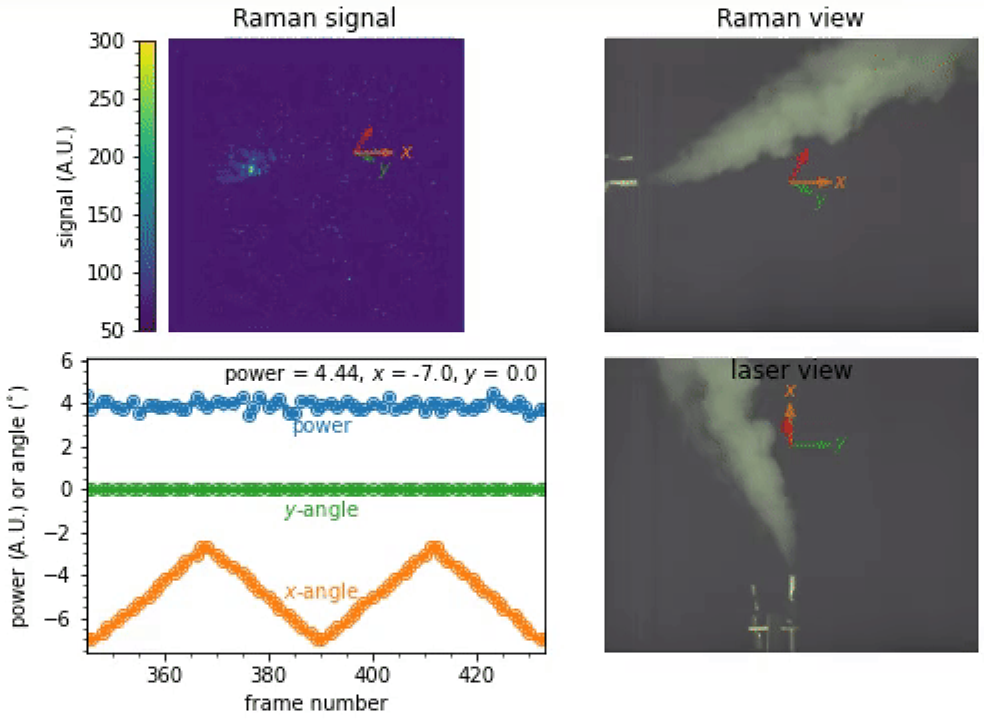
- Experiments performed at LLNL
- High laser power limits optics availability
- Raman signal polarization dependent (alignment critical)
- Daylight provided overwhelming background

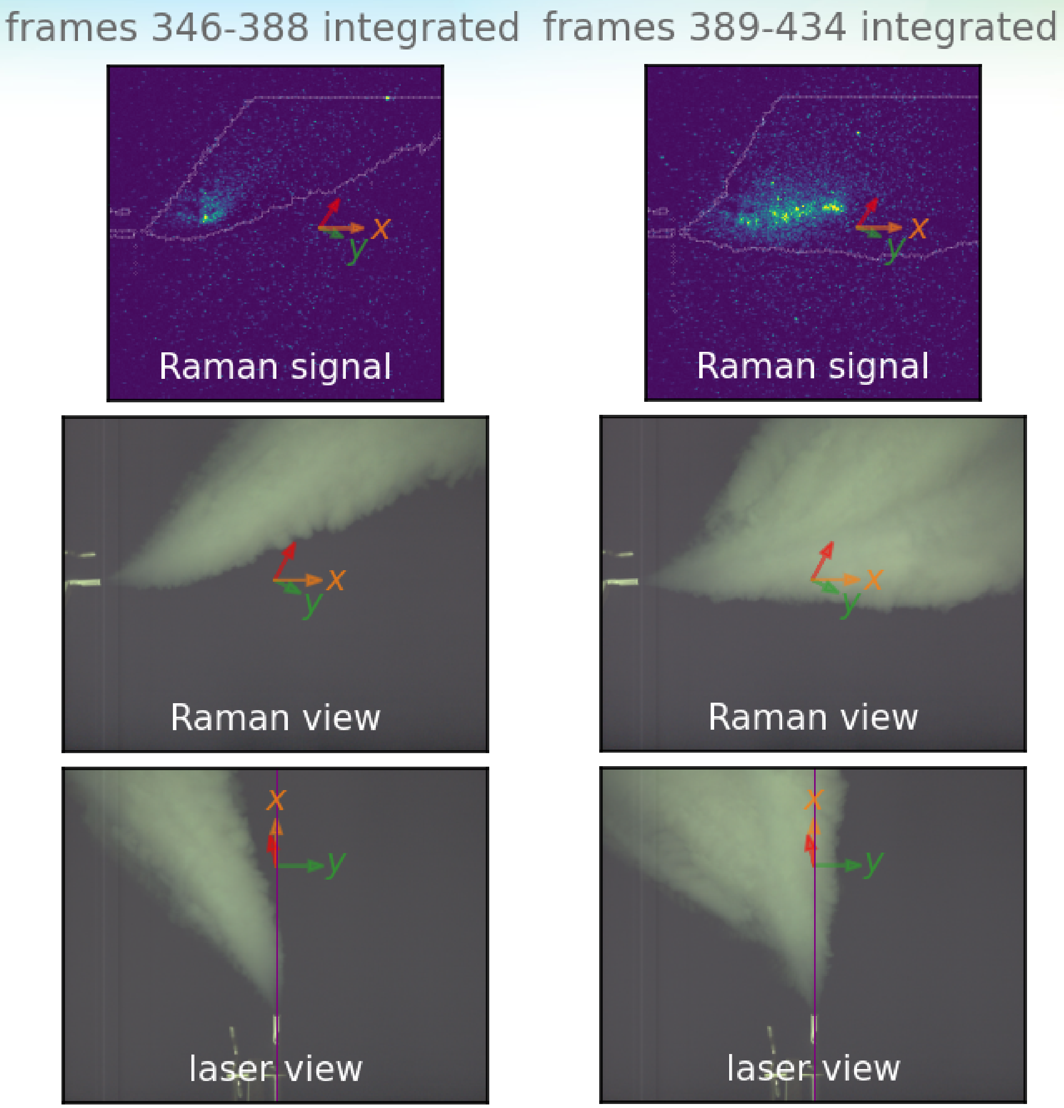
Experimental range:

