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

Project ID: SCS010
DOE Project Award #: WBS 6.2.0.801

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2023 DOE Hydrogen Program Annual Merit Review and Peer Evaluation Meeting

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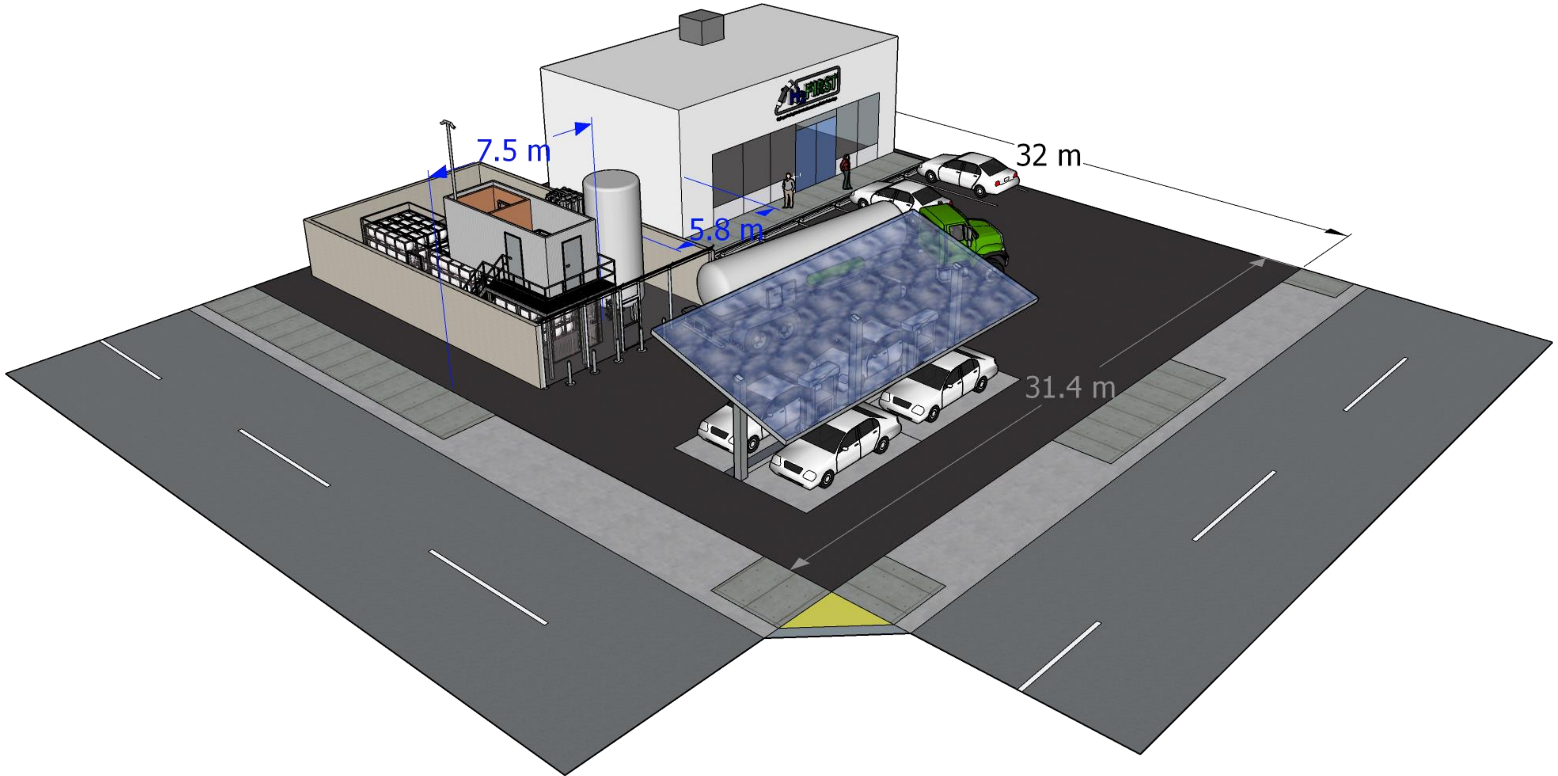
Project Goal

