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

Project ID: SCS010

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Overview

Timeline

- Project start date: Oct. 2003
- Project end date: Sept. 2017*
  * Project continuation and direction determined by DOE annually

Barriers

A. Safety Data and Information: Limited Access and Availability

G. Insufficient technical data to revise standards

Budget

- FY16 DOE Funding: $510 k
- Planned FY17 DOE Funding: $500 k
- Partner funding:
  - $175k committed stakeholder funds (CaFCP Auto OEM Group, Linde, Shell)

Partners

- **Stakeholder CRADA**
  - Bki (contractor for California Fuel Cell Partnership)
  - Fire Protection Research Foundation (research affiliate of NFPA)
- **Industry & Research**
  - NFPA 2 code committee
  - HySAFE

Relevance

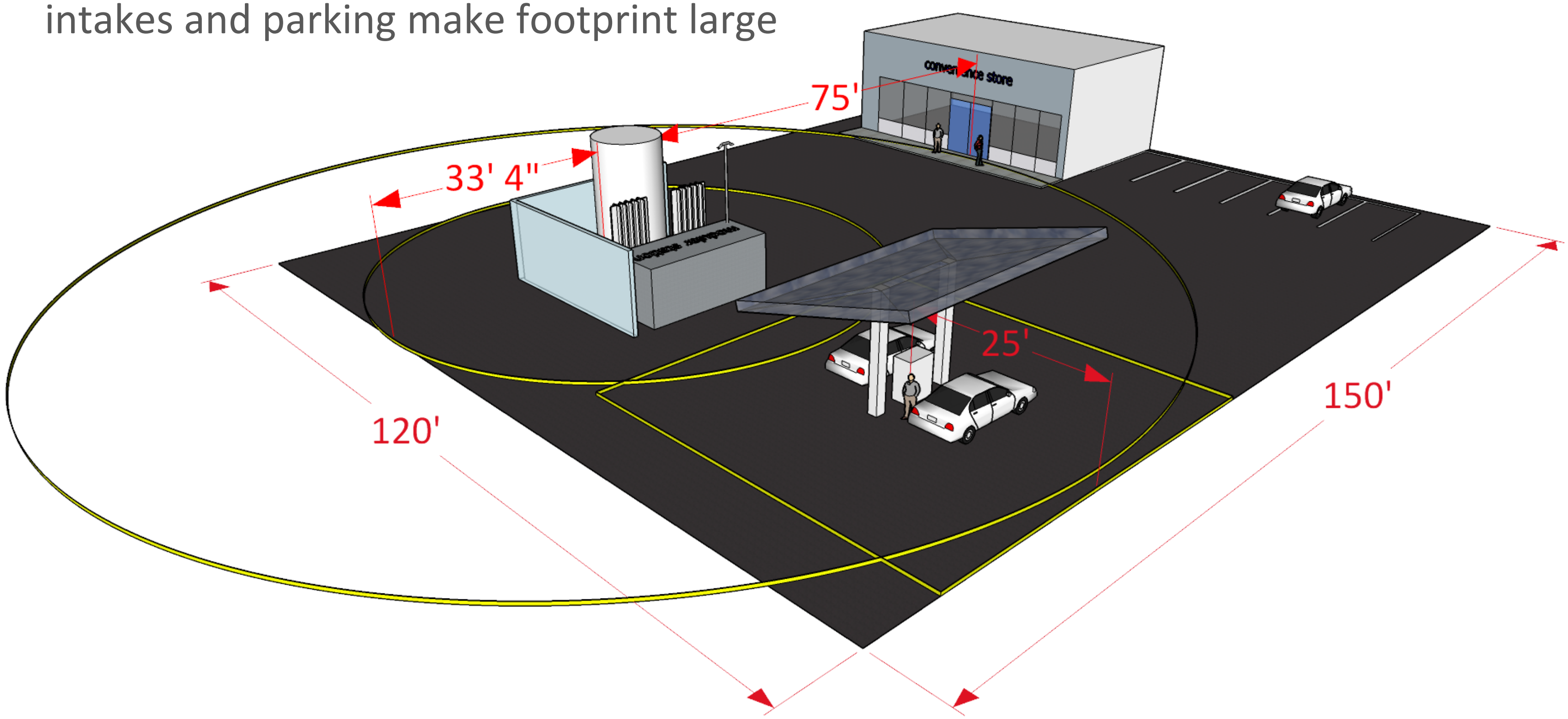
Objectives:

- 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	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

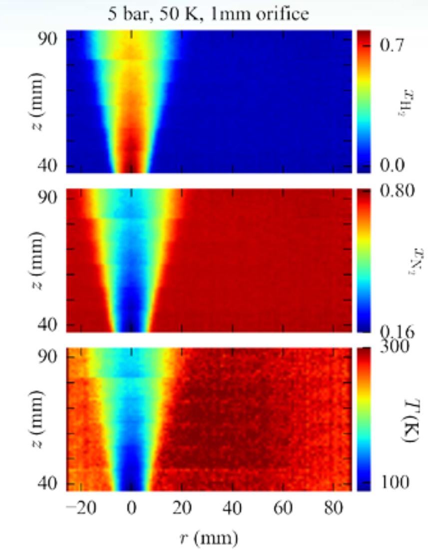
Relevance: Current separation distances for liquid hydrogen are based on consensus, not science

- Previous work by this group led to science-based, reduced, gaseous H_2 separation distances
- Higher energy density of liquid hydrogen over compressed H_2 makes it more economically favorable for larger fueling stations
- Even with credits for insulation and fire-rated barrier wall 75 ft. offset to building intakes and parking make footprint large

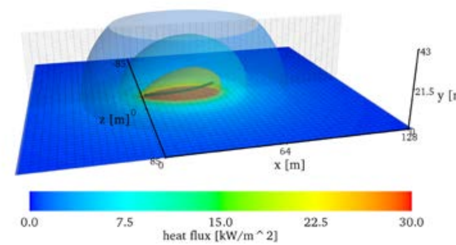


Approach (Sandia H_2 SCS): Coordinated activities that facilitate deployment of hydrogen technologies

- 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

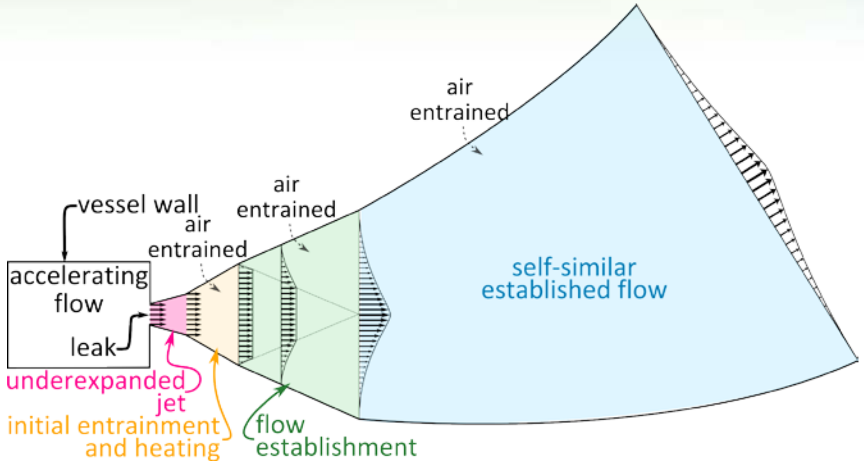
Issue: Cryogenic H_2 releases have been outdoors and/or instrumented with low fidelity sensors, with experimental uncertainty too high for model validation