- Low and high humidity
- Calm and windy conditions

➢ Experiments are measuring cryogenic hydrogen dispersion in real-world scenarios

Accomplishment: Demonstrated that hydrogen is concurrent with the visible plume





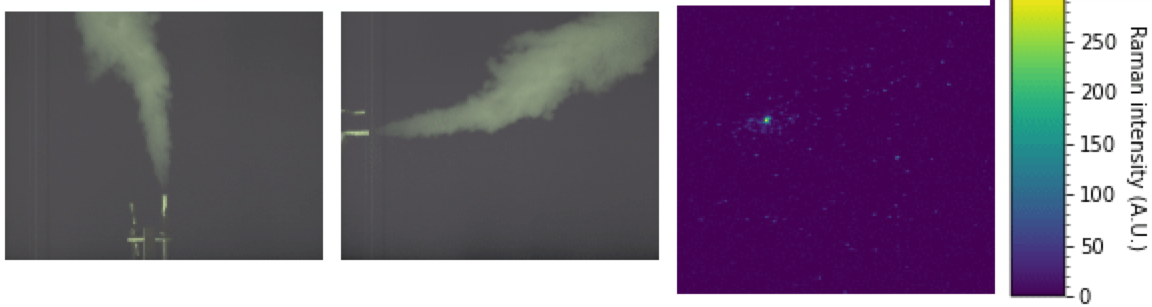
- As wind blows the visible plume off, then back on of the laser-line, the Raman signal disappears, then increases

Accomplishment: Demonstrated that humidity has little effect on hydrogen/visible plume trajectory

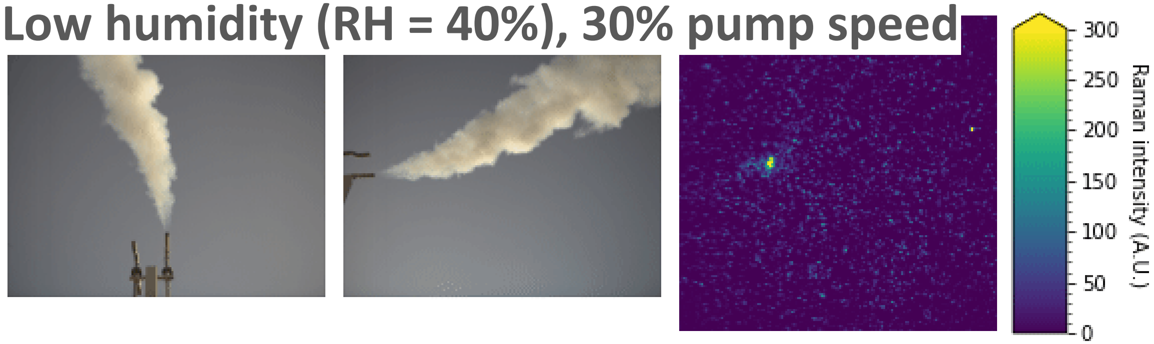
- Additional humidity does not lead to larger (wider) visible plume
- Buoyancy not affected by humidity (trajectories similar)
- Raman signal similar for all (19 -74%) relative humidity

