Sandia National Laboratories

H2FC Hydrogen and Fuel Cells Program

SAND2017-4818C

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

Project ID: SCS010

Ethan S. Hecht

With contributions from: Pratikash Panda, Anthony McDaniel, Radoslav Bosinoski

Sandia National Laboratories

June 6, 2017

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND NO. 2011-XXXXP

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

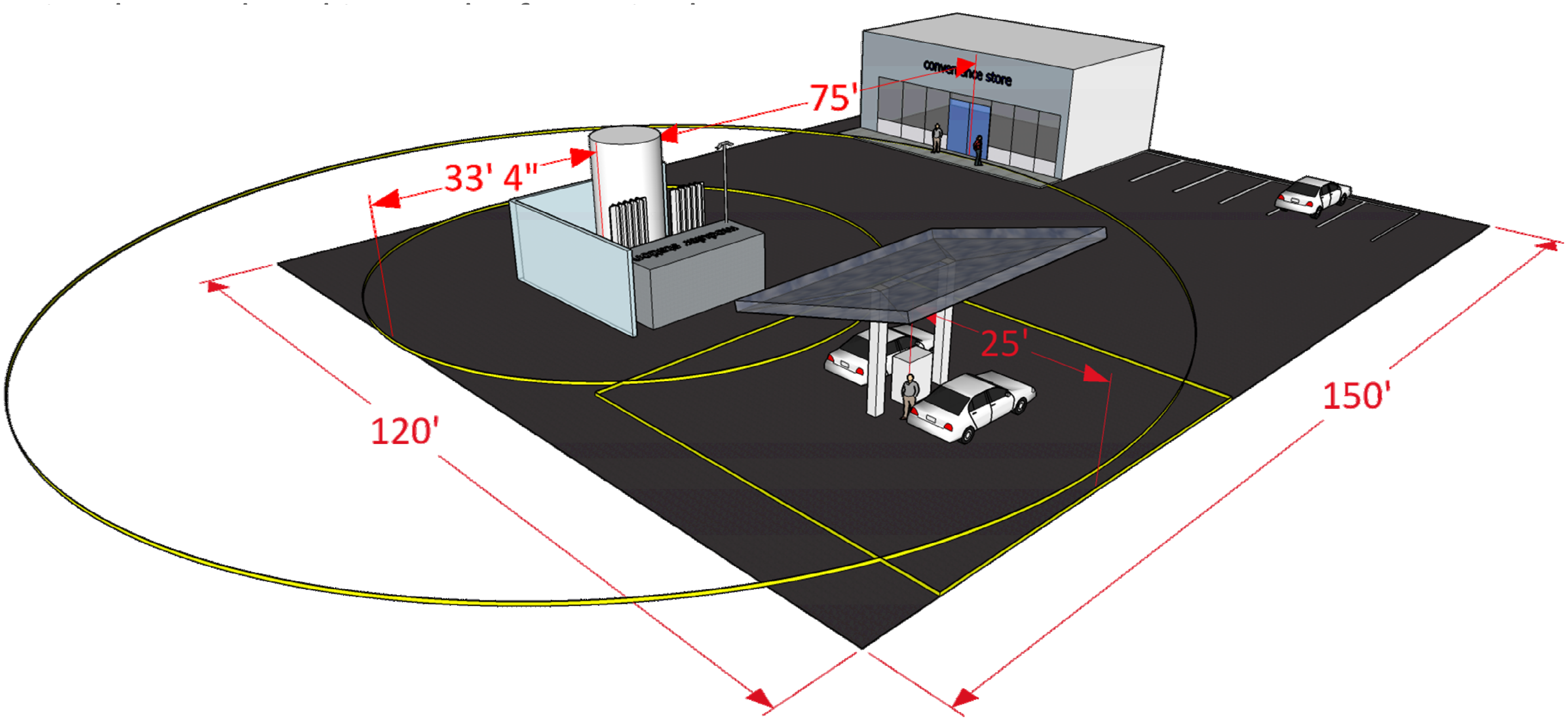
Objectives:

- 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

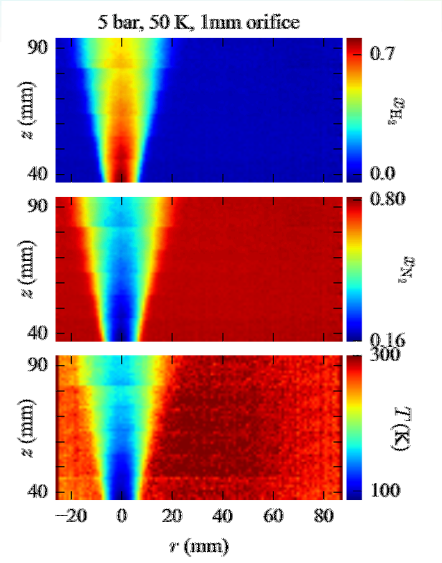
Relevance: Current separation distances for liquid hydrogen are based on consensus, not science

- 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

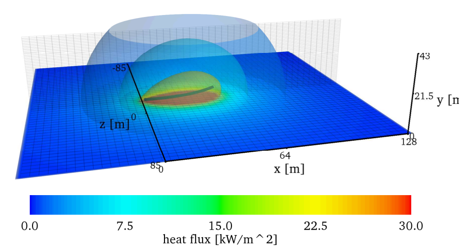


Approach (Sandia H_2 SCS): Coordinated activities that facilitate deployment of hydrogen technologies

- 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

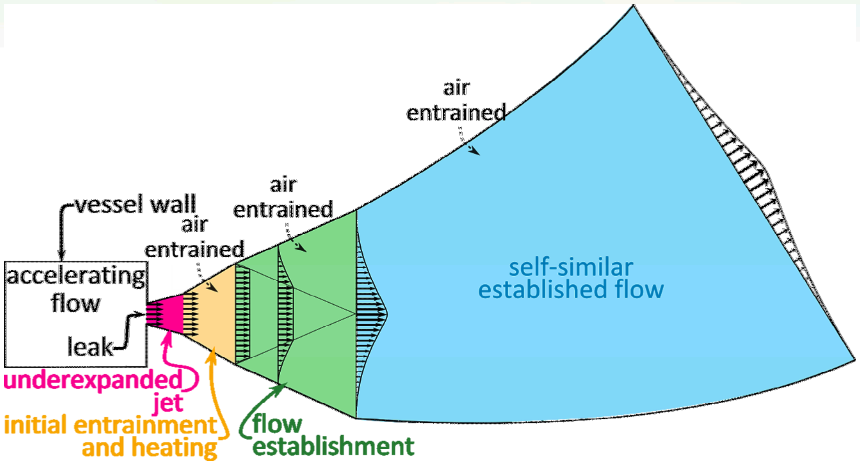
Issue: Cryogenic H_2 releases have been outdoors and/or instrumented with low fidelity sensors, with experimental uncertainty too high for model validation

