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SAND2022-5466C

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

Project ID: SCS010

DOE Project Award #: WBS 6.2.0.801

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Sandia National Laboratories

2022 Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting

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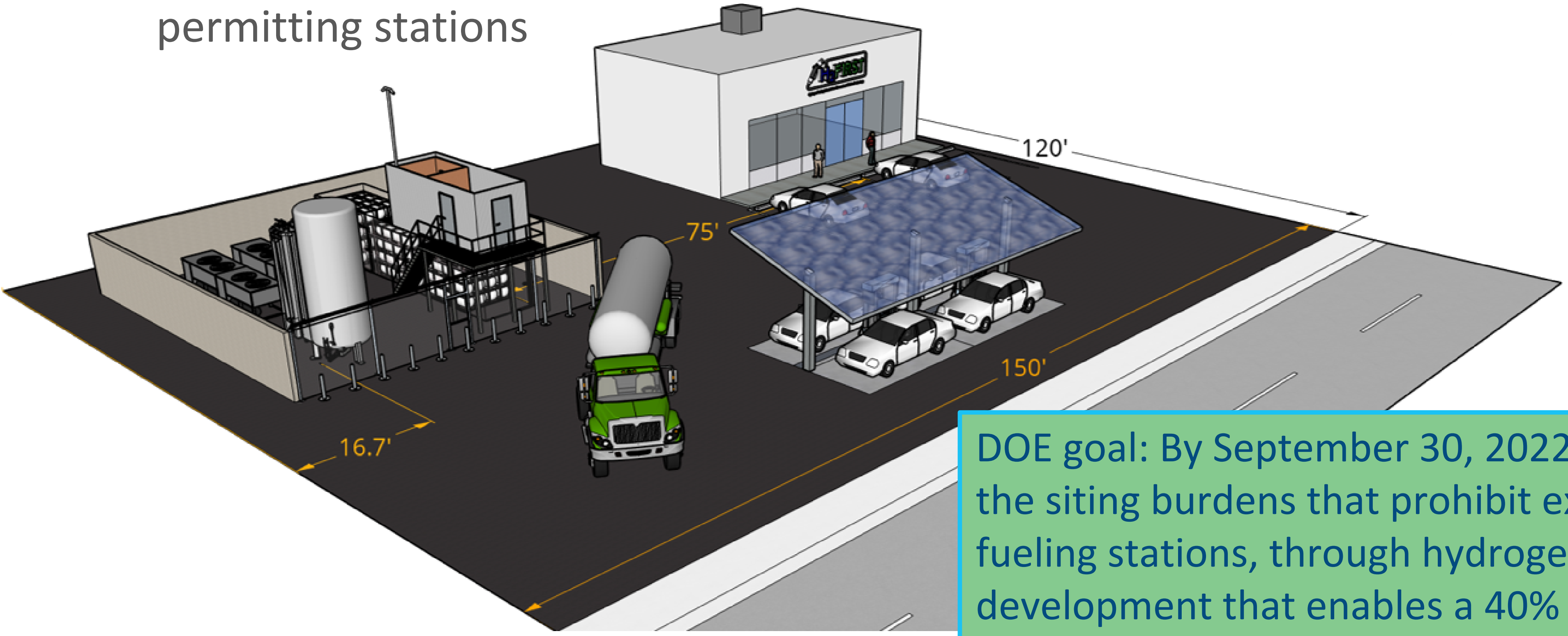
Project Goals

- 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 H_2 systems and enable use of that information for revising regulations, codes, and standards (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. 2022*
  * Project continuation and direction determined by DOE annually

Budget

- FY21 DOE Funding: $700 k
- Planned FY22 DOE Funding: $700 k

Partners

- **Industry & Research**
  - NREL
  - NFPA 2 code committee
  - CGA G-5.5 testing task force
  - Chart Industries
  - Air Products

Relevance: Providing data and analyses to support regulations, codes, and standards (RCS) for hydrogen and fuel cell technologies

- Conducting research to generate the valid scientific bases needed to define requirements in developing RCS
- Developing and enabling widespread dissemination of safety-related information resources and lessons learned

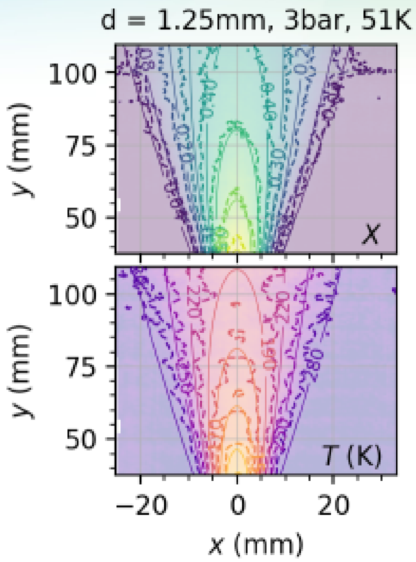
Liquid hydrogen example:

- Motivation:
  - 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), needed for HD vehicles
  - even with credits for insulation and fire-rated barrier wall, current 75 ft. offset to building intakes and parking make footprint large
- Background:
  - current separation distances in NFPA 2 for liquid hydrogen are based on consensus without documentation of decision basis
  - liquid hydrogen was likely not envisioned for use outside an industrial environment
  - previous work by our group led to science-based, reduced, gaseous H_2 separation distances

- Expected outcome: smaller separation distances, guided by data and analysis from this project, can lead to reduced infrastructure footprints which can enable construction of safe, large refueling stations in more locations, increasing zero-emission vehicle (FCEV) use across sectors

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

HyRAM+
Hydrogen Plus Other Alternative Fuels Risk Assessment Models

models

model needs

Enable Hydrogen Infrastructure through Science-based Codes and Standards
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