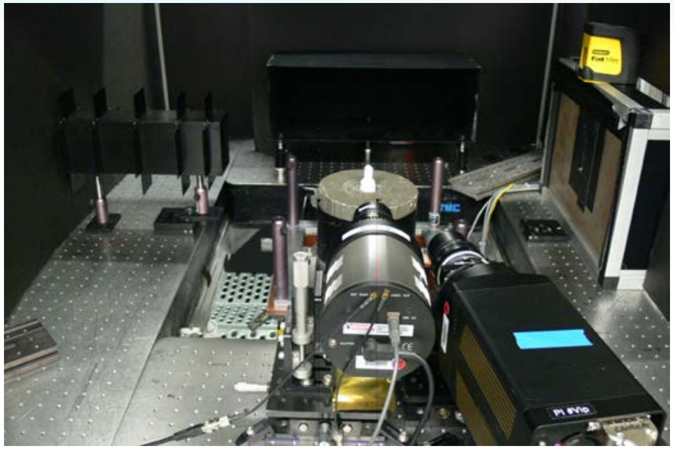
- SNL Approach (FY17 goals):
  - Perform lab-scale cryogenic hydrogen dispersion validation experiments with precise control of boundary conditions and high-fidelity imaging diagnostics (described in next slides)
  - Design large indoor experiments to enable the modeling of pooling and vaporization of liquid hydrogen (described in remaining challenges)

Issue: Low fidelity sensors and very specific vent geometries in previous accumulation experiments

- SNL Approach (FY17 goal): Design an experimental platform with flexible vent/source geometry and high-fidelity, accurate concentration measurements (task to begin in Q4)

Approach (FY17 Hydrogen Behavior): Validate model for cryogenic hydrogen dispersion

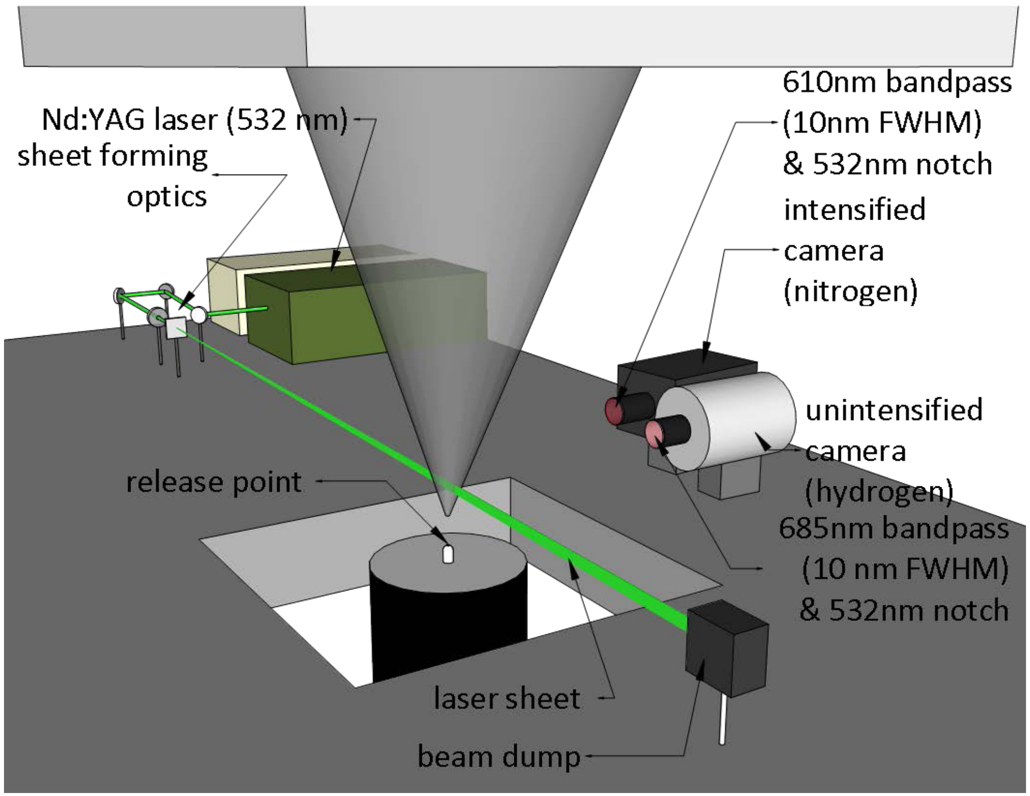




- Previously developed model requires validation data
  - Several model parameters based on empirical data
  - Data only from warm hydrogen or other warm gases
  - Are more physics required?
- Use experimental platform commissioned in FY16 to generate cryogenic hydrogen releases

> ➢ Milestone (FY17Q2): Measure dispersion field of < 40 K hydrogen (milestone complete) and incorporate validated model into HyRAM (FY18 milestone)

Accomplishment: Developed and implemented Raman imaging technique to measure cryogenic plumes