➢ Condensation of water vapor has minimal influence on dispersion

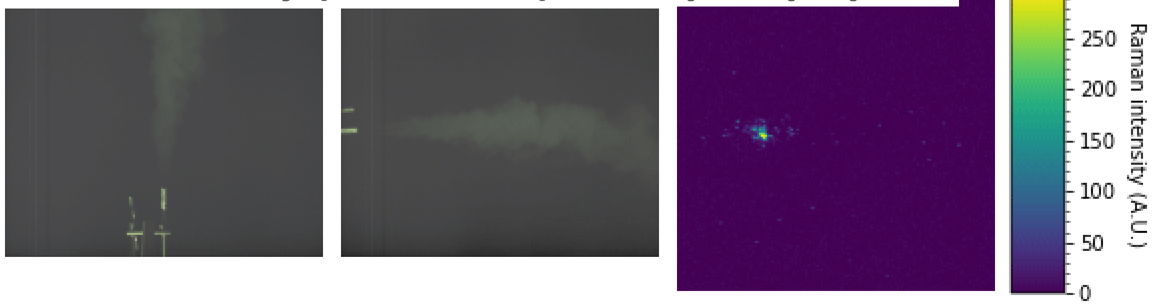
High humidity (RH = 74%), 30% pump speed



Low humidity (RH = 40%), 30% pump speed

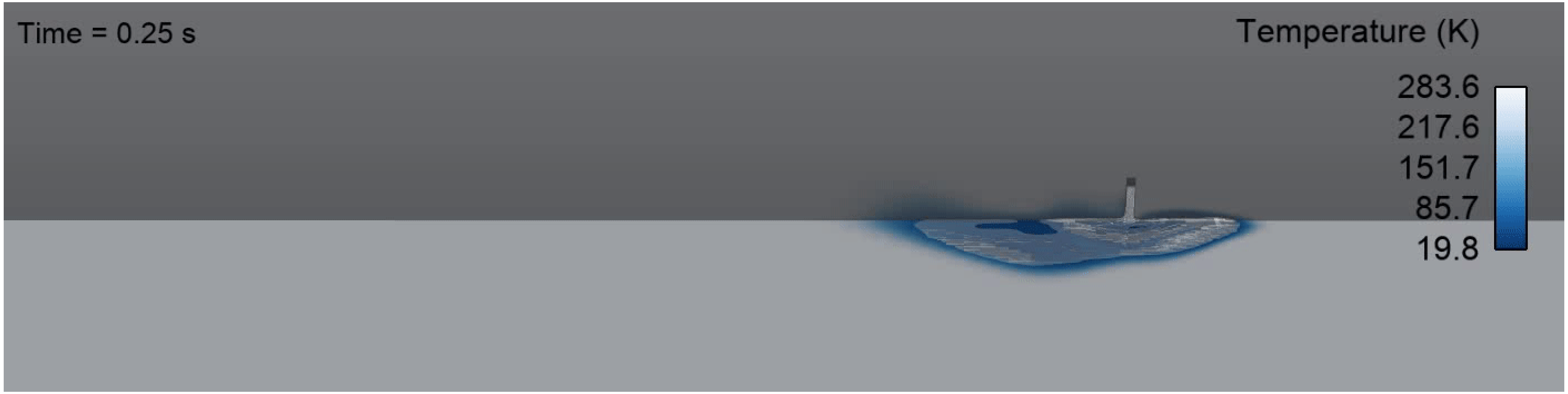


Low humidity (RH = 19%), 40% pump speed



Progress: Fluent modeling is being validated and will be used to plan pooling experiments

- Validating simulation methods based on HSL experiments
- Cross-Wind Test Facility (planned location for experiments) can only support a limited amount of unignited fuel
- Simulations will be used to determine flammable mass in experiments for a given release rate to ensure safety
- Simultaneously developing reduced order models for pooling and vaporization