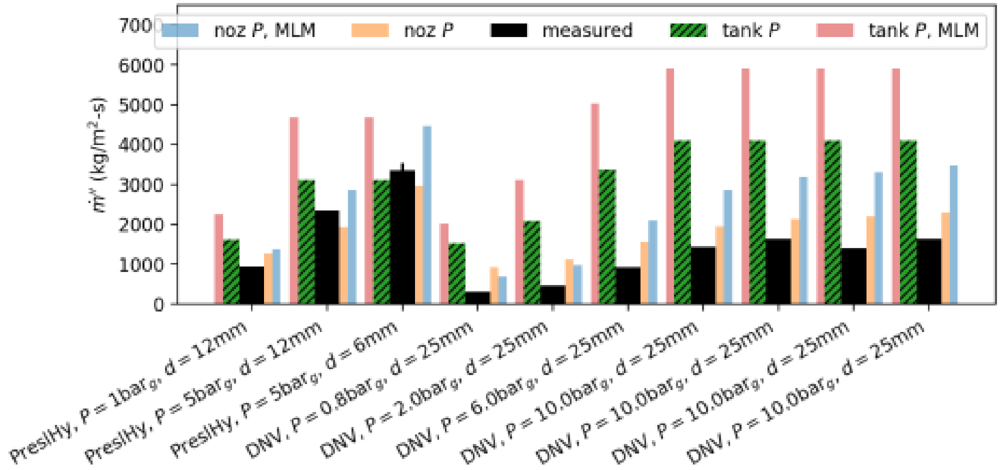
- Issue: Current separation distances for liquid hydrogen lack documentation of basis
  - Updated analysis for repeatable, revisable, verified liquid hydrogen separation distances
  - Built consensus for proposed changes to NFPA 2; changes were accepted in a verbal vote
- Issue: There is limited data on the behavior of H_2 blended with natural gas
  - Performed dispersion measurements on 0, 25, 50, 75 and 100% H_2 in CH_4
  - Characterizing ignition of blended gas buoyant jets
- 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
  - Performing CFD modeling to assist with planning experiments
  - Developing validated reduced order models for incorporation into HyRAM+
  - Performing experiments in large indoor facility with well-characterized cross-wind
  - **FY22 milestone:** Complete experimental campaign measuring vaporizing liquid hydrogen pool – in progress

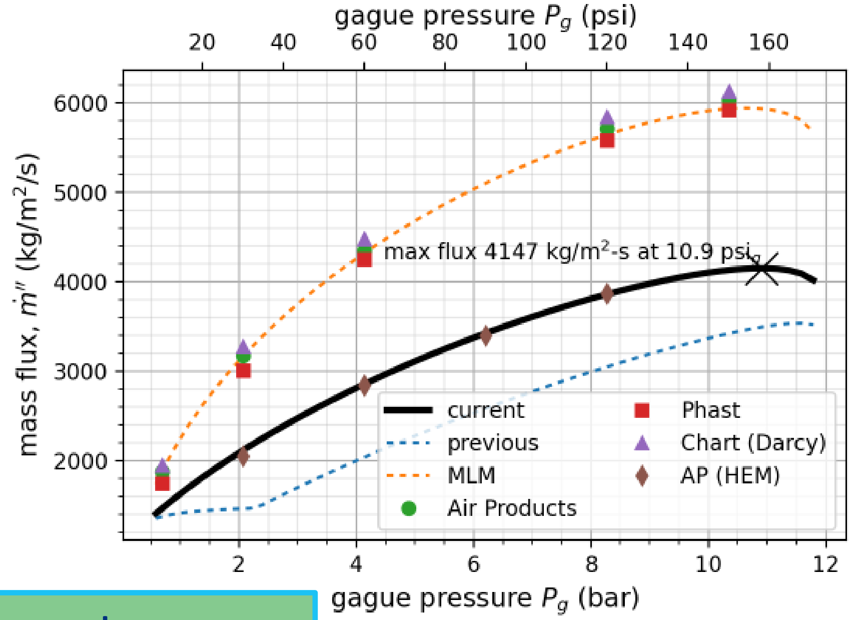
➢ Deliver validated scientific analyses of critical scenarios and provide the science to enable revisions to the 2023 edition of NFPA 2

Accomplishment: Revised choked flow calculations – a key calculation for updated bulk liquid exposure distances in NFPA 2

- Some calculations (saturated liquid or 2-phase releases) previously relied on uncertain 2-phase flow speed of sound
- New calculation searches for maximum mass flux using more reliable enthalpy data only
- For saturated liquid results in a higher (and more realistic) mass flow rate
- No change in flow rate for gases

Predictions (green striped bars) match or provide conservative estimate of measured flowrates (black bars)





Calculations are repeatable in several implementations. Current calculation (black line) has increased flux over previous (blue dashed) but is less conservative than metastable liquid model (MLM).