- Provide a science & engineering basis for the release, dispersion, ignition, and combustion behavior of hydrogen across its range of use (including high pressure, cryogenic, and blends)
  - Develop models and tools to facilitate the assessment of the safety (risk)
  - Enable use of models and data for revising and developing regulations, codes, and standards (RCS) and permitting infrastructure



Overview

Timeline

- Project start date: Oct. 2003
- Project end date: Sept. 2023*

  * Project continuation and direction determined by DOE annually

Barriers

- Conduct research to generate the valid scientific bases needed to define requirements in developing regulations, codes and standards
- Enable the safe deployment of new hydrogen technologies

Budget

- FY22 DOE Funding: $1M
- Planned FY23 DOE Funding: $1M

Partners

- **Industry & Research**
  - NREL
  - Chart Industries
  - Air Products
- **Codes & Standards Development**
  - NFPA 2

Potential Impact: Data and analyses to support updates and new regulations, codes, and standards (RCS) for hydrogen 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 logistically and economically viable for larger fueling stations needed for HD vehicles
- even with credits for insulation and fire-rated barrier wall, previous 75 ft. offset to building intakes and parking resulted in a large fueling station footprint

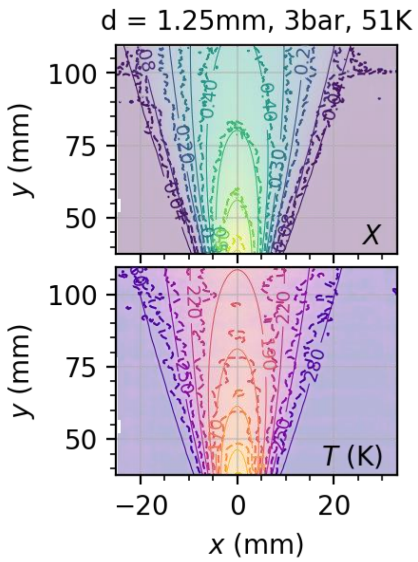
Background:

- previous separation distances in NFPA 2 for liquid hydrogen 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

- Impact: updated separation distances, guided by data and analysis from this project, facilitate 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

- Analysis was updated and documented for repeatable, revisable, verified liquid hydrogen separation distances
- Built consensus for updates to NFPA 2; changes published in 2023 edition

Issue: There is limited data on the behavior of H_2 blended with natural gas

- Performed dispersion, ignition and flame experiments on 0, 25, 50, 75 and 100% H_2 in CH_4
- Characterized ignition and dispersion 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

- Performed 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
- Complete experimental campaign measuring vaporizing liquid hydrogen pool – in progress

Accomplishment: Documented calculations of updated bulk liquid separation distances in 2023 version of NFPA 2