Response to previous Reviewer's comments (comments from 2019)

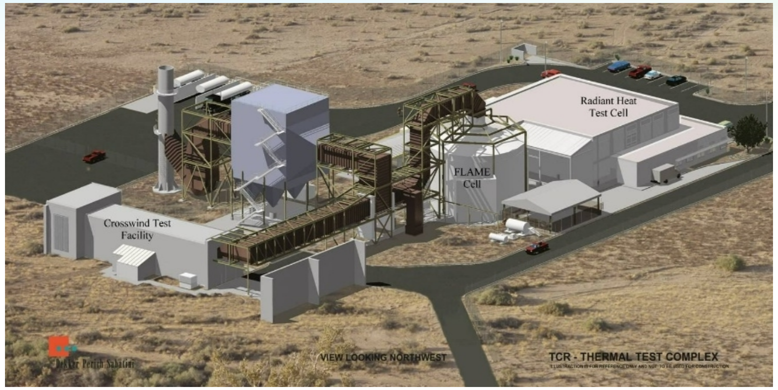
- The timeline continues to slide, and it is critical not to miss important submission deadlines for NFPA documents. The lack of large-scale release testing is being addressed with the development of a project to perform these tests, but the schedule is vague and needs to be accelerated.
  - We continue to progress along several fronts simultaneously. While the experimental schedule slipped a bit, we are continuing to work closely with the NFPA 2 storage task group. We submitted the placeholder proposal for the current code-cycle, with the intention of updating based on completion of the experimental, modeling, and detailed justification. We are also attempting to accelerate the experimental schedule (pooling and vaporization) as much as safely possible.
- 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 is included in the future work section.

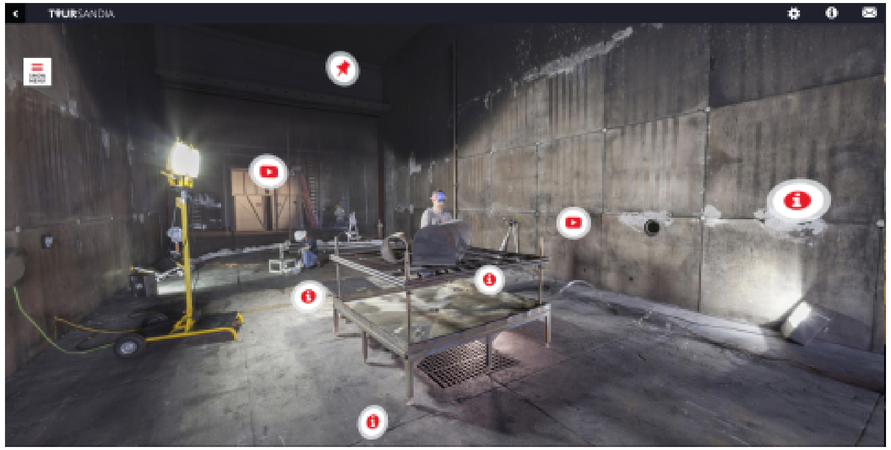
Collaborations enable this research and expand impact

- Experiments at LLNL facility
- 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: Consensus is needed to get proposed NFPA 2 changes accepted, and additional experiments are needed

- Consensus of the approach and assumptions in the separation distance analysis is needed so that the changes proposed to NFPA 2 can be accepted
- Additional experiments are needed to address additional phenomena:
  - 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