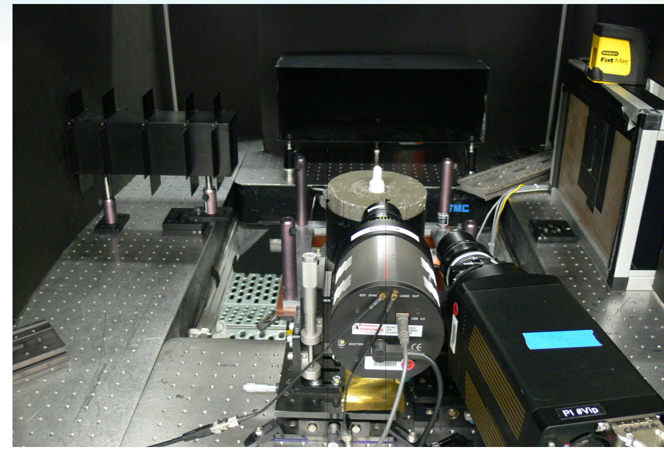
- SNL Approach (FY17 goals):
  - Perform lab-scale cryogenic hydrogen dispersion validation experiments with precise control of boundary conditions and high-fidelity imaging diagnostics (described in next slides)
  - Design large indoor experiments to enable the modeling of pooling and vaporization of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

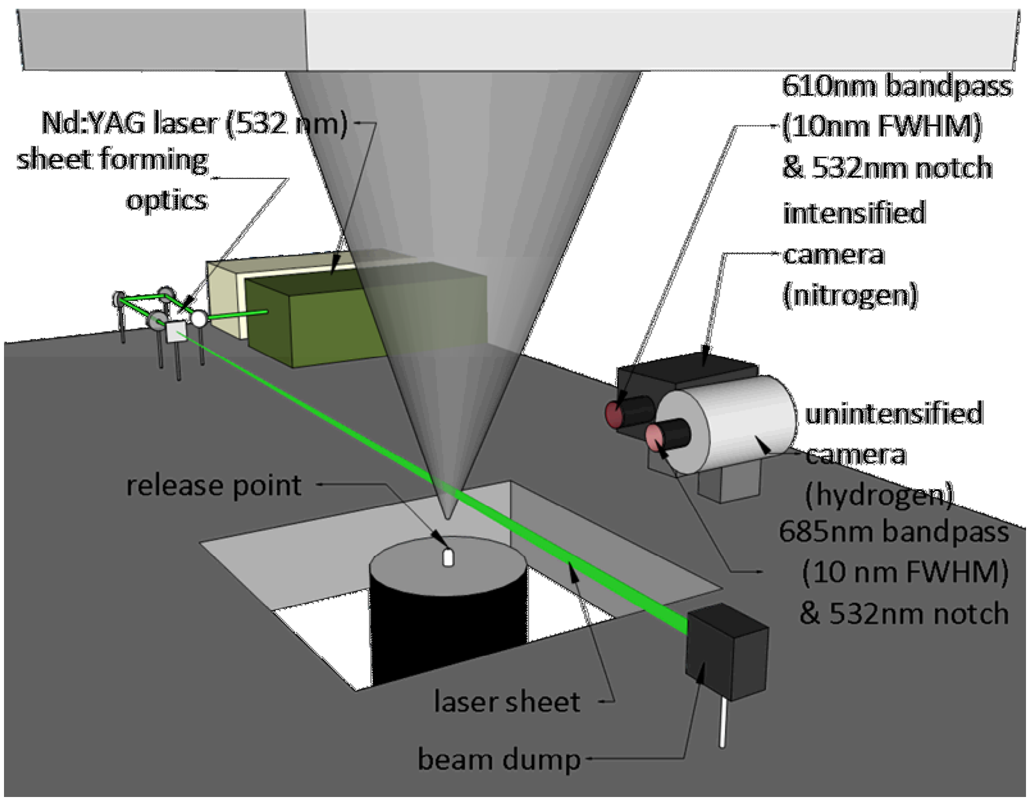




- Previously developed model requires validation data
  - Several model parameters based on empirical data
  - Data only from warm hydrogen or other warm gases
  - Are more physics required?
- Use experimental platform commissioned in FY16 to generate cryogenic hydrogen releases