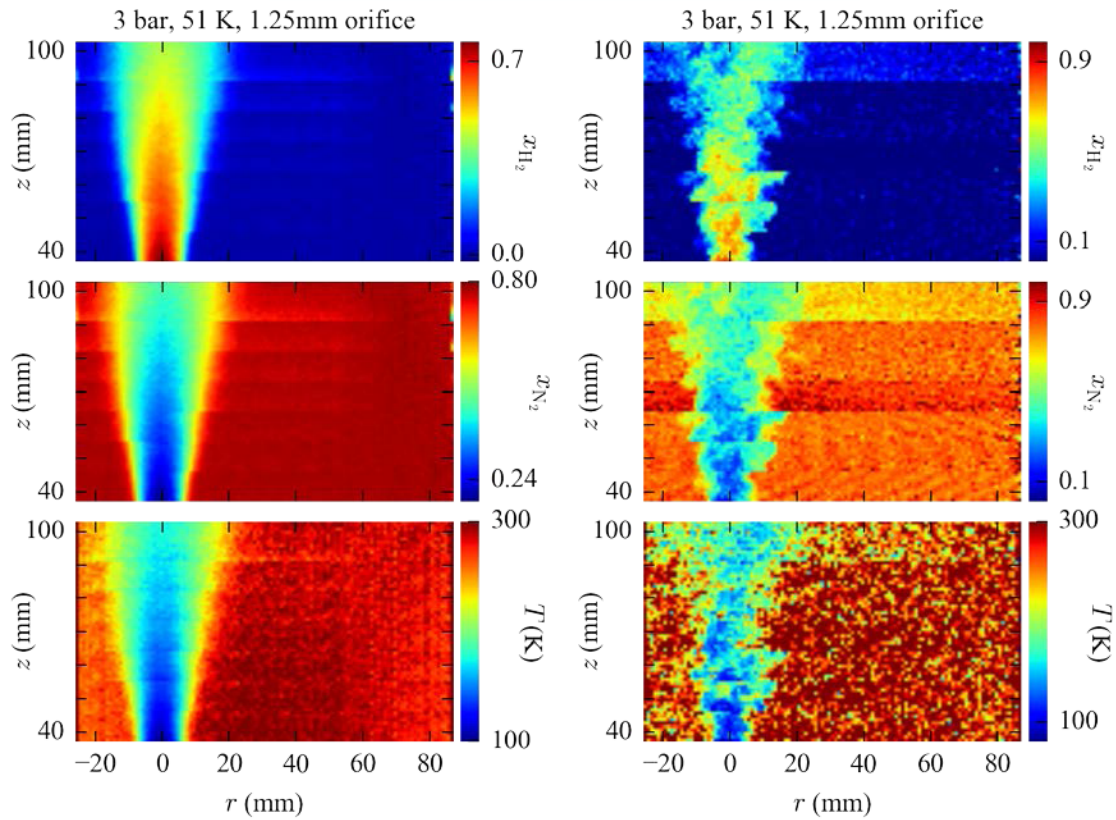


- Conventional Rayleigh signal overwhelmed by Mie scattering off of condensed water vapor in jet
- Filtered Rayleigh had insufficient Mie scattering light suppression (OD≈3)
- Raman scattering enables higher optical density filters
  - 10 nm FWHM bandpass filters at wavelengths of interest
  - OD of 12 @ all wavelengths
  - OD of 18 @ 532 nm

➢ Enables simultaneous measurement of concentration and temperature in 2D

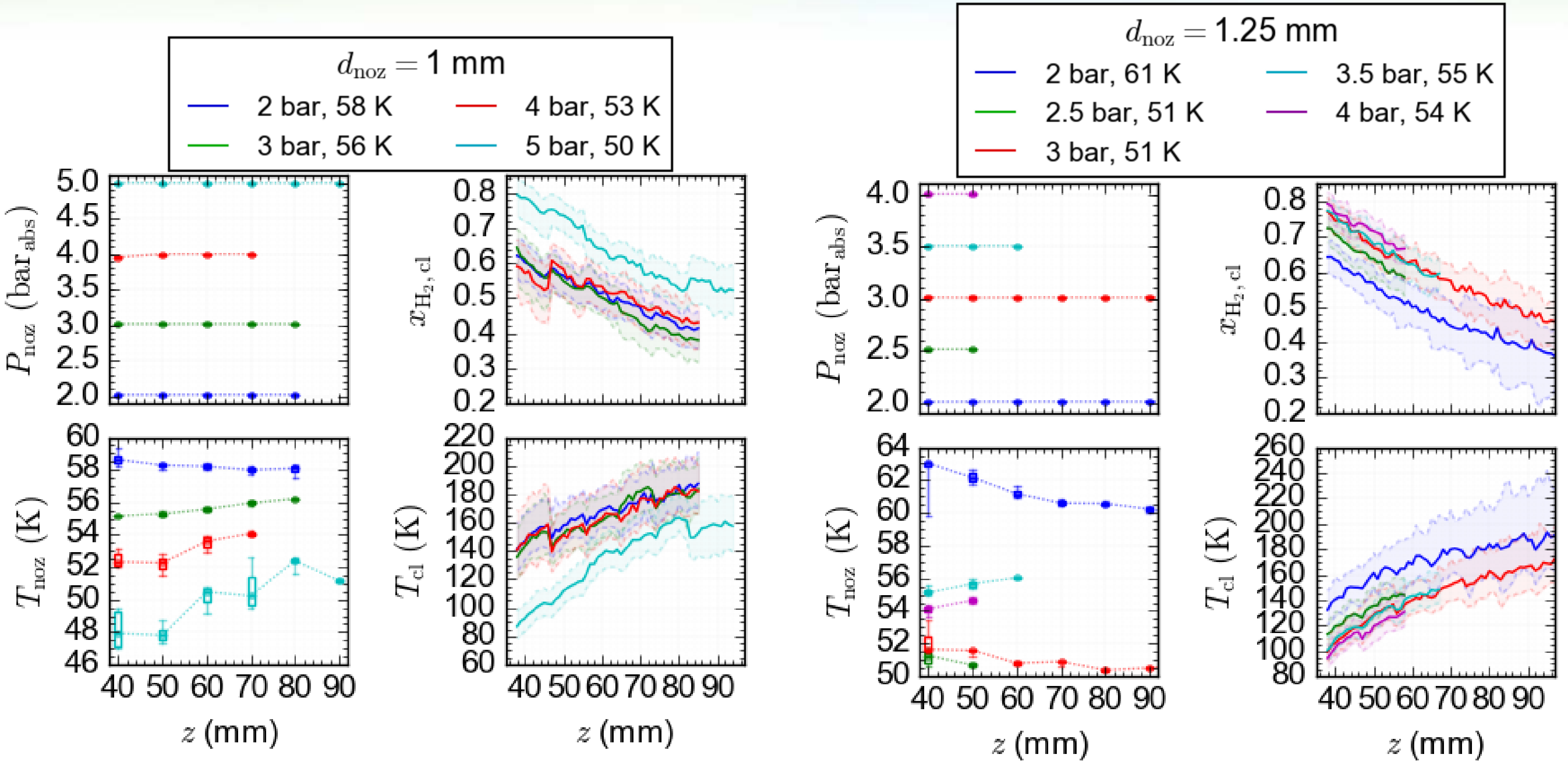
Accomplishment: Measured concentration and temperature fields of cryogenic hydrogen releases

T_{noz} [K]	P_{noz} [bar_{abs}]	d [mm]	T_{throat} [K]	n_{hts}
58	2	1	43.5	4
56	3	1	41.9	4
53	4	1	39.6	4
50	5	1	37.4	5
61	2	1.25	45.7	6
51	2.5	1.25	38.2	2
51	3	1.25	38.2	6
55	3.5	1.25	41.2	3
54	4	1.25	40.4	2