- 5% leak rate based on risk assessment (see SCS011)
- Exposure placed into 3 groups
- HyRAM+ physics models used to calculate distances to different hazard levels
- Each exposure group distance is the maximum distance to several hazards
- Calculations and assumptions (and resulting separation distances) can be updated as the scientific basis progresses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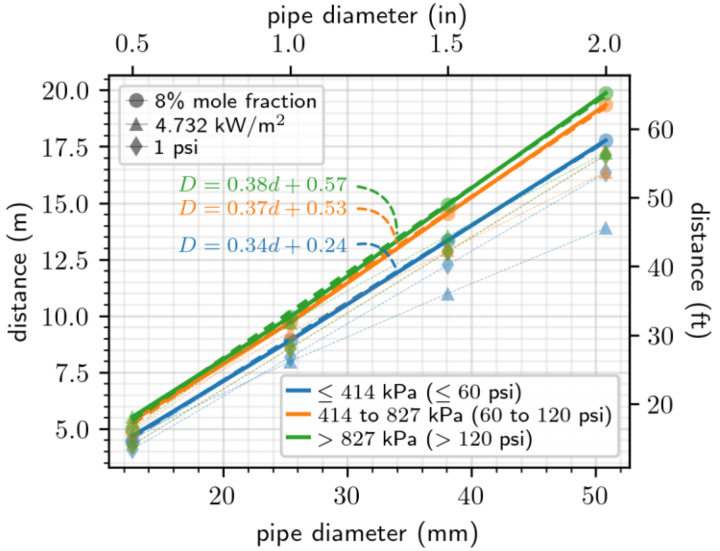
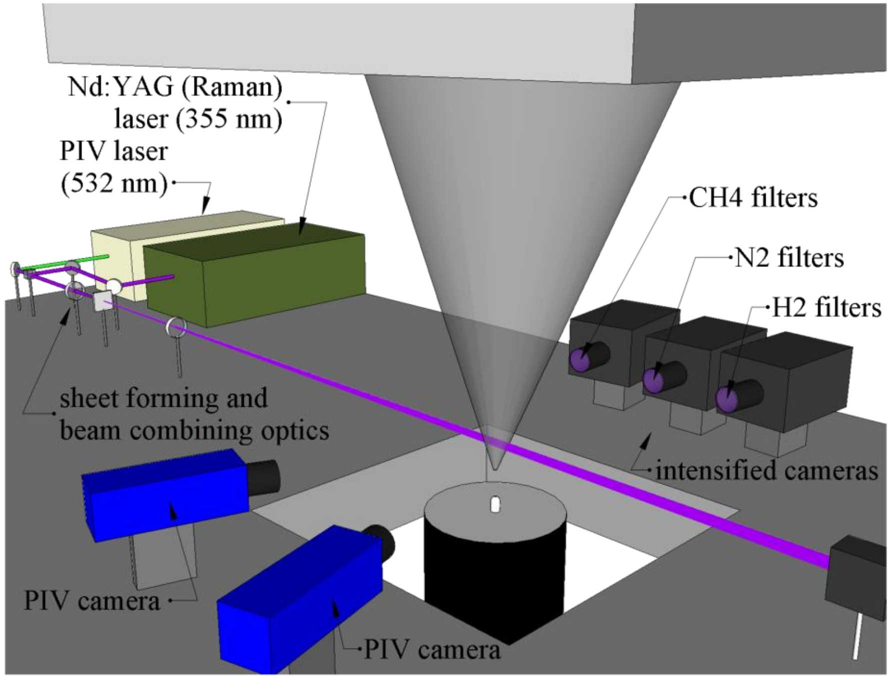
Technical Justifications for Liquid Hydrogen Exposure Distances