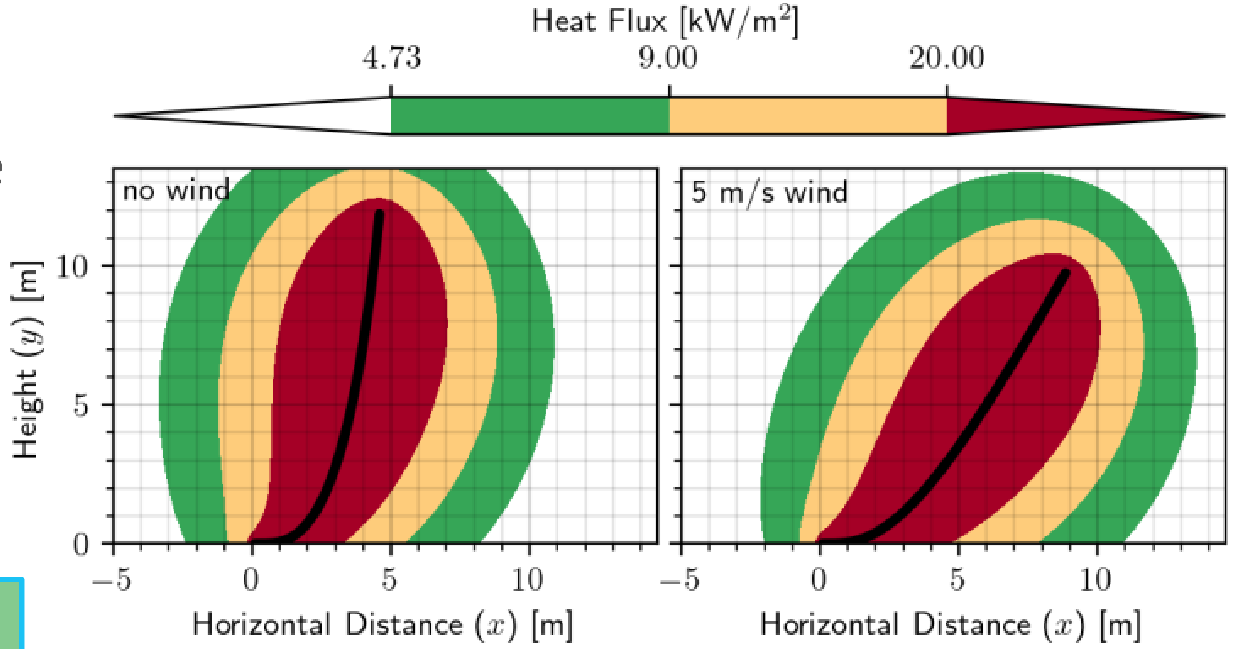
➢ Model improvements were needed to match data and ensure calculations result in science-based separation distances

Accomplishment: Enabled wind effects in jet flame simulations

- Saturated liquid flows have a low velocity
- High temperature flames have a lot of buoyancy
- Wind effect added to x-momentum balance
- Wind extends birds-eye view of exposure distances
- Predicted heat fluxes closer to experimental data with unsteady wind

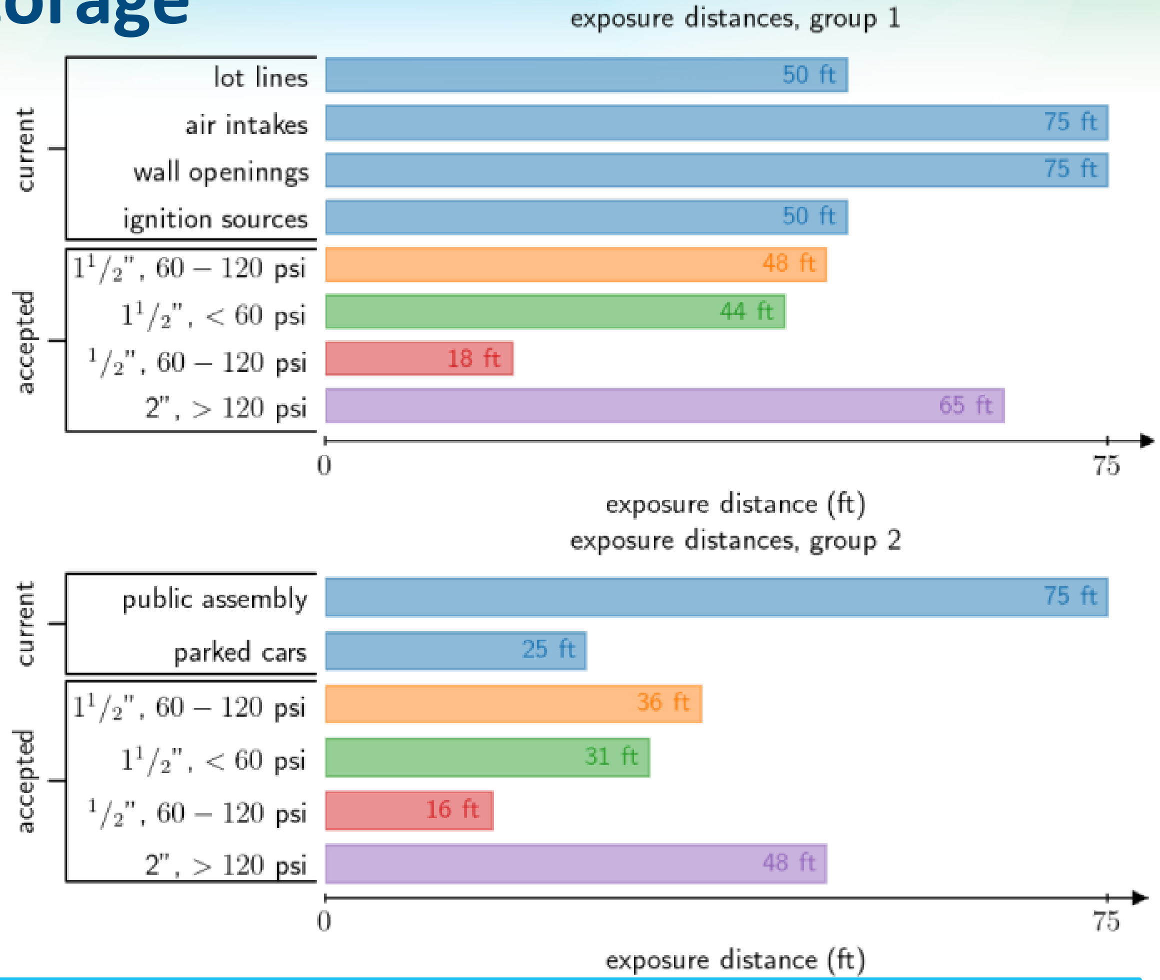
➢ Model improvements were needed to match data and ensure calculations result in science-based separation distances