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

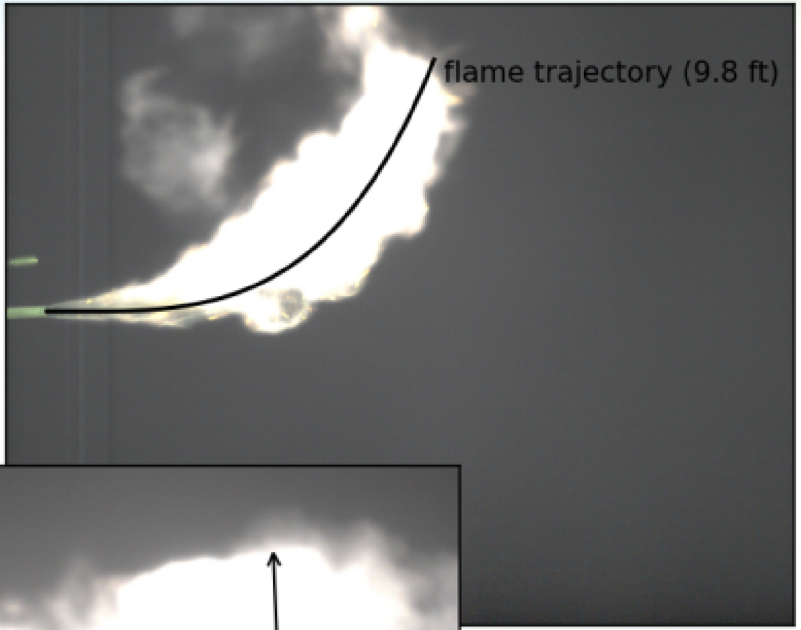
- Remainder of FY21
  - Publish justification and build consensus for proposals to NFPA 2 2023 with reduced separation distances for liquid hydrogen infrastructure
  - Final analysis of vent-stack experimental data
    - Quantification of hydrogen concentrations from signal
    - Statistical analysis of all signals (Raman, visible, weather conditions)
  - Finalize R&D plans for pooling/vaporization experiments
  - Begin planning wall mitigation experiments
- FY22
  - 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
  - Improve the understanding of hydrogen ignition phenomena
  - Refine simulations and analyses of scenarios driving separation distances in NFPA 2 and enable the continued science-based revision of the liquid hydrogen separation distances in NFPA 2

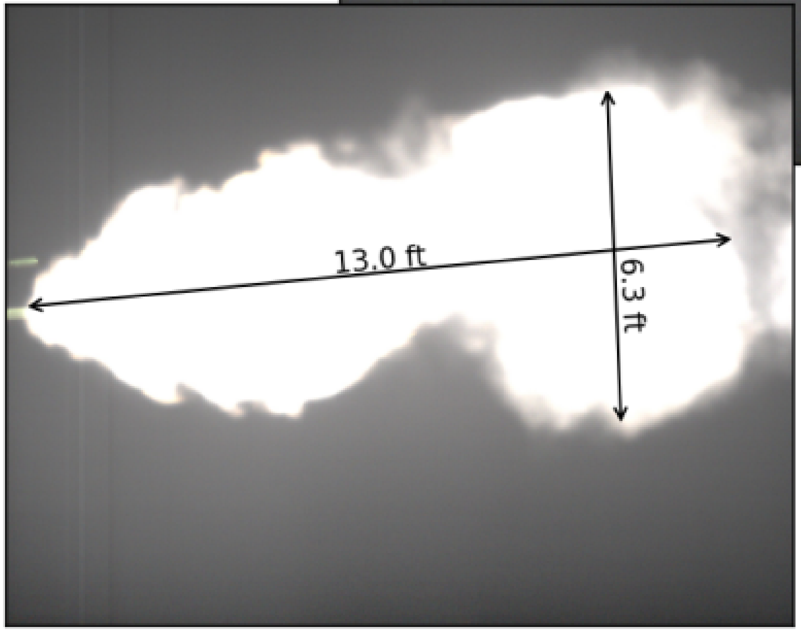
Summary

- **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**:
  - Developed analysis and provided science-based proposal of bulk liquid hydrogen setback distances for the 2023 edition of NFPA 2, based on operating pressure and system pipe size
  - Executed vent-stack dispersion experiments for a range of conditions at LLNL LH_2 pad
    - Hydrogen is concurrent with the visible plume
    - Hydrogen dispersion and visible plume is not greatly affected by relative humidity
  - Refined CFD capabilities for liquid hydrogen to enable planning of pooling and evaporation experiments
- **Future work**:
  - Perform additional large-scale experiments and develop models for pooling and evaporation
  - Use models to advise NFPA 2 code committee on hazards and harm from liquid hydrogen and build consensus to justify LH_2 infrastructure siting reductions in 2023 edition of NFPA 2