➢ 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

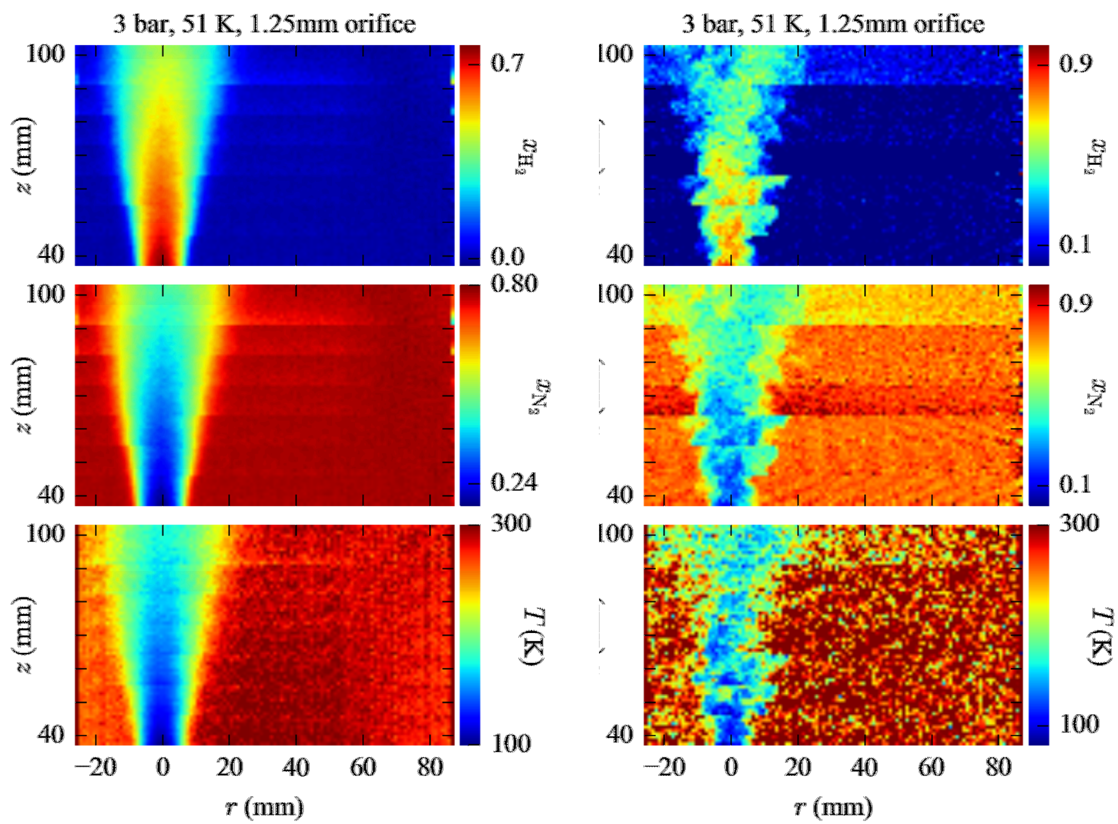


- Conventional Rayleigh signal overwhelmed by Mie scattering off of condensed water vapor in jet
- Filtered Rayleigh had insufficient Mie scattering light suppression (OD≈3)
- Raman scattering enables higher optical density filters
  - 10 nm FWHM bandpass filters at wavelengths of interest
  - OD of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

➢ Enables simultaneous measurement of concentration and temperature in 2D

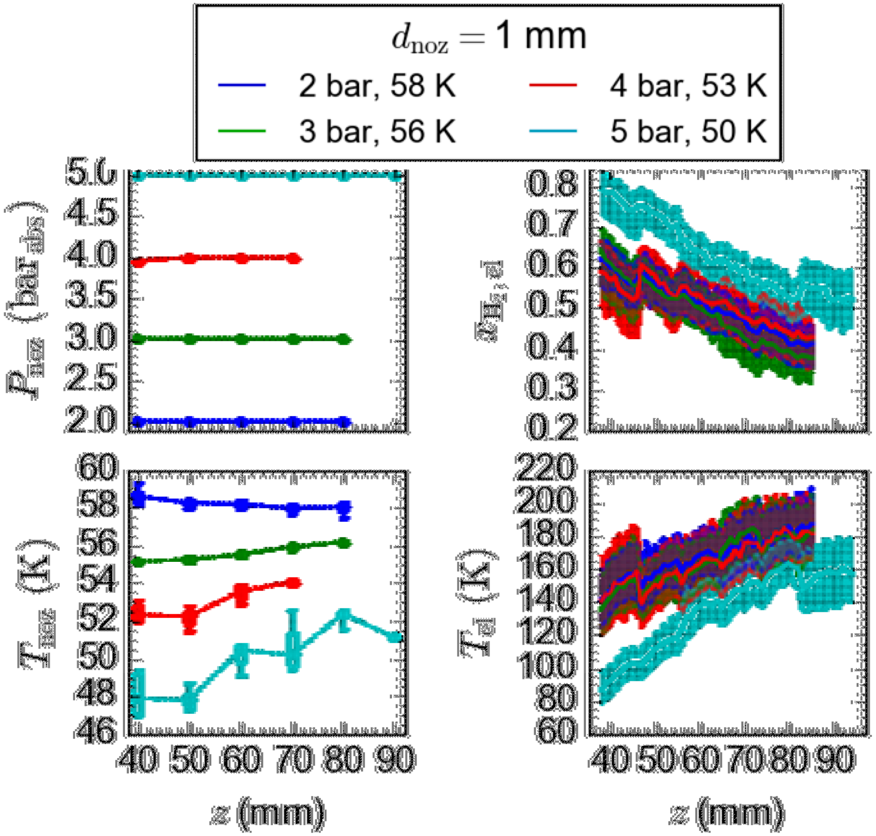
Accomplishment: Measured concentration and temperature fields of cryogenic hydrogen releases

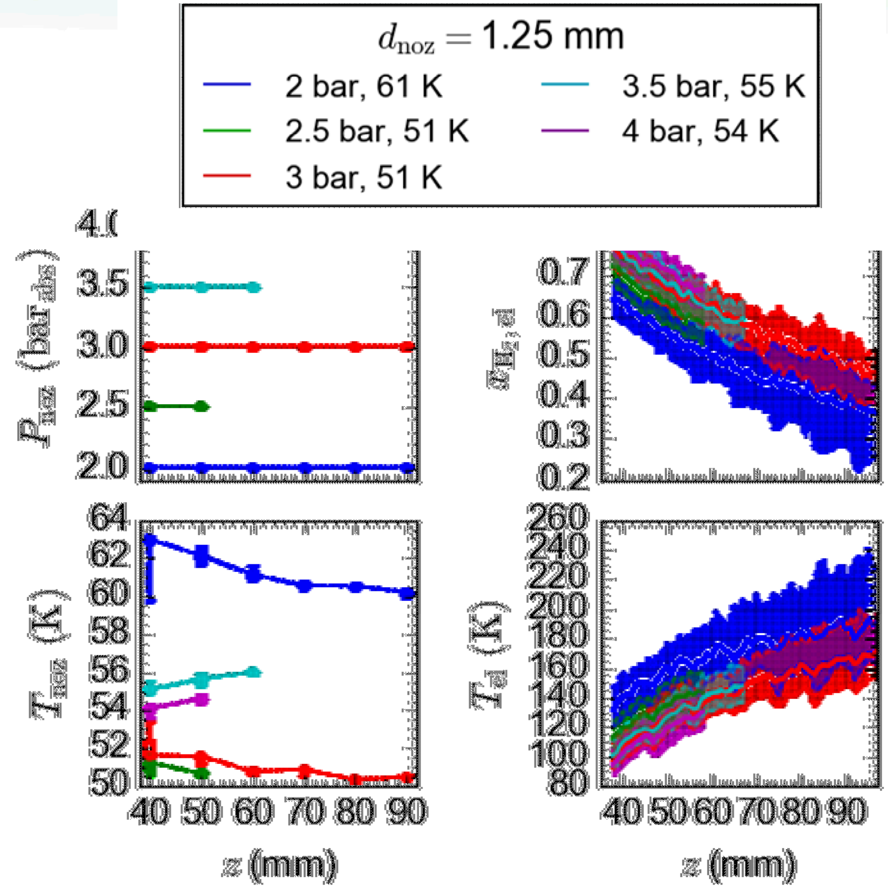
T_{noz} [K]	P_{noz} [bar_{abs}]	d [mm]	T_{throat} [K]	n_{hts}
58	2	1	43.5	4
56	3	1	41.9	4
53	4	1	39.6	4
50	5	1	37.4	5
61	2	1.25	45.7	6
51	2.5	1.25	38.2	2
51	3	1.25	38.2	6
55	3.5	1.25	41.2	3
54	4	1.25	40.4	2