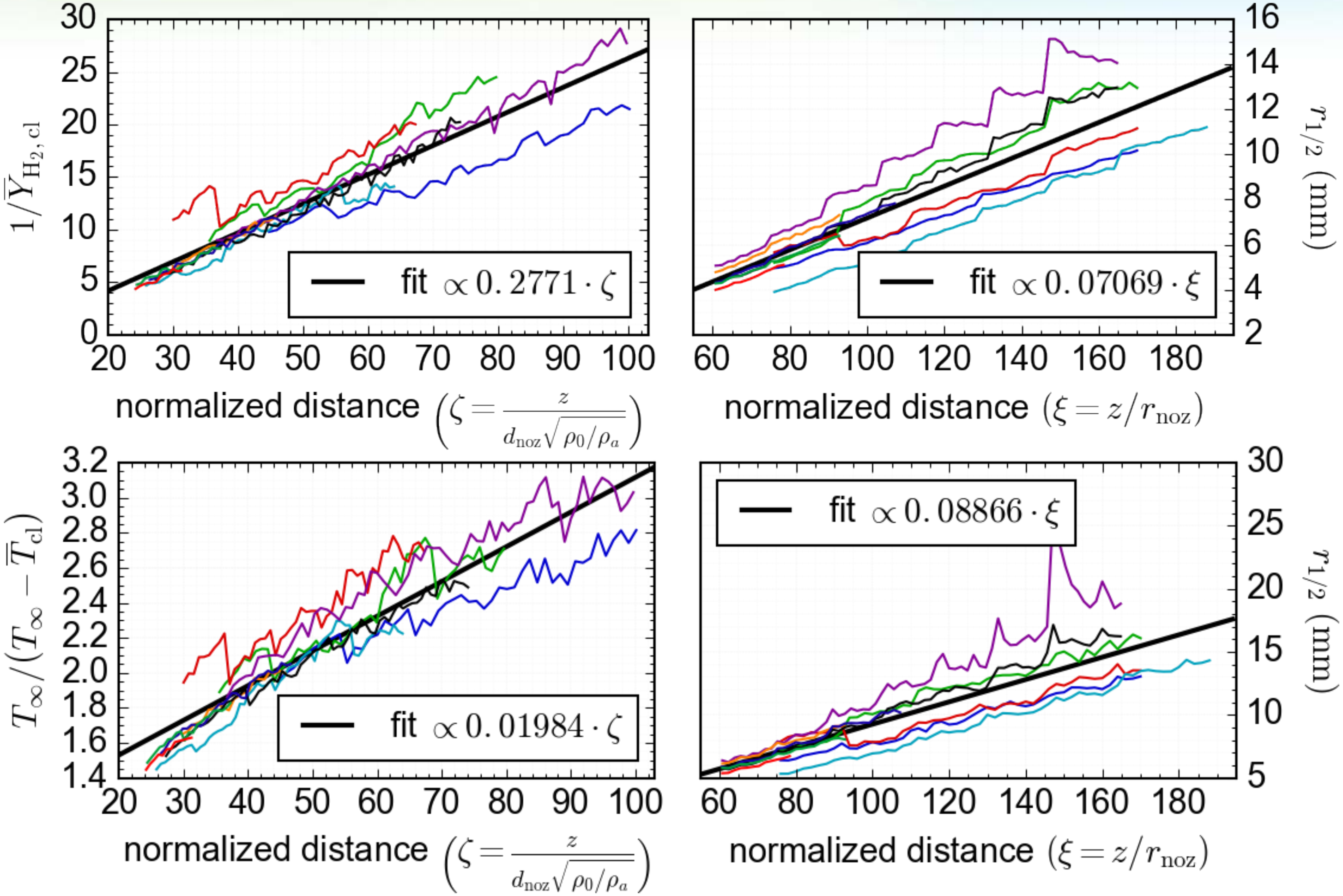
- Two-dimensional images are superior to centerline only measurements for model validation

Accomplishment: Measured temperatures as low as 85 K, 38 mm from the release point

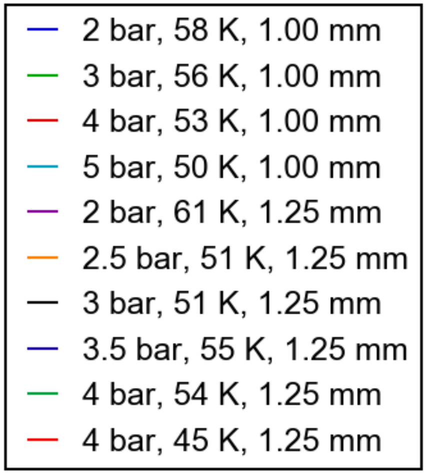


- Control of pressure, and measurement of temperature at nozzle enables data to be used for model validation

Accomplishment: When normalized properly, centerline and half-width decay rates scale linearly

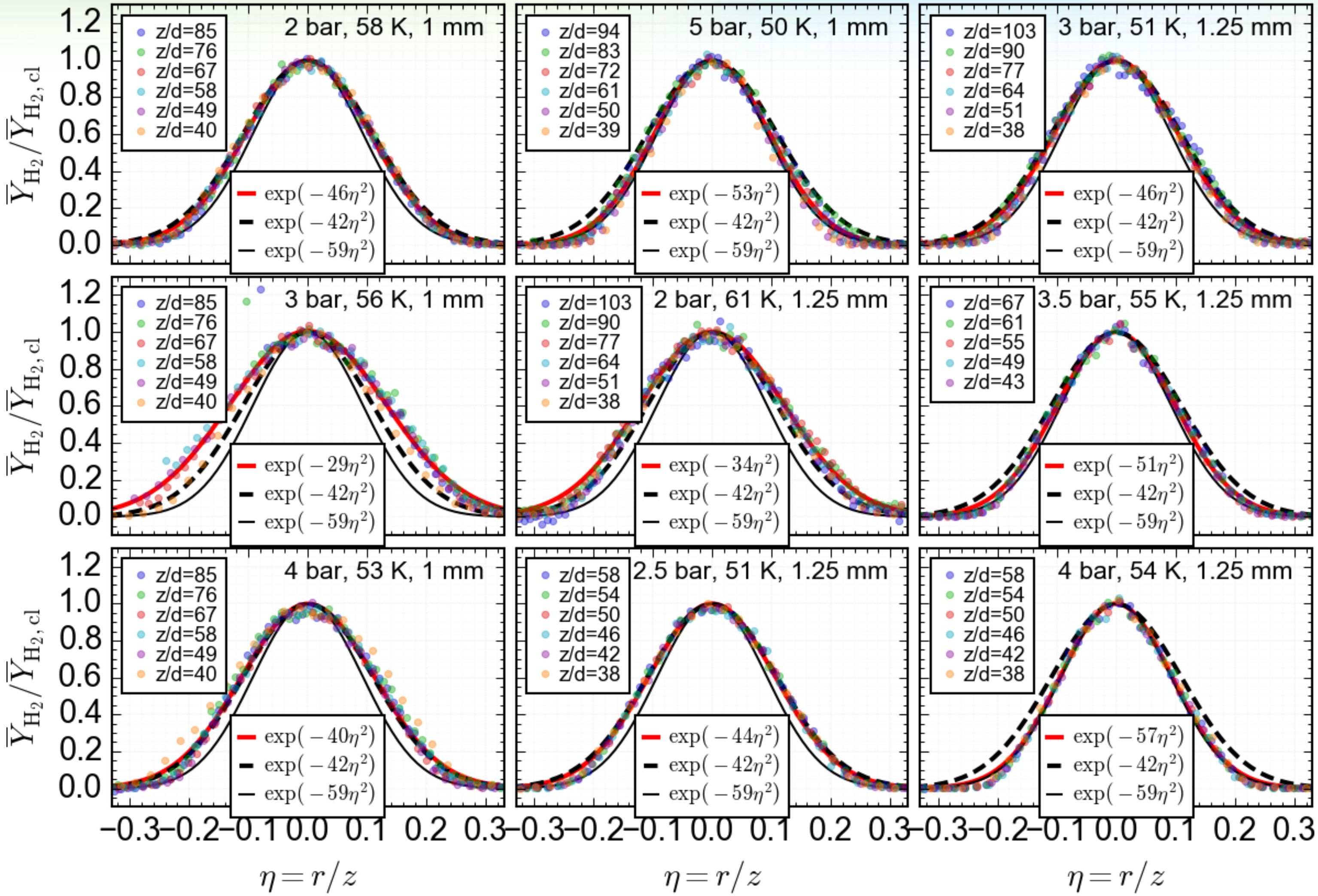


- Literature inverse mass-fraction decay rate: 0.21–0.271
- Literature mass-fraction half-width spreading rate: 0.1–0.11 mm