Flame from 5% leak area of 1.5" pipe of saturated liquid hydrogen at 160 psi without and with 11 mph (5 m/s) wind in the x-direction



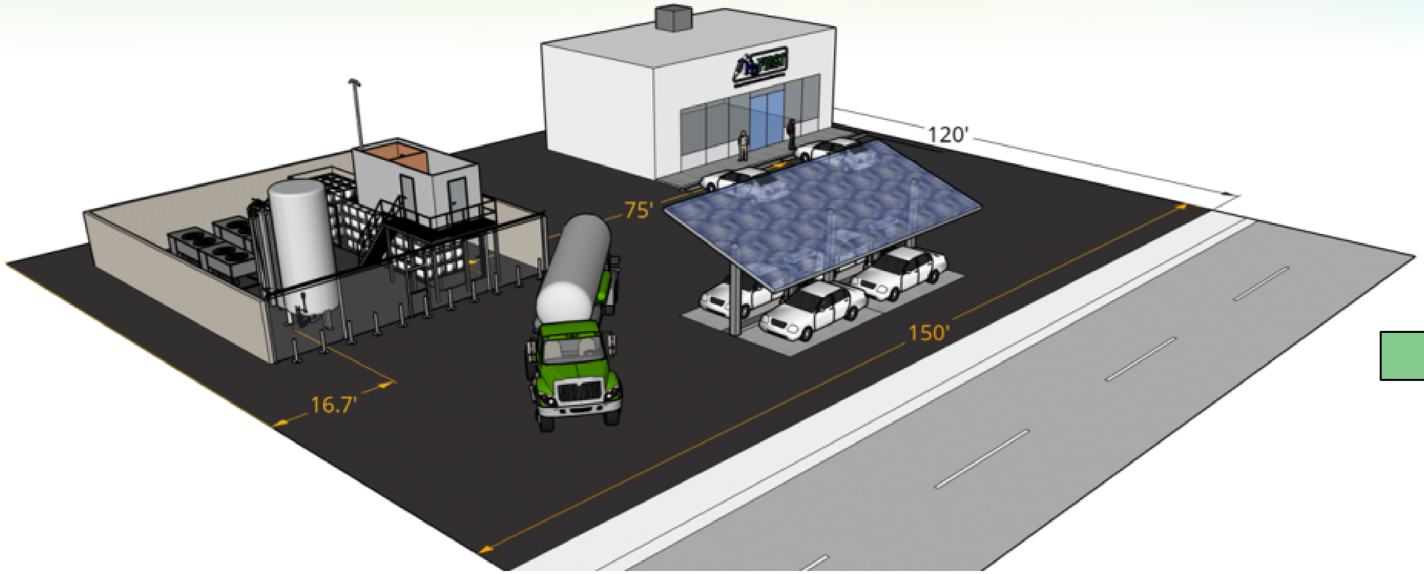
Accomplishment: Used physics models to develop updated setback distances for bulk liquid hydrogen storage

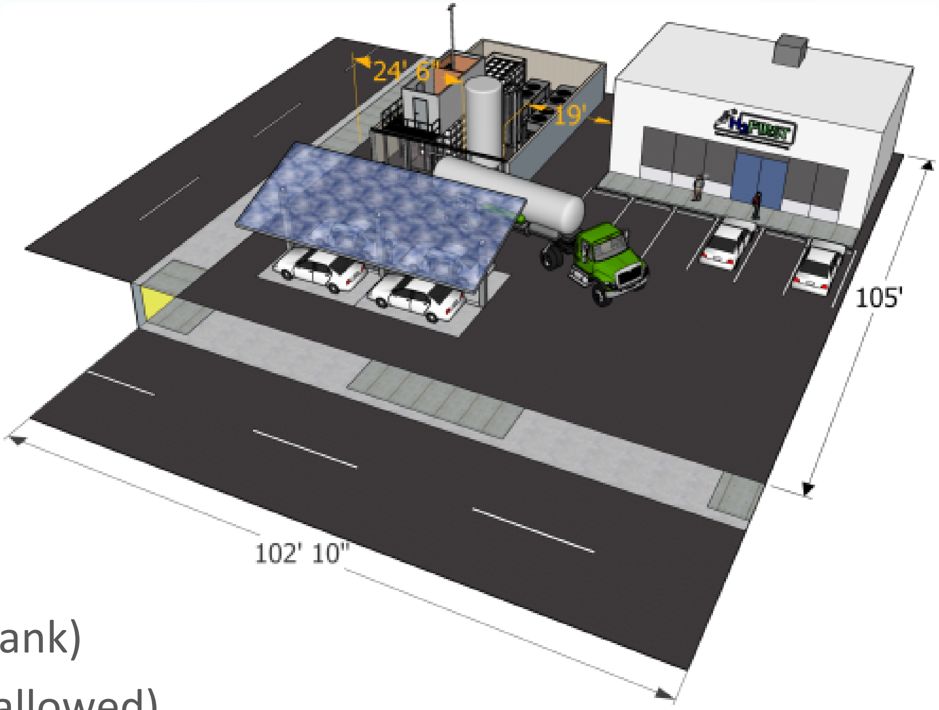
- Separation distances grouped in a similar manner as gaseous exposures
- Conservative assumption on leak size (5% area)
- Updated harm criteria (e.g., heat flux level), and criteria includes overpressure from delayed ignition
- Distances function of pipe size and system pressure instead of tank volume
- Calculated through consequence modeling as maximum distance to each harm criteria (for each group) from a characteristic (5% area) leak