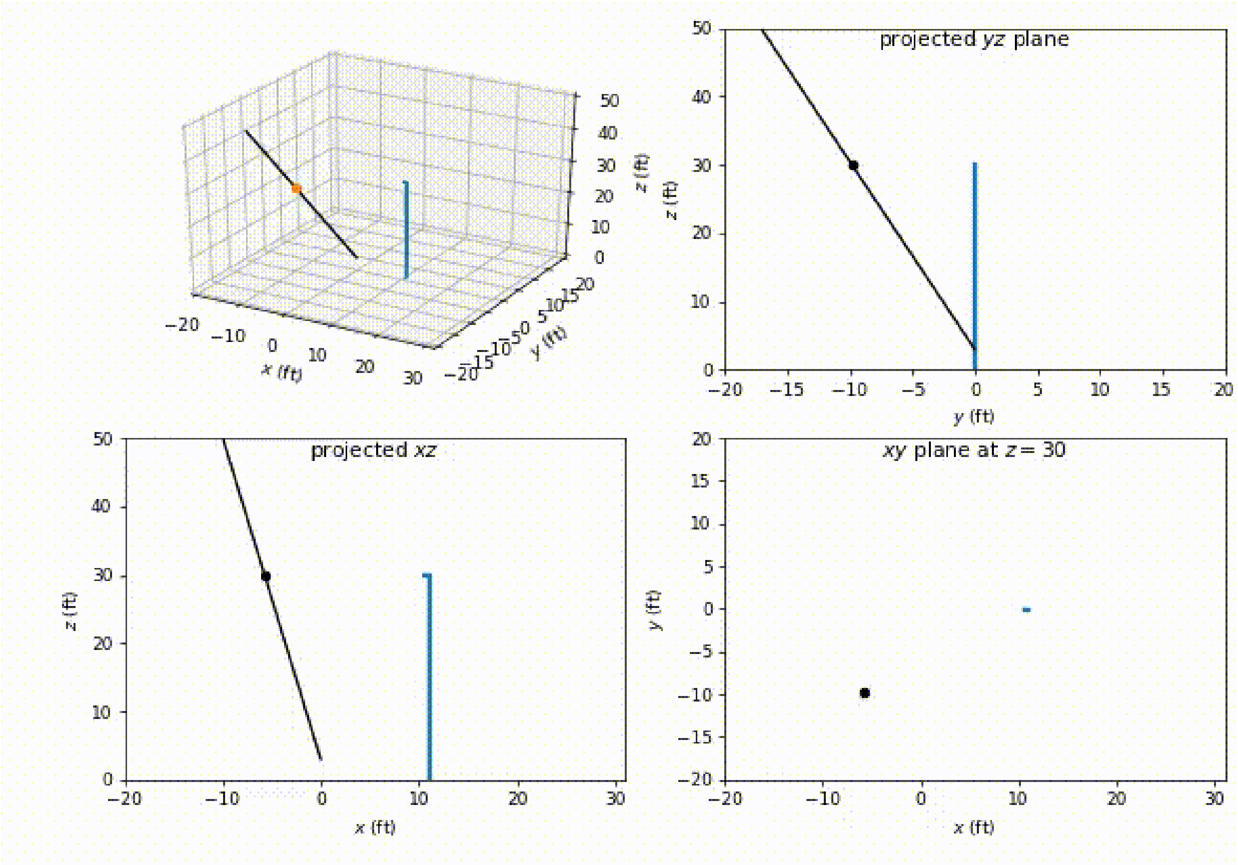
TECHNICAL BACKUP SLIDES

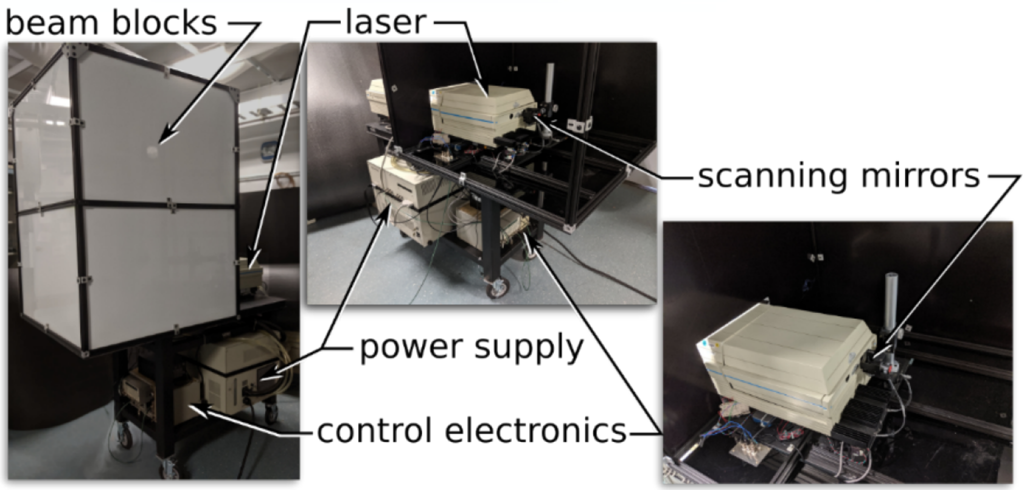
High laser power has resulted in ignition, but the flame was safely extinguished without harm (to personnel or equipment)