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

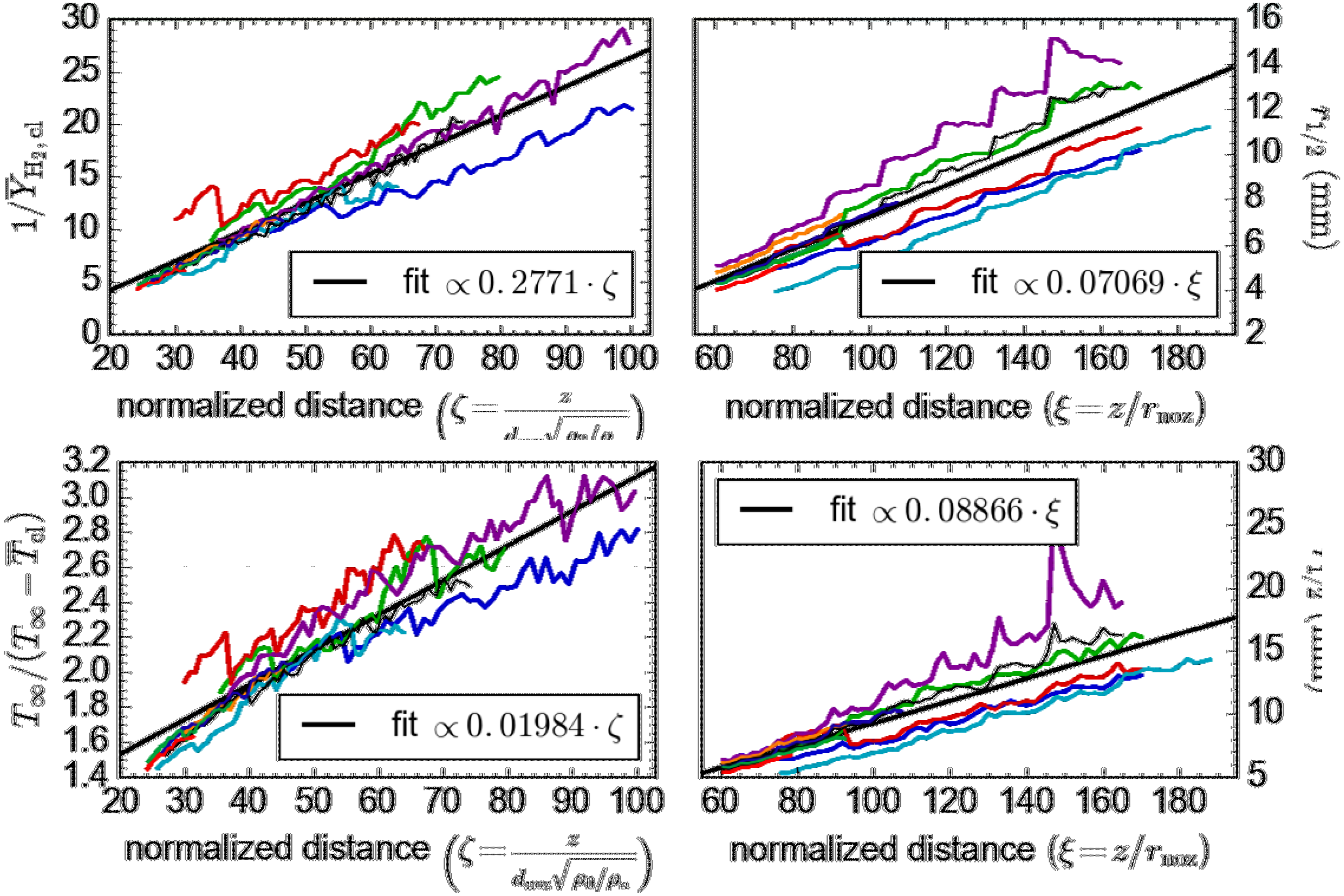
Accomplishment: Measured temperatures as low as 85 K, 38 mm from the release point



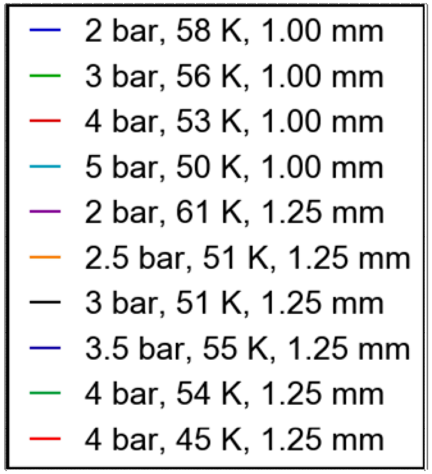


- Control of pressure, and measurement of temperature at nozzle enables data to be used for model validation