➢ 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: Showed that reduced footprint will be enabled by updated tables and language in NFPA 2

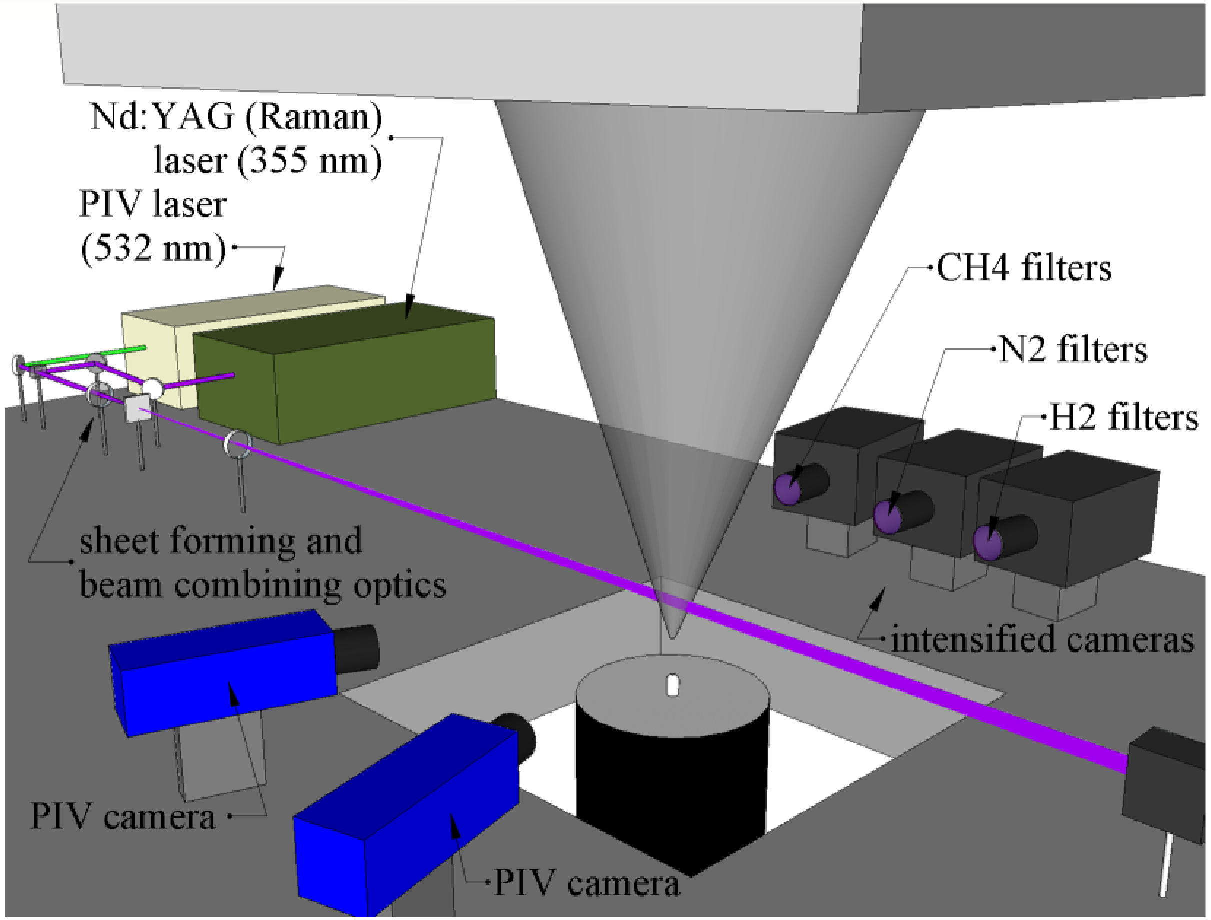




- Distance to air intakes reduced from 75 ft to 24’6”
  - For 1.5” diameter piping, >120psi tank (vs 3,500-15,000 gal [4000 kg] tank)
  - Reduction of calculated distance enabled due to walls (previously not allowed)
- Liquid and gaseous portions of the system are divided by source valve
- Distance to lot lines increased from 16.7’ to 24’6”

> ➢ Using accepted separation distances, DOE goal of 40% reduction in footprint can be met (18,000 ft^2 -> 10,800 ft^2)