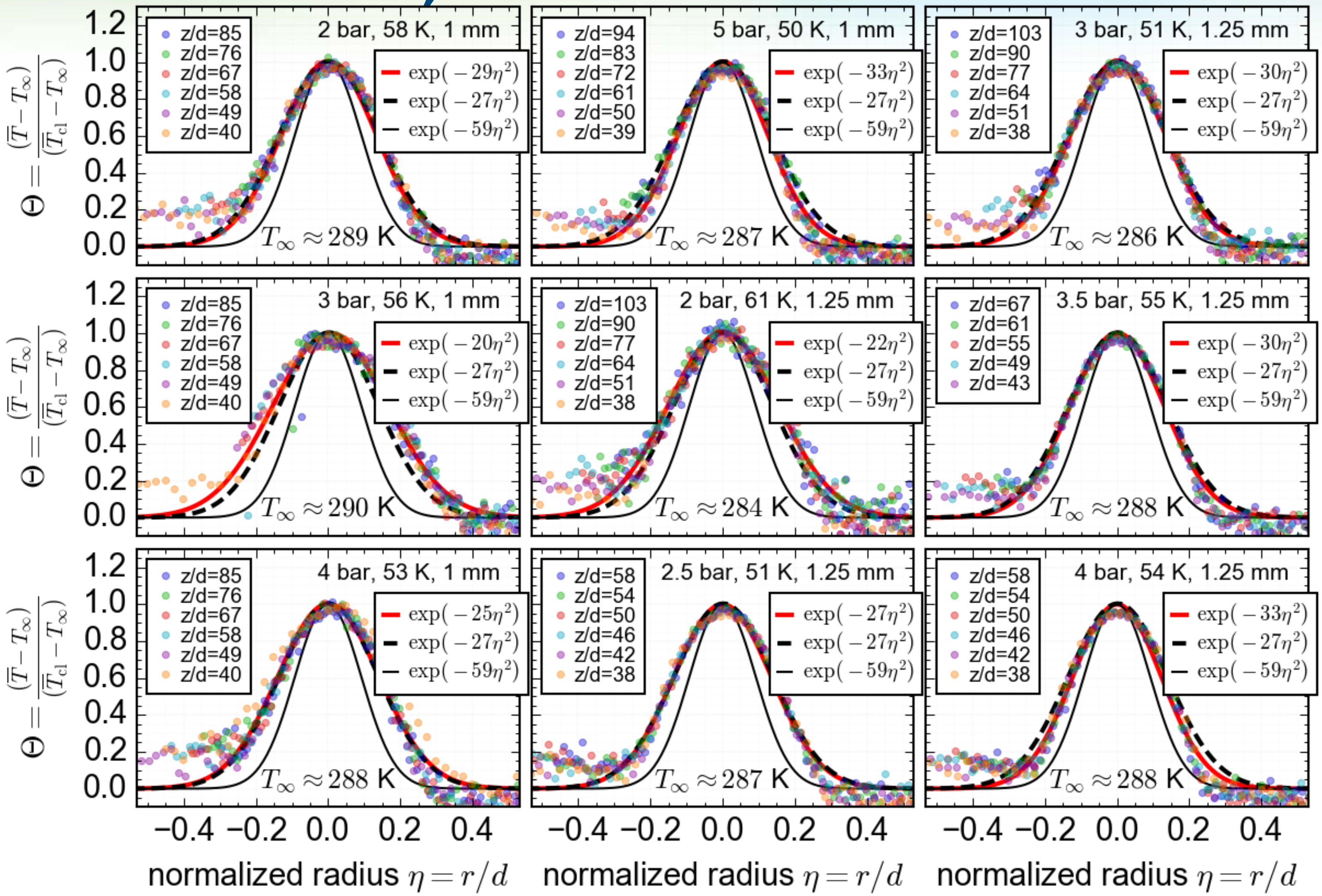
➢ First ever measurements of temperature needed for model energy balance

Accomplishment: Radial profiles are self-similar, but wider than literature data of warm releases



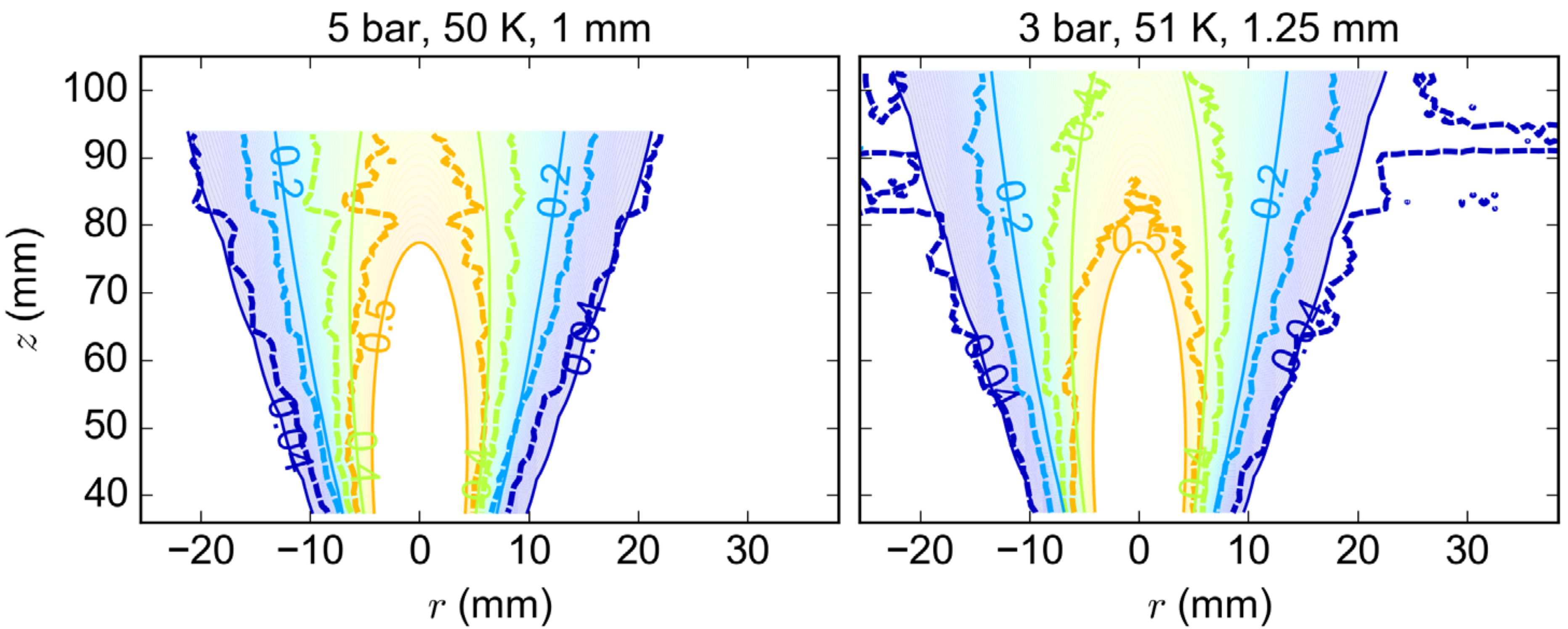
➢ Different profiles implies different modeling parameters from warm releases