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

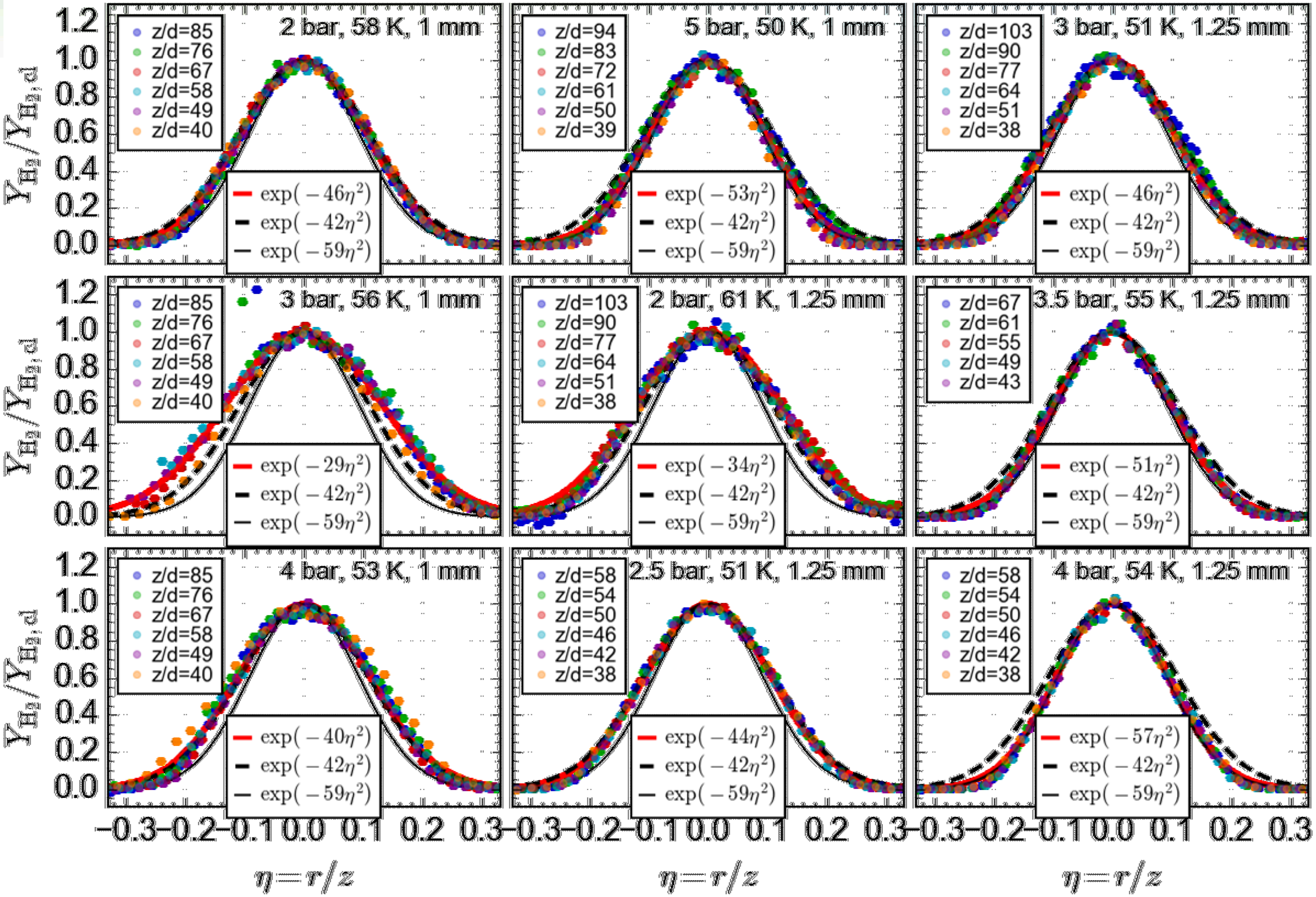


- Literature inverse mass-fraction decay rate: 0.21–0.271
- Literature mass-fraction half-width spreading rate: 0.1–0.11 mm



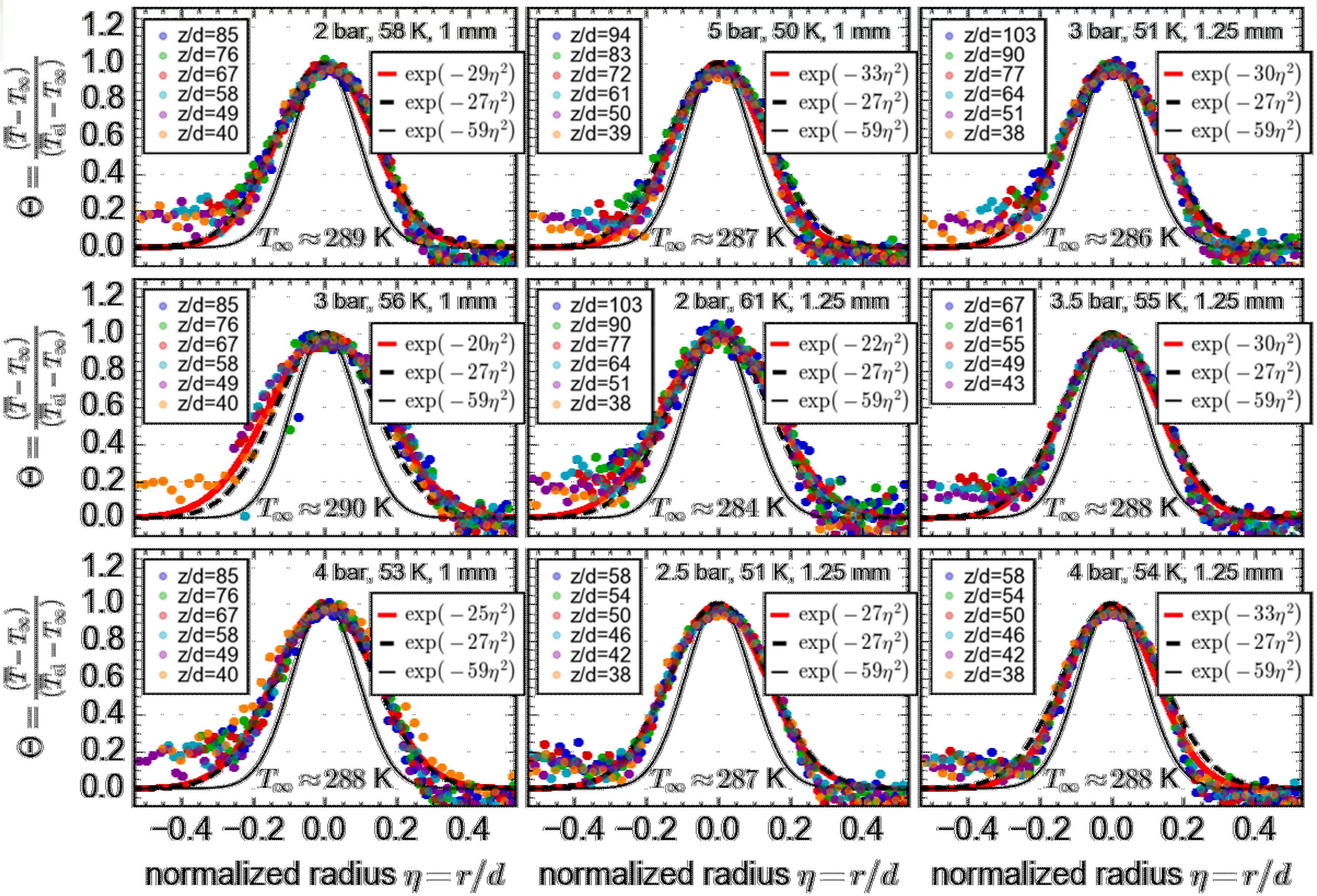
➢ First ever measurements of temperature needed for model energy balance