Brian D. Ehrhart, Ethan S. Hecht, Benjamin B. Schroeder

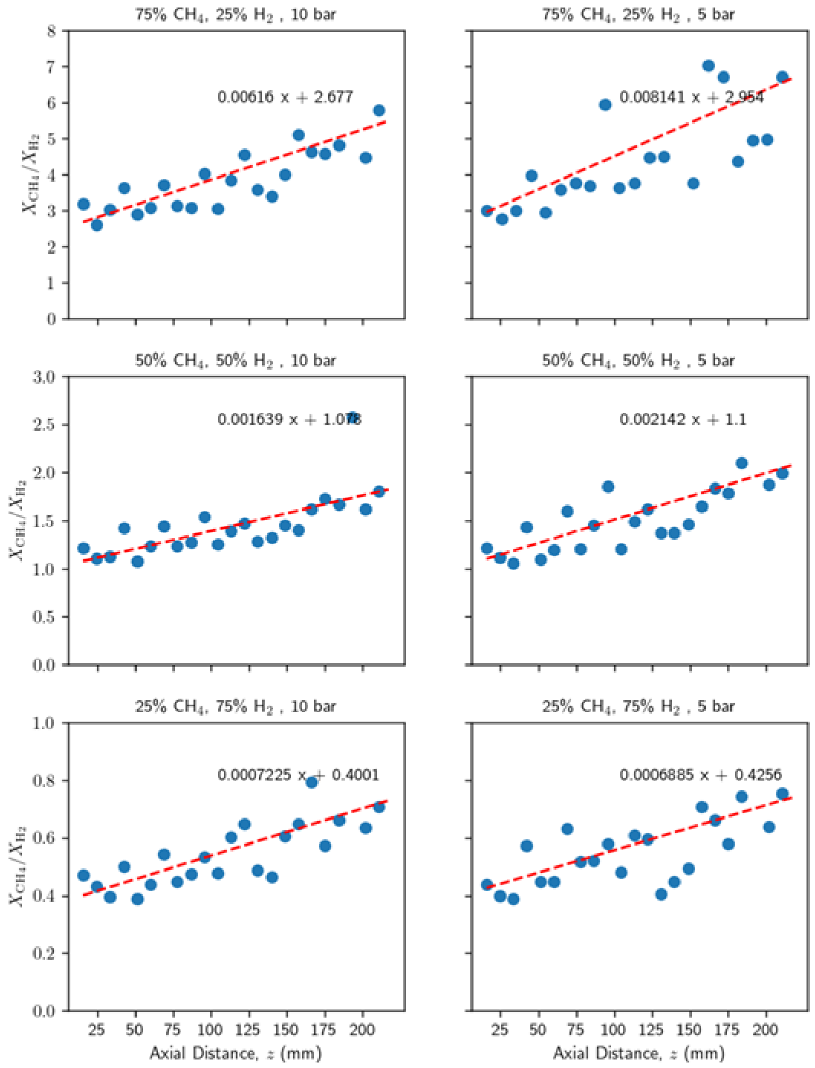


> ➢ Ensuring that distances and calculations are well-documented, retrievable, repeatable, revisable, independently verified, and use experimental results to verify the models

Accomplishment: Preliminary analysis of unignited H_2/CH_4 blend dispersion shows that ratio of constituents does not remain constant