Accomplishment: Unignited dispersion data of H_2/CH_4 blends has been collected

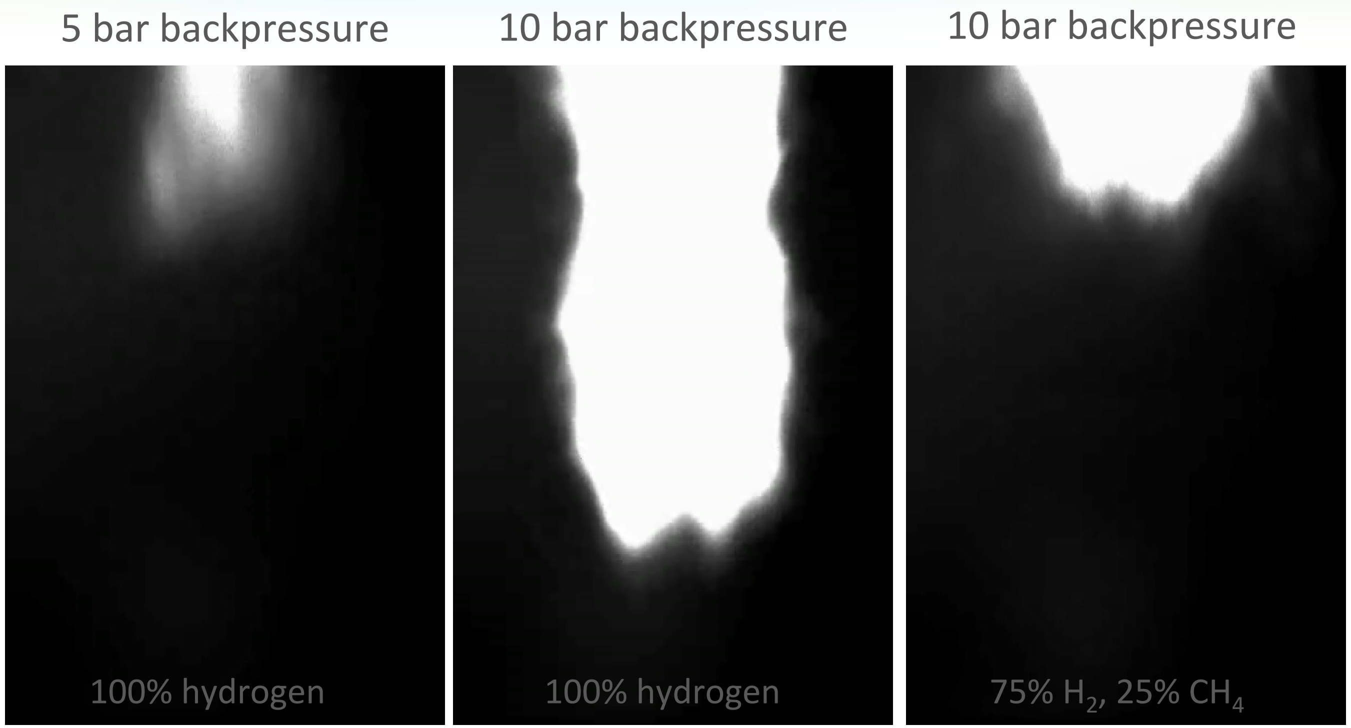


- Raman scattering from H_2 and CH_4 measured
- Blends of 25, 50, 75 vol-% H_2-CH_4 along with pure H_2 and pure CH_4 measured
- Data analysis underway to map out concentrations
- Will elucidate behavior of blends (do H_2 and CH_4 remain well-mixed?)
- Additional velocity information (PIV) to be collected
- Concentration and velocity data can help explain different ignition phenomena (when blends ignite/do not ignite)

➢ Data is critical to validating models for blend dispersion

Progress: Measuring under which conditions buoyant jets of pure hydrogen and blends of H_2/CH_4 ignite into jet flames

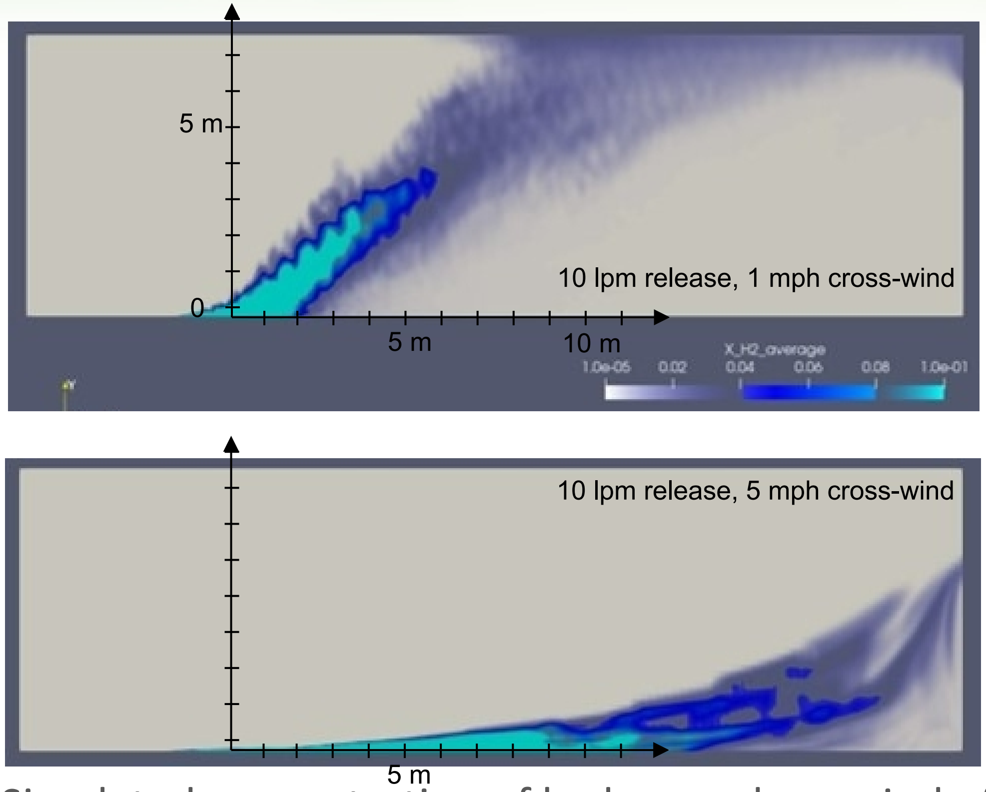
- Laser spark ignition non-intrusively forms a plasma at a precise location
- Flame speed high enough for hydrogen to ignite into jet flame under certain conditions
  - Jet flame forms for releases with less than 2 bar or over 6 bar backpressure
  - Extinction (blow off) between 3 and 5 bar (ignition kernel still forms)
- Reduced flame speed of CH_4 prevents ignition of blends with 25% or more CH_4 from forming jet flames (1 mm diameter nozzle, up to 10 bar backpressure)
- Behavior being studied further for additional conditions



Chemiluminescence of laser spark ignition of gases through a 1mm diameter nozzle (15/1000 speed). Pure hydrogen at moderate pressure (left) and 25% CH_4 (right) show flame blow-off while pure hydrogen at a higher pressure (center) ignites into a jet flame.