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



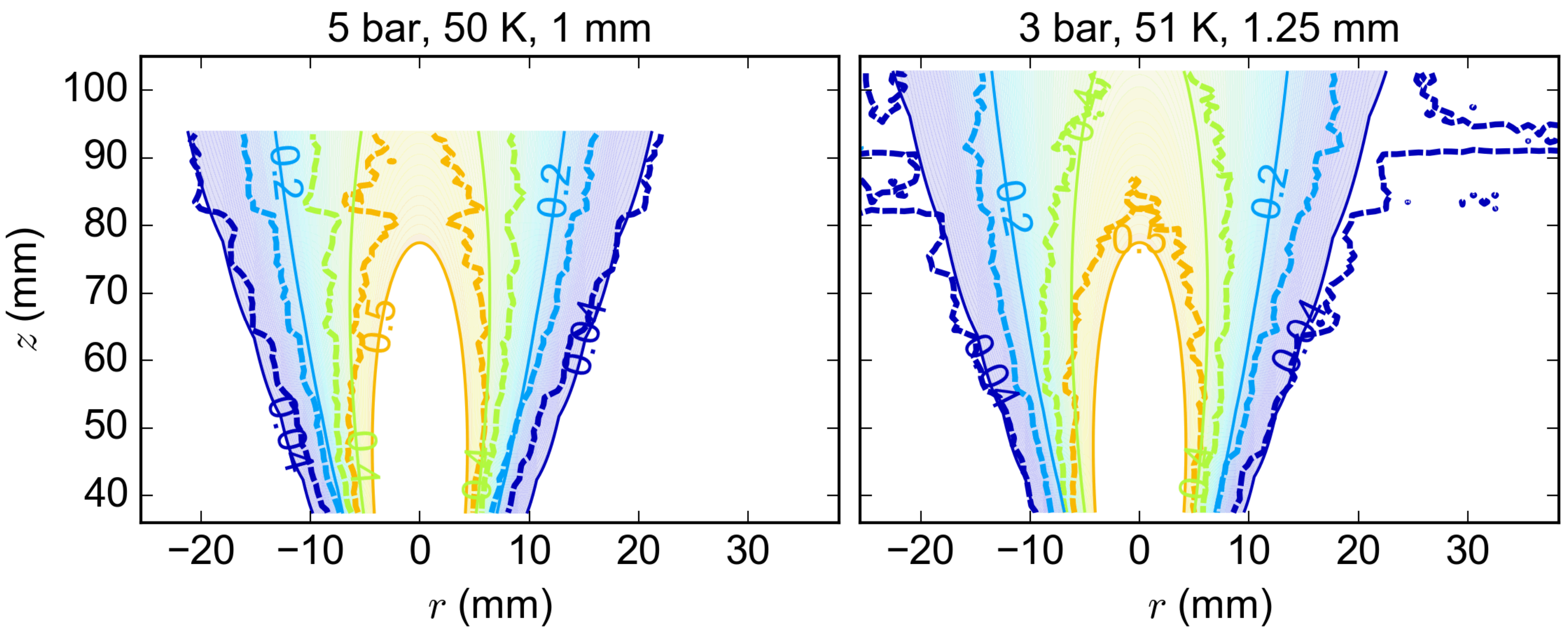
- Different profiles implies different modeling parameters from warm releases

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



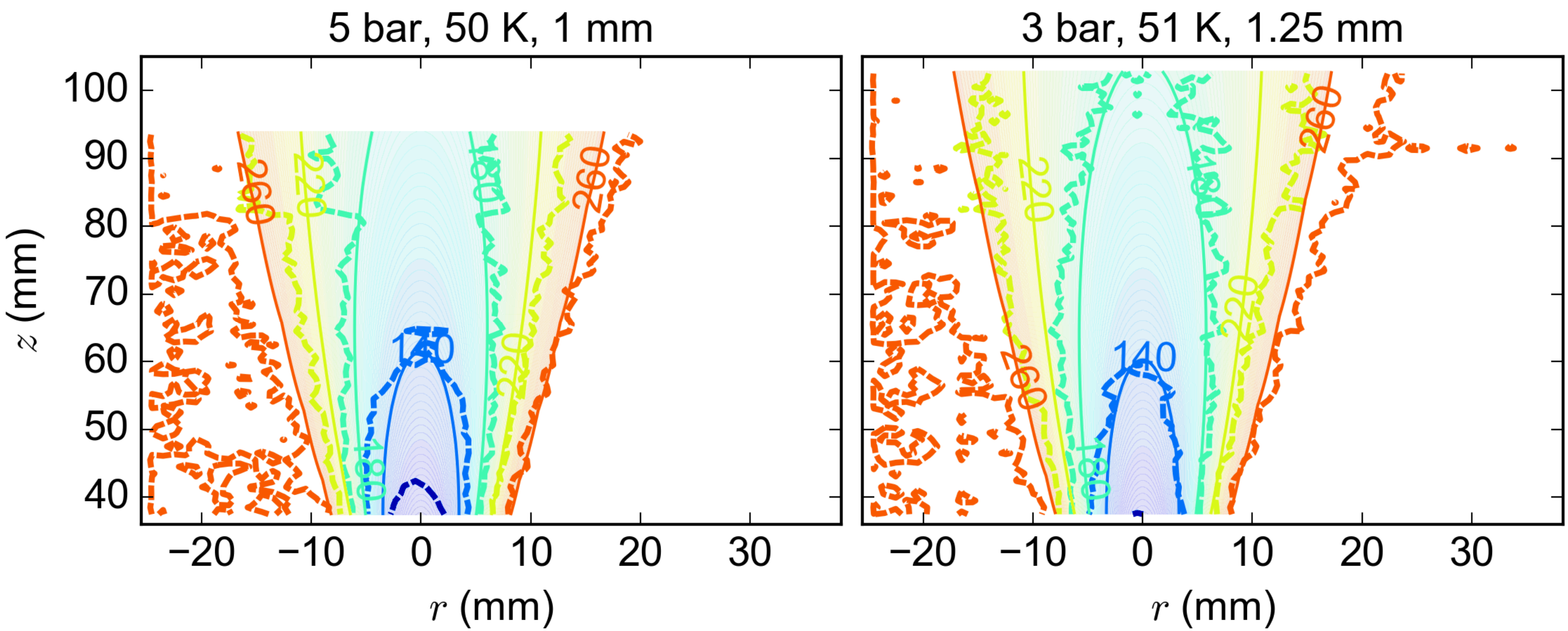
➢ Data can be used to validate relative spreading ratio in model