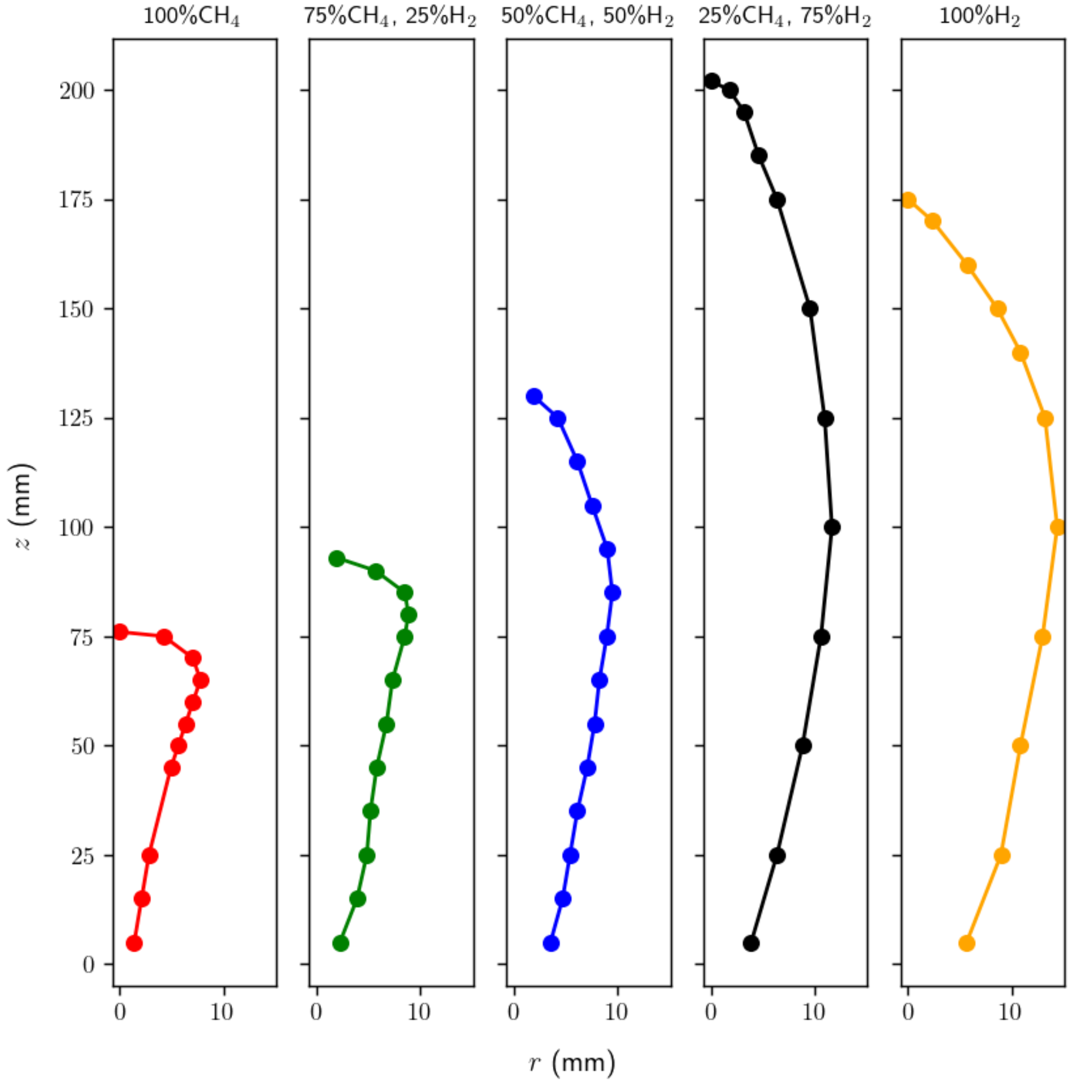


- Mole fraction ratio of CH_4/H_2 is 3, 1, and 0.33
- Ratio of CH_4/H_2 increases downstream
- Likely that H_2 is diffusing radially more rapidly than CH_4 and there is therefore less along the centerline



➢ Preliminary analysis suggests that centerline mole fraction of methane decreases more slowly than hydrogen

Accomplishment: Adding hydrogen to methane increases radial and axial extent of ignition boundary