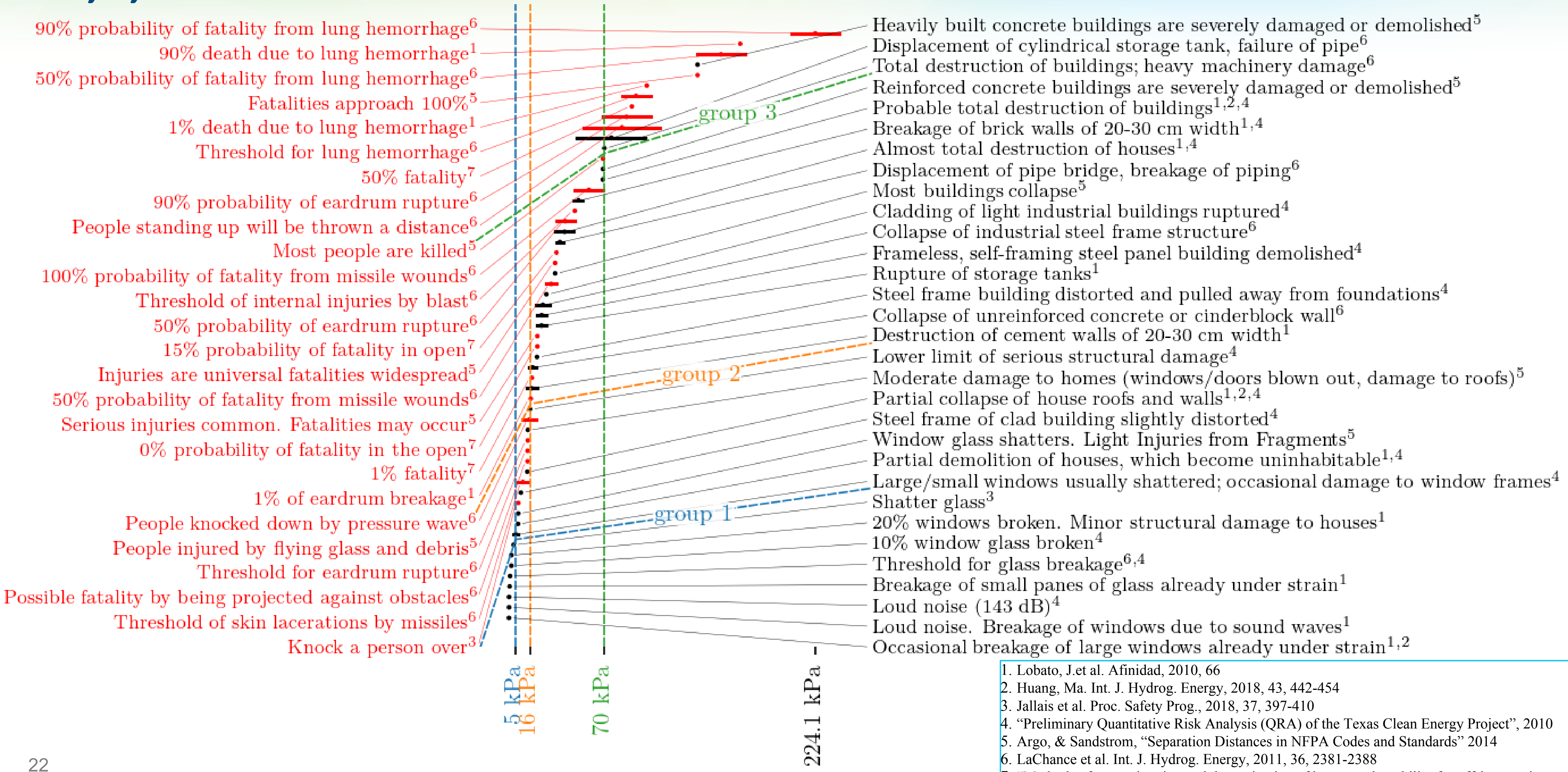


Rastering of the laser is needed to maintain power while covering a large area





Overpressure harm criteria have reviewed, with selection of Groups 1,2, and 3 criteria