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

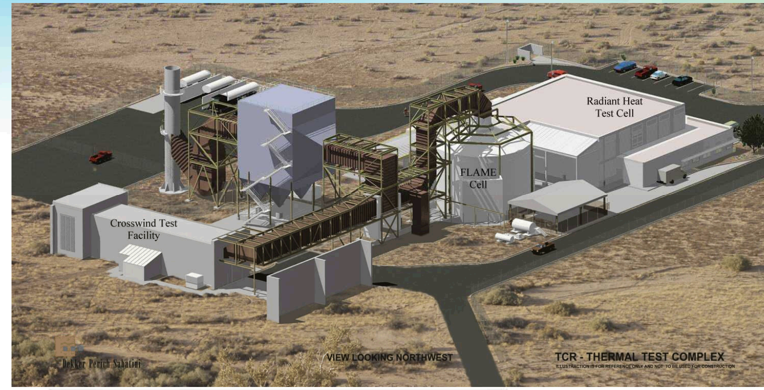
H_2 behavior (SCS010) collaborations

- 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

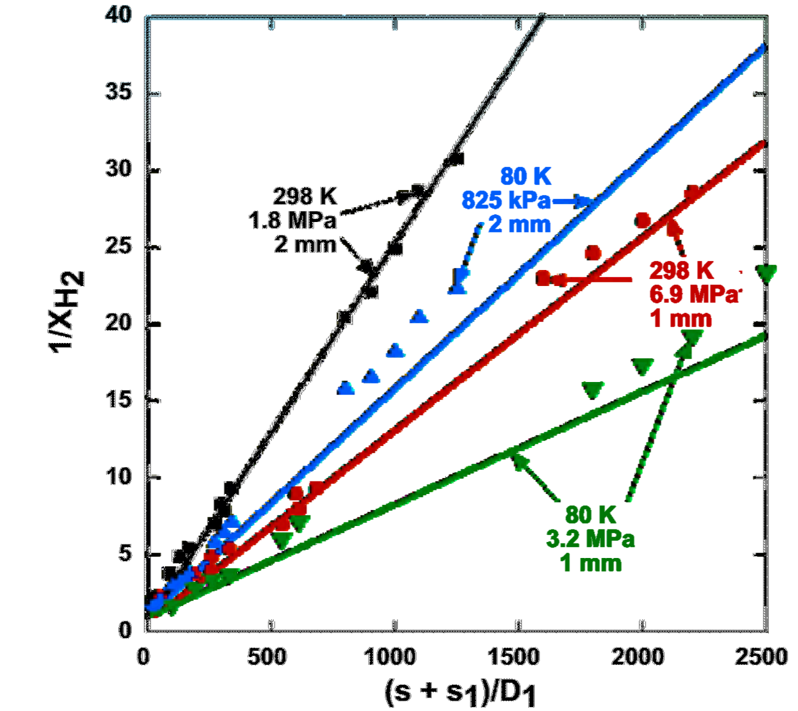
Summary

- **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)

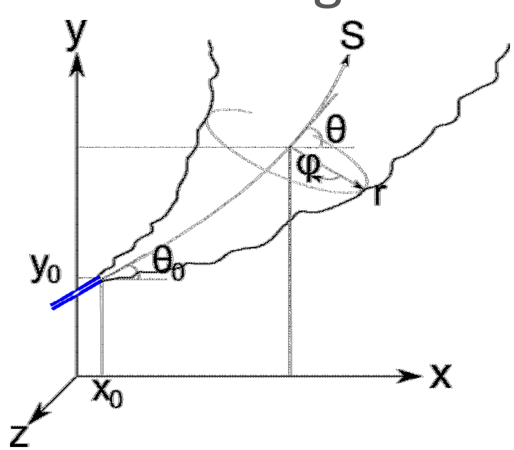
TECHNICAL BACKUP SLIDES

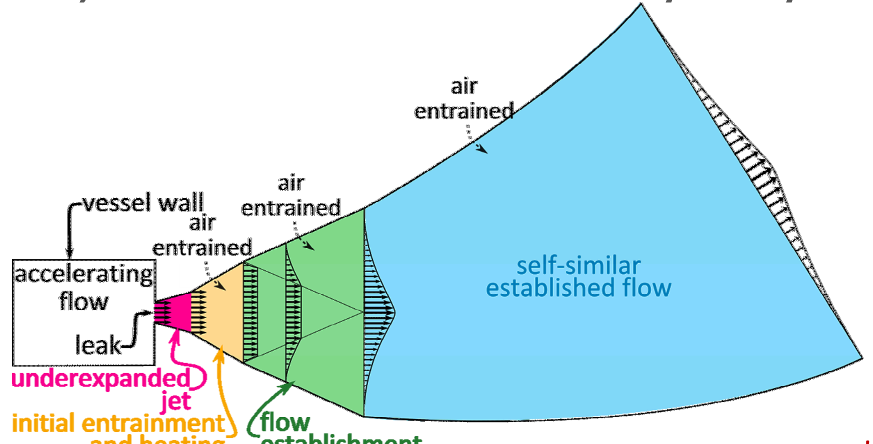
A conceptual model needs to further validation