➢ Small leaks of blends at moderate pressures may be unlikely to form jet flames

Progress: Computational simulations have informed liquid H_2 pooling experimental design

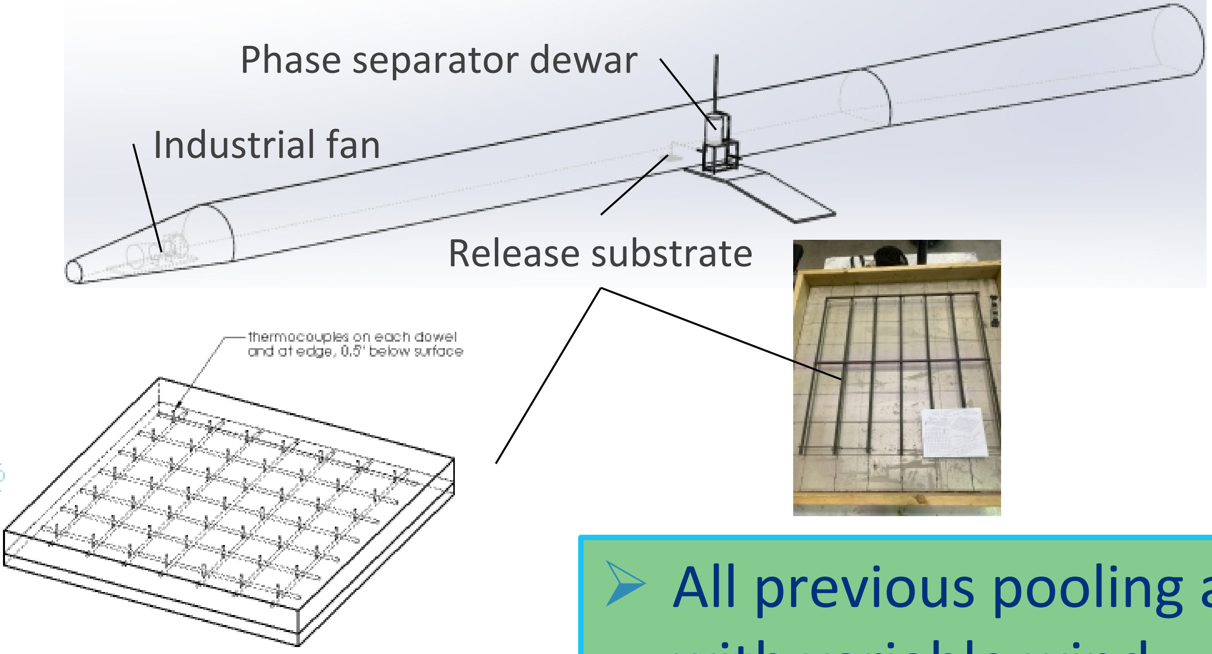


Simulated concentration of hydrogen downwind of the release for different experimental conditions

- Simulations of saturated H_2 vapor release from various pool diameters
  - Eliminates complexities of 2-phase flow modeling
  - Pool size is
    - highly uncertain (challenging to measure)
    - likely to fluctuate
    - different for different substrates (concrete, steel)
- Dispersion profile (downwind concentrations) fairly independent of pool size
- Informs where to put sensors

➢ 5 mph wind keeps the plume near the floor; sensor density to be increased near the floor for this condition

Progress: Liquid hydrogen pooling and vaporization experiments to take place at the end of July



- Releases to take place in 18’ diameter shock tube in Albuquerque for control of cross-wind
- Visible and IR imaging of pool dimensions and condensed moisture in plume
- Thermocouple measurements in substrate (for heat flux and pool dimensions) and in plume (for temperature and concentration)
- Verification of temperature-concentration correlation through application of NREL’s HyWAM sensors
- Well controlled crosswind, supplied by 100,000 cfm fan providing 1 and 5 mph crosswinds
- Measurements with variations in wind speed, LH_2 flowrate and substrate (concrete and steel)

➢ All previous pooling and dispersion measurements have been outdoors with variable wind – this data will be suitable for model validation

Response to reviewer comments

- There is still a good deal of model validation and testing to be performed, and the timelines and cost for this work are not well-defined or -identified. The codes and standards bodies would benefit from more results sooner. Presentation of more future planning would be beneficial.
  - With the data and models in-hand we were able to propose changes to NFPA 2 and build consensus around the updated language and separation distance tables. The work of updating the bulk liquid hydrogen section of NFPA 2 has crystalized paths towards reducing conservatism and updating NFPA 2 further. Pooling experiments are to be completed this FY. We agree that there is additional testing and work that is needed in several areas. Some specific reviewer suggestions are included below.
- Several suggestions for future work:
  - Condensation of air and formation of oxygen enriched in LH_2 pools, shock sensitivity, and risk (industry representatives claim this is not a hazard, but the project should consider HSL's surprise occurrence)
  - Vapor cloud formation from cryogenic releases, formation of condensed air within such releases, combustion yields, overpressure, and acoustic hazards
  - Barrier/wall design to loft vapors into a safer region for dissipation and to mitigate overpressure should ignition occur
  - The impact of explosions based on releases with delayed ignition, as well as jet explosions from large releases
  - ➢ Each of these suggestions has merit. We are laying out plans for addressing these phenomena in the future work section as time and budget permits.