Accomplishment: Radial profiles of temperature are also self-similar, and wider than mass fraction



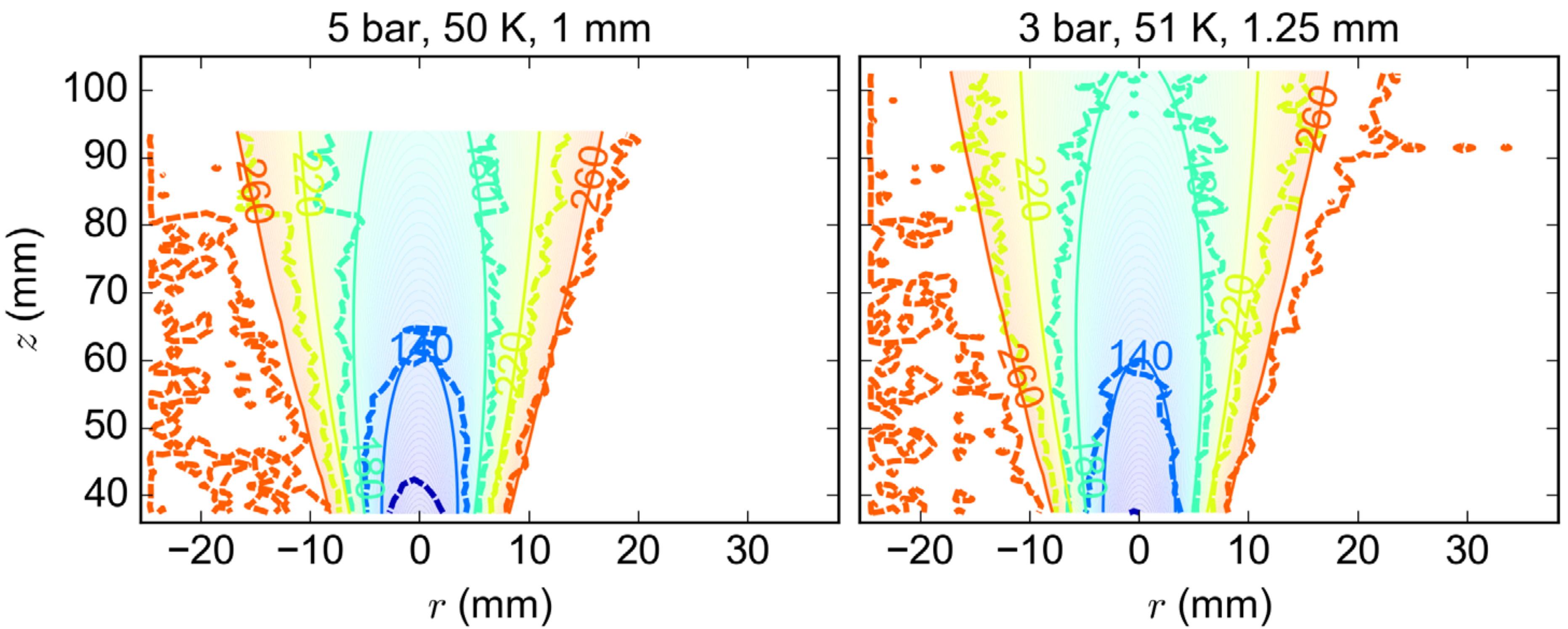
- Data can be used to validate relative spreading ratio in model

Progress: Initial comparisons to model show slower centerline mole-fraction decay rate than predictions



➢ Expansion model and/or entrainment rate may need to be adjusted

Progress: Initial comparisons to model show good agreement in terms of temperature



- Improved data analysis may yield reduced noise

Response to last year's Reviewer's comments

- The project needs more emphasis on adding liquid hydrogen capability. It would be helpful if the project could address releases in a container that did not trap hydrogen under a roof, thereby limiting the concentration.
  - We recognize the ability to predictively model liquid hydrogen releases as being a critical barrier to code revisions; this work focuses directly on model validation. We are close to having a valid model for some aspects of liquid hydrogen stations. We are also planning some enclosure experiments to improve our simulations of scenarios with walls.
- The proposed work to evaluate cold/liquid releases does not appear adequate to meet the needs of the project if the intent is to address large-scale releases.
  - The large-scale releases being planned (described in the following slides) will address the shortcomings of the lab-scale experiments, enabling modeling of larger releases.
- The project should add benchmarking against other fuels.
  - We are planning on running similar (cryogenic release) experiments with methane (as a surrogate for natural gas), with funding from the vehicle technologies office.

Note: While this work was presented during the 2016 AMR, it was not independently reviewed. Since there are such close ties to SCS-011: Hydrogen behavior and Quantitative Risk Assessment, some relevant comments were taken from there.

Collaborations have enabled this research and expanded impact

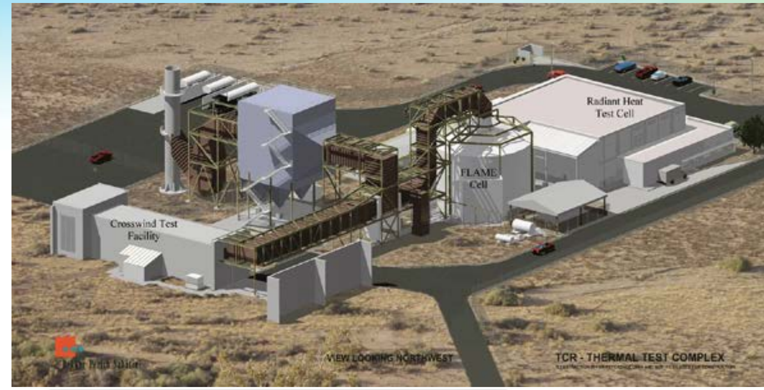
H_2 behavior (SCS010) collaborations

- CRADA with **BKi** to fund 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
- **HySafe**
  - Panelist for HySAFE Research Priority workshop on Hydrogen Safety

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: Phenomena from large-scale releases are not well understood



Need experiments to characterize:

- Pooling
- Evaporation from LH_2 pools

Planning underway for experiments at Sandia (Albuquerque) facilities:

- Thermal test complex
  - Flame cell
    - Up to 3m diameter pool
    - 18.3 m dia. x 12.2 m high
    - Well characterized conditions for model validation
  - Crosswind test facility
    - Dispersion in controlled crosswind
    - Single-direction flow
    - Well-characterized ambient conditions
- Severe Accident Phenomena/Analysis (Surtsey)
  - 100 m^3 pressure vessel with 6 levels of instrumentation ports

Proposed future work

- Remainder of FY17
  - Complete Raman imaging characterization of cryogenic hydrogen releases
  - Conclude development/validation of the ColdPLUME model for predictive dispersion modeling
  - Develop R&D plans for large-scale experiments
  - Develop research plans and design enclosure/accumulation experiments
- FY18
  - Integrate validated ColdPLUME model into publicly released HyRAM
  - Conduct large-scale release experiments to characterize hydrogen pooling, evaporation, and interaction with atmosphere
  - Complete enclosure/accumulation experiments and develop predictive models of risk for unintended releases of hydrogen in containers
- Out years
  - Simulate 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