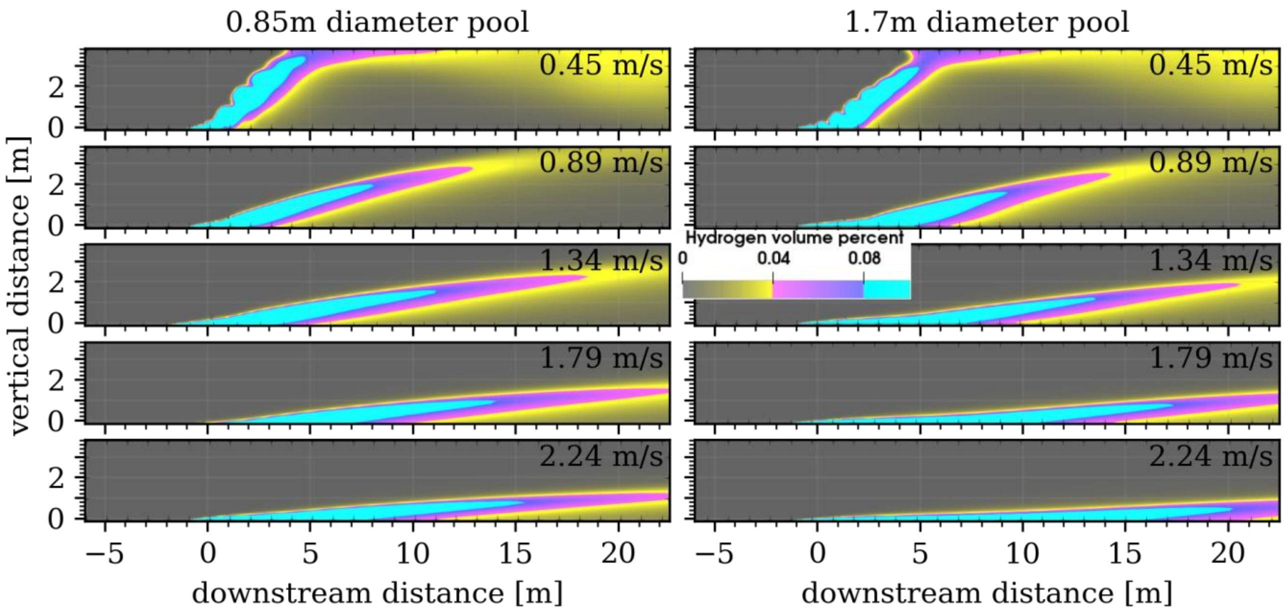


- Volumetric flowrate (and velocity) kept constant
- Ignition boundary is the point at which a flame kernel can form (not the point at which a jet flame can ignite)
- Higher flame speed of hydrogen extends ignition boundary
- Maximum axial extent for 25% CH_4, 75% H_2 possibly due to slower radial diffusion of methane

➢ Blending hydrogen has implications for safety distances – for an equivalent volumetric leak, ignition sources must be kept further from leak point

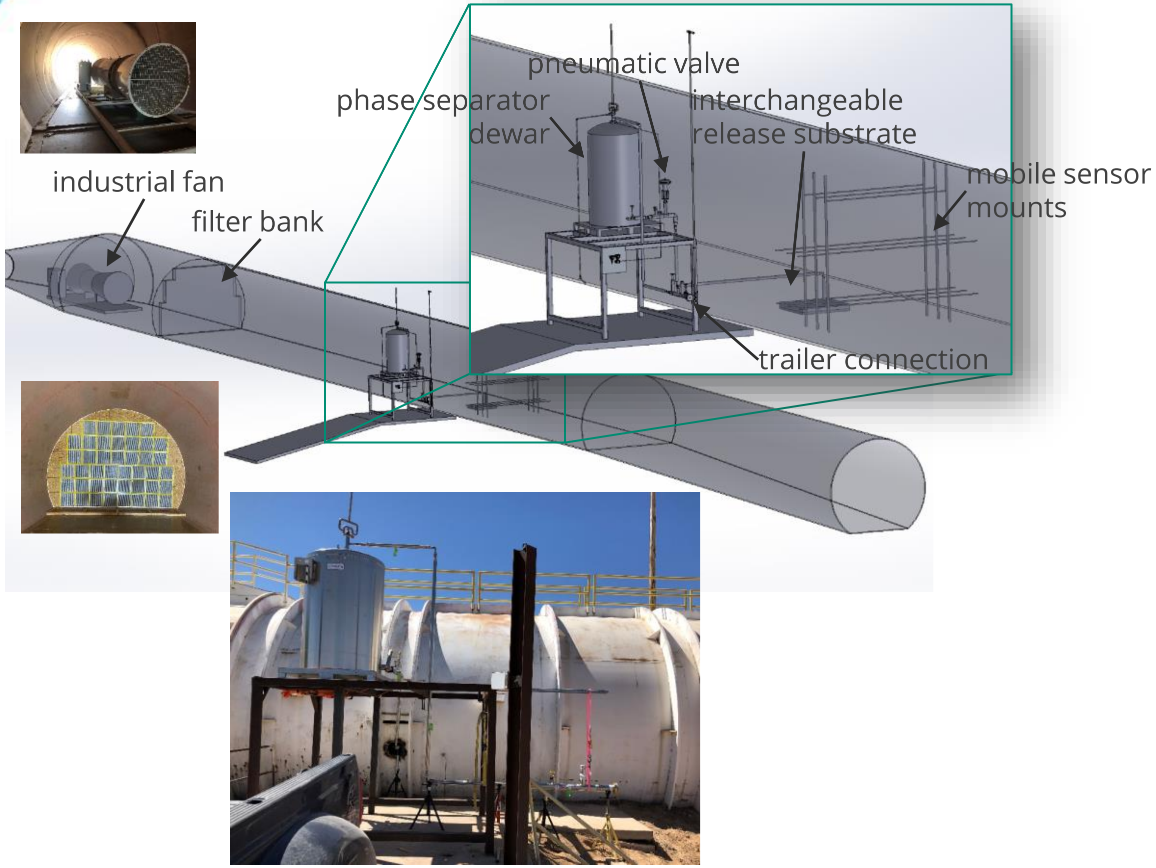
Accomplishment: Simulations were used to determine sensor placement and wind speeds for upcoming experiments