Collaborations enable this research and expand impact

- NFPA 2 Technical Code Committee (Industry)
  - Regular attendance with expert advisory role
  - Close collaboration with Air Products and Chart Industries in subtask group to develop updated NFPA 2 bulk liquid hydrogen separation distances
- CGA G-5.5 testing task force (Industry)
  - Providing hardware for and analysis support of measurements of LH2 vent stack flames
- Chart Industries and Air Products (Industry)
  - Subs providing hardware and design assistance on the pooling and vaporization experiments
- NREL (National Lab)
  - Collaboration to instrument pooling and vaporization experiments with HyWAM sensors

Remaining challenges and barriers: Execution of pooling and vaporization experiments, studying other phenomena of interest

- Logistical challenges for successful completion of pooling and vaporization experiments
  - Need hardware onsite (e.g., phase separator tank, HyWAM sensors, LH2 tanker)
  - Scheduling challenges with other activities at the site
- Additional experiments are needed to understand and develop validated models for additional phenomena:
  - Study mitigation of liquid hydrogen leaks/flames from walls
    - Effects on unignited dispersion and accumulation
    - Reduction in heat flux/overpressure
  - Understand air condensation into LH2 and the formation of more hazardous (oxygen enriched) mixtures

Proposed future work

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

- Remainder of FY22
  - Execute pooling and vaporization experiments
    - Validate pooling and vaporization models
    - Incorporate pooling models into HyRAM+
  - Complete lab-scale experiments with (H_2/CH_4) blends
    - Analysis and publication of dispersion data
    - Analysis and publication of ignition data
    - Measurements, analysis, and publication of radiation data
    - Incorporate buoyant jet and jet flame models of blends into HyRAM+
- FY23: Develop additional experiments and modeling tools
  - Experiments and models on the effect of walls mitigating radiation, dispersion, and overpressure hazards from liquid hydrogen
  - Models for air condensation into LH_2
  - Improved models on the physics of ignition of hydrogen and H_2/CH_4 blends

Summary

- **Relevance**: Address lack of safety data, technical information relevant to development of safety codes & standards.
- **Approach**: Provide a scientific foundation enabling the development/revision of codes & standards.
  - 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
- **Accomplishments and Progress**:
  - Revised several models in HyRAM+ for liquid hydrogen, enabling final analysis and science-based bulk liquid hydrogen setback distances for the 2023 edition of NFPA 2, based on operating pressure and system pipe size, and teamed to build consensus around proposed changes
  - Begun gathering data on H_2/CH_4 blend behavior, including dispersion and ignition
  - Significant progress towards execution of pooling and vaporization experiments
- **Future work**:
  - Execution of pooling and vaporization experiments
  - Analysis and publication of data and models
    - Pooling and vaporization
    - Blends of H_2/CH_4
  - Improve understanding of and develop valid modes for additional phenomena related to hydrogen safety (e.g. walls, air condensation into LH_2)

TECHNICAL BACKUP SLIDES AND ADDITIONAL INFORMATION

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

Publications and presentations

- E.S. Hecht, “Lab-scale dispersion of cryogenic hydrogen jets.” Presented at the PreSLHy Dissemination Conference (online), May 5, 2021. SAND2021-5510 C
- E.S. Hecht, B. Ehrhart, “Updated Justification for LH2 Exposure Distance Proposal.” Presented at the NFPA 2 Storage task group meeting (online), May 18, 2021 (SAND2021-6058 PE)
- E.S. Hecht, N. Killingsworth, “Effect of wind on cryogenic hydrogen dispersion from vent stacks,” paper at the International Conference on Hydrogen Safety, 21-24 September 2021 (SAND2021-7706 C)
- E.S. Hecht, N. Killingsworth, “Effect of wind on cryogenic hydrogen dispersion from vent stacks,” presentation at the International Conference on Hydrogen Safety (online), 21-24 September 2021 (SAND2021-11592C)
- E.S. Hecht, B. Ehrhart, “Analysis to support revised distances between bulk liquid hydrogen systems and exposures,” paper at the International Conference on Hydrogen Safety, 21-24 September 2021 (SAND2021-7705 C)
- E.S. Hecht, B. Ehrhart, “Analysis to support revised distances between bulk liquid hydrogen systems and exposures,” presentation at the International Conference on Hydrogen Safety (online), 21-24 September 2021 (SAND2021-11475C)
- D.M. Machalek, G. Bran Anleu, E.S. Hecht, “Influence of non-equilibrium conditions on liquid hydrogen storage tank behavior,” paper at the International Conference on Hydrogen Safety, 21-24 September 2021 (SAND2021-7886C)
- D.M. Machalek, G. Bran Anleu, E.S. Hecht, “Influence of non-equilibrium conditions on liquid hydrogen storage tank behavior,” presentation at the International Conference on Hydrogen Safety (online), 21-24 September 2021 (SAND2021-11265C)
- E.S. Hecht, “Overview of NFPA 2 public comment 49/NFPA 55 public comment 16.” Presented to the NFPA 2 Storage Task Group, Sept. 17, 2021. (SAND2021-11589PE)
- E.S. Hecht and B.D. Ehrhart, “Hydrogen Plus Other Alternative Fuels Risk Assessment Models (HyRAM+) Version 4.0 Technical Reference Manual.” SAND2021-14813. November 2021.
- E.S. Hecht and A.M. Glover, “Detection and monitoring tools for quantification of hydrogen releases, benchmark against methane.” Presented at the Clean Hydrogen JU Expert Workshop on Environmental Impacts of Hydrogen (virtual meeting), March 31 - April 1, 2022. (SAND2022-3617 C)
- E.S. Hecht, “Experiments and Analysis on Hydrogen Behavior in Support of Science-Based Liquid Hydrogen Codes and Standards.” Presented at the U.S. Drive Codes and Standards Tech Team virtual meeting, Jan. 13, 2022. (SAND2022-0354 PE)