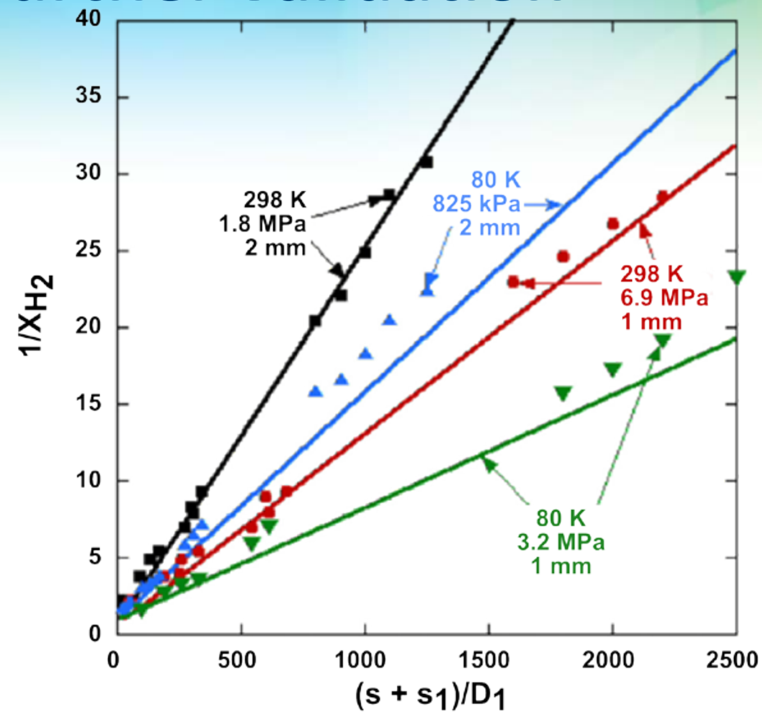
Summary

- **Relevance**: Address lack of safety data, technical information relevant to development of 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**:
  - Raman imaging used to characterize concentration and temperature profiles of cryogenic hydrogen releases
  - Preliminary analysis suggests that mixing of cryogenic hydrogen jets is different from warm hydrogen jets, requiring new empirical model parameters
  - Experiments on-going
    - Push to even lower temperatures
- **Future work**:
  - Modify ColdPLUME model as validation data dictates
  - Implement ColdPLUME into HyRAM
  - 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 inform 2022 edition of NFPA 2)

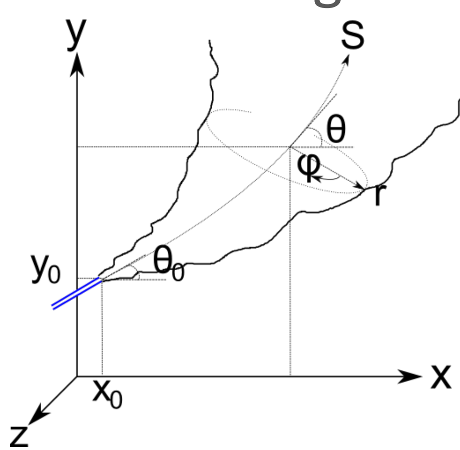
TECHNICAL BACKUP SLIDES

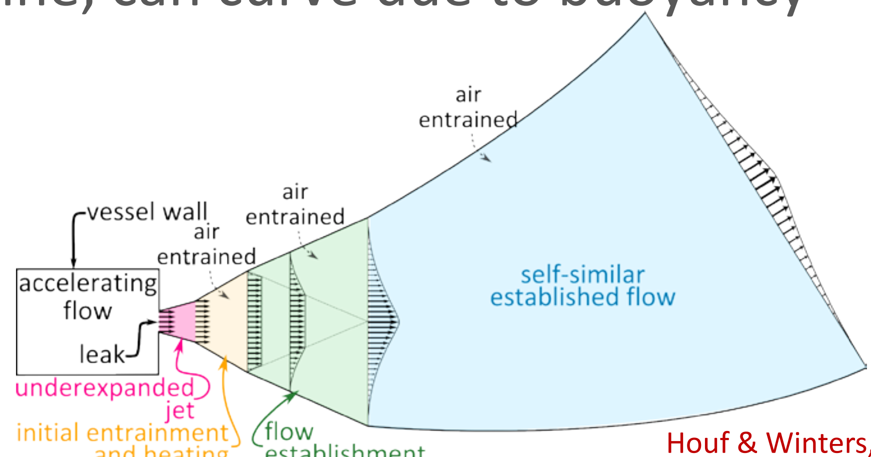
A conceptual model needs to further validation