- Plume will interact with ceiling at low cross-wind speed
- Pool size (uncertain) has minor effect on plume dispersion
- Wind speed has large effect on plume dispersion
- Angle of sensors to be changed with wind speed



➢ Simulations enable more meaningful experiments to be performed and improved data to be collected

Progress: Experimental equipment for LH2 pooling and dispersion studies is being installed



- Experiments will measure extent of pooling and vaporization rate for various controlled cross-winds
- Using thermocouples and HyWAM sensor array (in collaboration with NREL) for concentration measurements
- Pooling and heat flux measured with visible and IR cameras and embedded thermocouples
- Lead time on equipment procurement and contracting significantly longer than expected

➢ Data will be well suited for model validation, with careful control of boundary conditions

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.

- ➢ We were able to make updates to the bulk separation distances in NFPA 2. Documentation of these distances provides pathways towards reducing conservatism and updating NFPA 2 further as more information is gathered. 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

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

Pooling and vaporization experiments have been significantly delayed

- Contracts now in place and equipment is onsite
- Ignited experiments to follow unignited experiments

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 LH_2 and the formation of more hazardous (oxygen enriched) mixtures
- Simplified impinging flame models for accident scenarios in tunnels

Proposed future work

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

Remainder of FY23

- Complete pooling and vaporization experiments
  - Validate pooling and vaporization models
  - Incorporate validated pooling model into HyRAM+ (see SCS011)
- Complete lab-scale experiments with (H_2/CH_4) blends
  - Improve dispersion data analysis
  - Measure velocity of unignited jets
  - Develop ignition map for blends based on mean and RMS velocity and concentrations
- Set up ignited LH_2 tests
  - Measure heat flux and trajectory of jet flames and overpressure from delayed ignition
  - Assess influence of fire-rated walls on mitigation of hazards

FY24: Develop additional experiments and modeling tools

- Experimentally measure and develop model for heat flux from impinging jet flame (has application to tunnel safety)
- Models for air condensation into LH_2

Summary

Potential Impact: Enable infrastructure siting through updated and new safety codes & standards based on data and technical analyses

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 (including liquid hydrogen and blends) releases and subsequent combustion
- Generate validation data where it is lacking

Accomplishments and Progress:

- Documented scientific basis for bulk liquid hydrogen setback distances in 2023 version of NFPA 2, enabling future revisions
- Demonstrated that ignition envelop increases with hydrogen content in blends and preliminary analysis suggests that mole fraction of methane and hydrogen does not remain constant as blends disperse
- Contracts placed and began installing hardware for pooling and vaporization experiments

Future work:

- Execution of pooling and vaporization experiments
- Analysis and publication of data and models
  - Pooling and vaporization
  - Ignition map for 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, heat flux from impinging diffusion flames)