1. Lobato, J.et al. Afinidad, 2010, 66
2. Huang, Ma. Int. J. Hydrog. Energy, 2018, 43, 442-454
3. Jallais et al. Proc. Safety Prog., 2018, 37, 397-410
4. “Preliminary Quantitative Risk Analysis (QRA) of the Texas Clean Energy Project”, 2010
5. Argo, & Sandstrom, “Separation Distances in NFPA Codes and Standards” 2014
6. LaChance et al. Int. J. Hydrog. Energy, 2011, 36, 2381-2388
7. “Methods of approximation and determination of human vulnerability for offshore major accident hazard assessment.” 2010

Technology transfer activities

- HyRAM, an open source software contains validated models developed under this project (see HyRAM.sandia.gov or github.com/sandialabs/hyram)

- Analyses performed under this project are regularly presented to the NFPA 2 Hydrogen Storage Task group, resulting in changes to the fire code

Progress toward DOE targets or milestones

- 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
  - Proposed reduced separation distances to NFPA 2023 with the following feedback
    - The committee believes in the intent of the [proposed changes] but would like the public to have adequate time to review these changes prior to being incorporated. Additionally, the committee would like additional time to ensure that changes have the following attributes:
      - methodology used is well documented
      - retrievable - ex: SAND reports
      - repeatable - ex: someone else (independent) can be reasonably expected to have the same separation results
      - revisable - ex: all input assumptions are clearly defined and revisable at a later date
      - Independent verification of the model and method used
      - Sandia to complete testing and verify dispersion model
  - ➢ **Currently addressing the concerns listed above so that the proposed changes can be accepted and the liquid hydrogen footprint can be reduced**

Publications and presentations

- B. Roy Chowdhury and E.S. Hecht, "Dispersion of cryogenic hydrogen through high-aspect ratio nozzles," International Journal of Hydrogen Energy. 46 (23), 12311-12319. 2021. https://doi.org/10.1016/j.ijhydene.2020.09.072.
- X. Li, B. Roy Chowdhury, Q. He, D.M. Christopher, and E.S. Hecht, "Validation of two-layer model for underexpanded hydrogen jets," International Journal of Hydrogen Energy. 46, (23), (12320-12328) 2021. https://doi.org/10.1016/j.ijhydene.2020.08.204.
- S.G. Giannissi, A.G. Venetsanos, and E.S. Hecht, "Numerical predictions of cryogenic hydrogen vertical jets," International Journal of Hydrogen Energy. 46 (23), 12566-12576. 2021. https://doi.org/10.1016/j.ijhydene.2020.08.021.
- E.S. Hecht, and B. Roy Chowdhury, "Characteristic of cryogenic hydrogen flames from high-aspect ratio nozzles," International Journal of Hydrogen Energy. 46 (23), 12320-12328. 2021. https://doi.org/10.1016/j.ijhydene.2020.08.265.
- E.S. Hecht an B.D. Ehrhart. "HyRAM simulations of LH2 hazard distances," presented to the NFPA 2 storage task group, June 23, 2020. SAND2020-6054 PE.
- E.S. Hecht "Hydrogen detection via Raman scattering" Presentation at the NREL Technical Seminar--Next Generation Detection Strategies for Hydrogen Applications, SAND2020-11172 PE, Oct. 13, 2020
- T. Jordan and E.S. Hecht "Session: Progress in Safety Research, Topic: Low T (LH2/cryogenic) related" Presented at the Research Priorities Workshop, SAND2020-11941 PE, Oct 22, 2020
- E.S. Hecht "Developing a scientific basis for liquid hydrogen safety codes and standards in the United States" Presented at the 2020 International Gas Safety Seminar in Seoul, Korea. SAND2020-12805 C, Nov. 27, 2020
- E.S. Hecht and B.D. Ehrhart "Analysis to support revised distances between bulk liquid hydrogen systems and exposures" Abstract for the International Conference on Hydrogen Safety – 2021. SAND2020-14363A
- E.S. Hecht and N.J. Killingsworth "Effect of wind on cryogenic hydrogen dispersion from vent stacks" Abstract for the International Conference on Hydrogen Safety – 2021. SAND2020-14364A
- E.S. Hecht "Experiments and Analysis in Support of Science-Based Liquid Hydrogen Codes and Standards" Presented to the Codes & Standards Tech Team, SAND2021-0344 PE, Jan 14, 2021
- E.S. Hecht "Scientific justification for updating the bulk liquid separation distance tables in NFPA 2" Presented to the CGA Hydrogen Gap Analysis Task Force, SAND2021-4268 PE, April 8, 2021