- 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

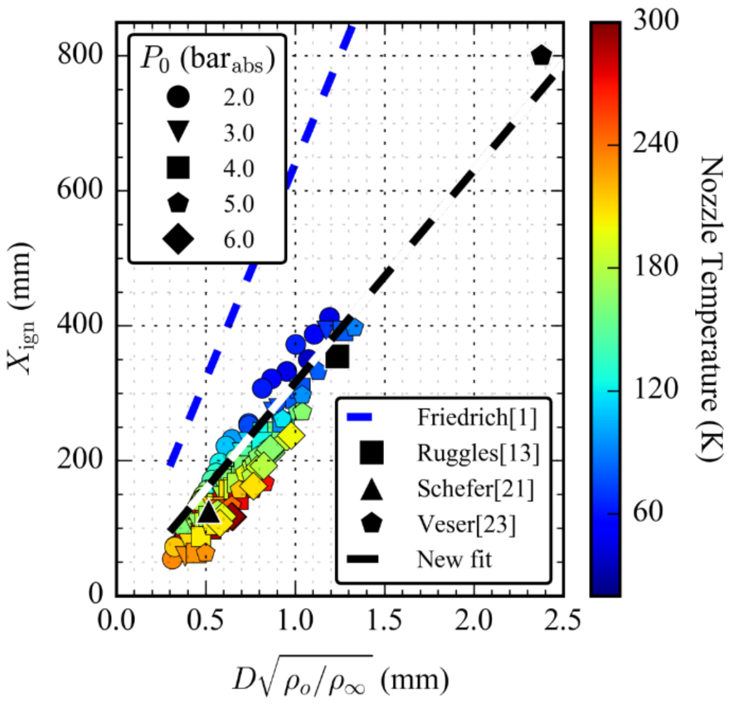


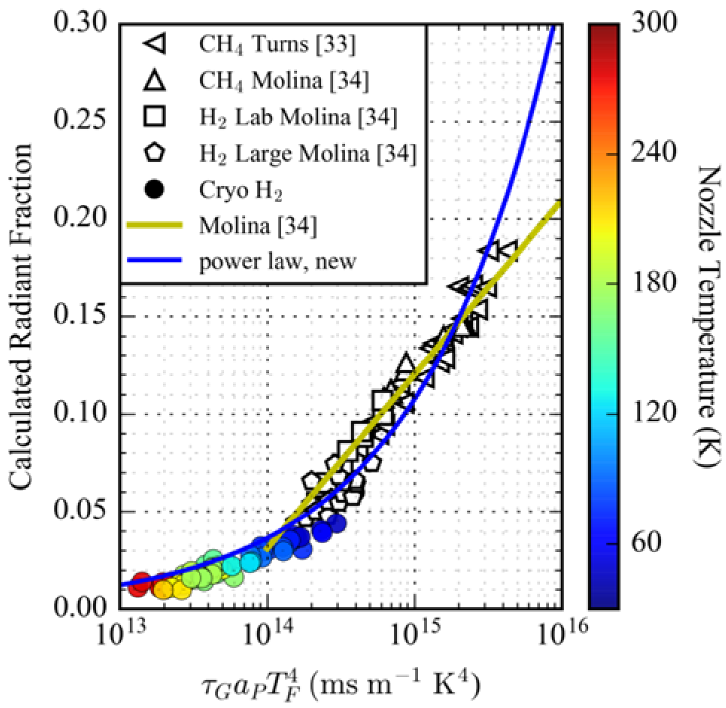


Houf & Winters, IJHE, 2013

(Air) icing at the nozzle likely improves mixing for temperatures < 50K

Ignition distance and radiant fraction were mapped out last FY

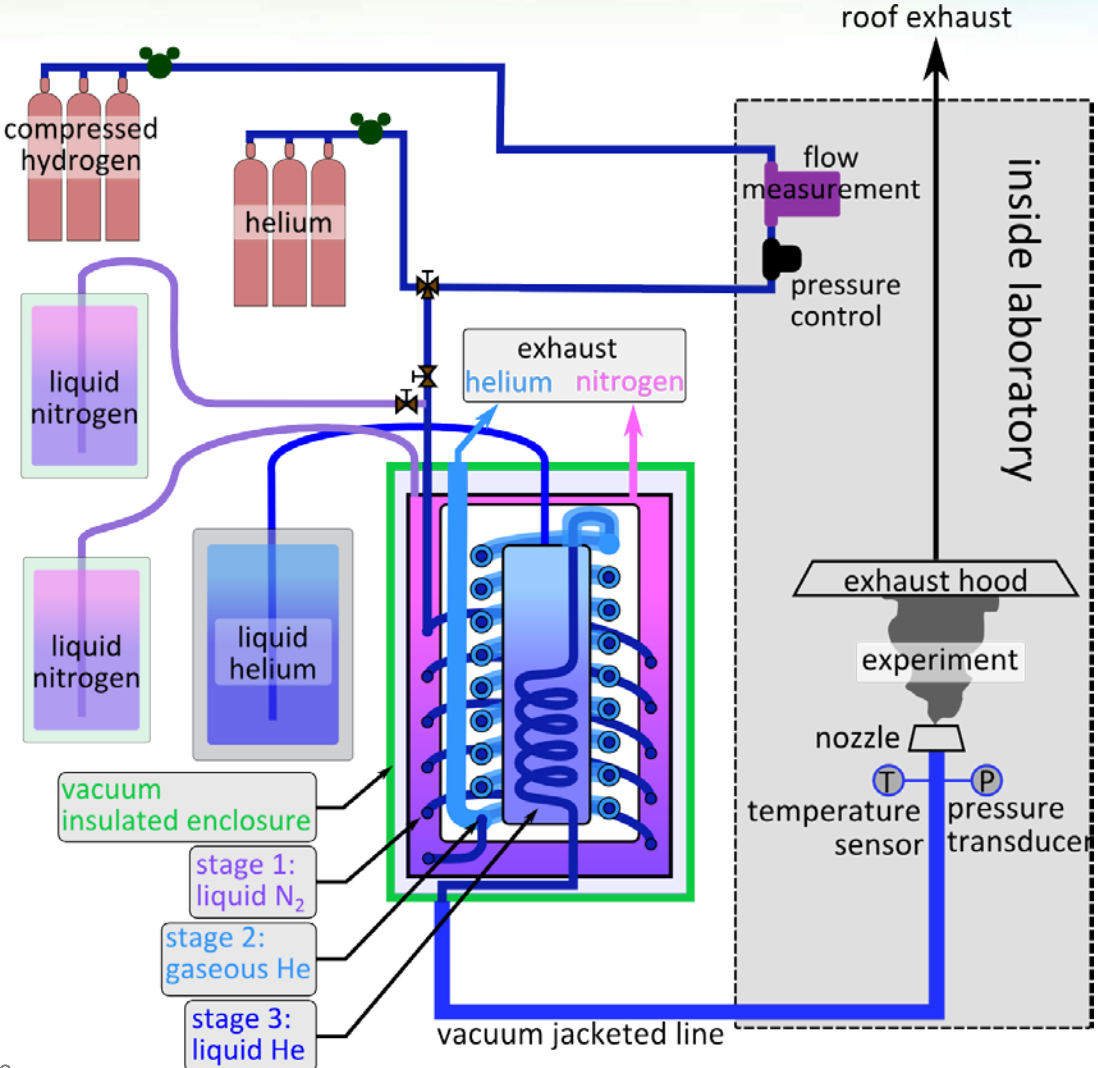


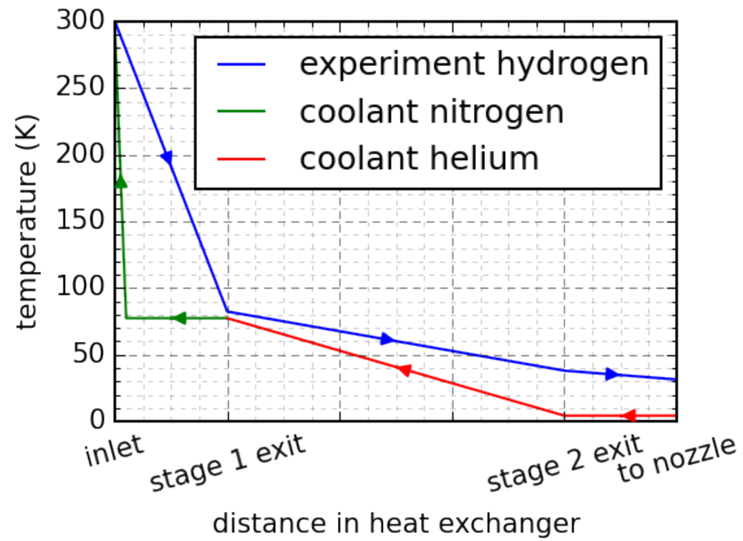


Two high priority scenarios identified by the NFPA 2 code committee are initially targeted for modeling

- ✓ Flow from vent of ultra-cold hydrogen (e.g. trailer venting excess pressure after normal LH_2 delivery or burst disk rupture)
  - Are vent stacks appropriately designed?
  - Separation distance from air intakes and overhead utilities
  - Vertical discharge, 3” diameter pipe, 20-140 psig
- ❑ Release from pipe containing liquid H_2 (e.g. leading from tank to vaporizer or vaporizer itself - caused by thermal cycles or ice falling from vaporizers)
  - Requires ability to model flashing, pooling and evaporation from pools
  - Need to model concentration plume and heat flux from a subsequent fire
  - Horizontal discharge, ¾”-2” diameter pipe, 20-140 psig

We are running an experiment, releasing ultra-cold hydrogen in the laboratory





- Accurate control/measurement of boundary conditions