- 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

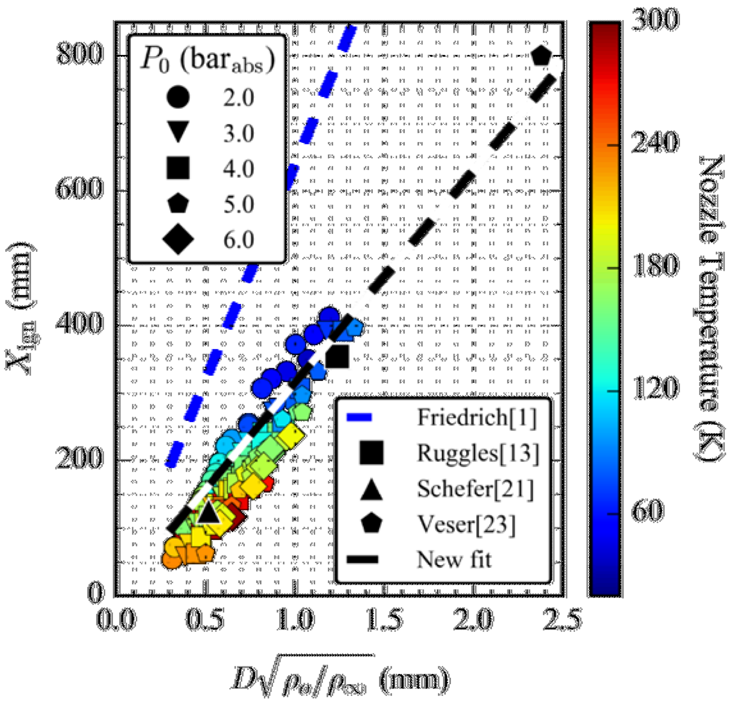


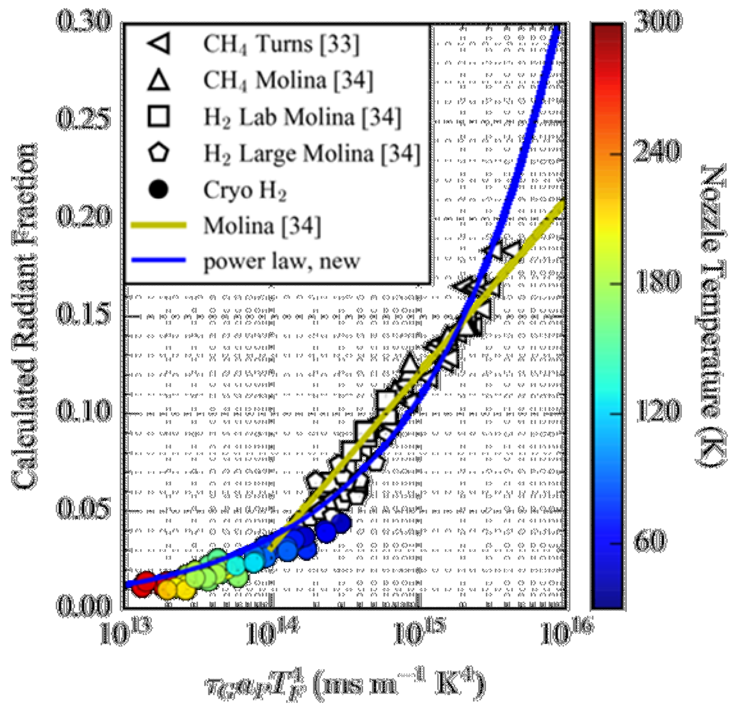


, IJHE, 2013

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

Ignition distance and radiant fraction were mapped out last FY

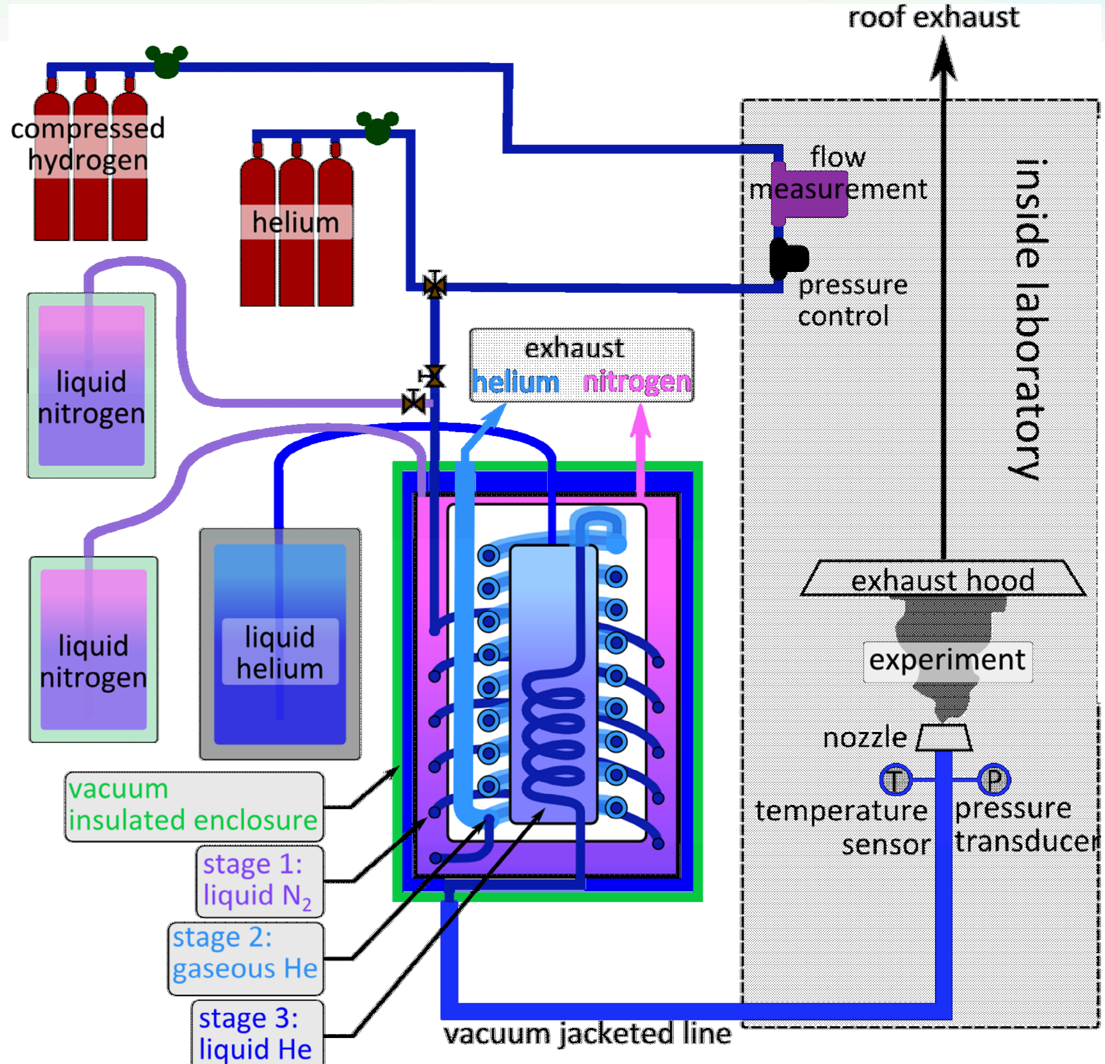


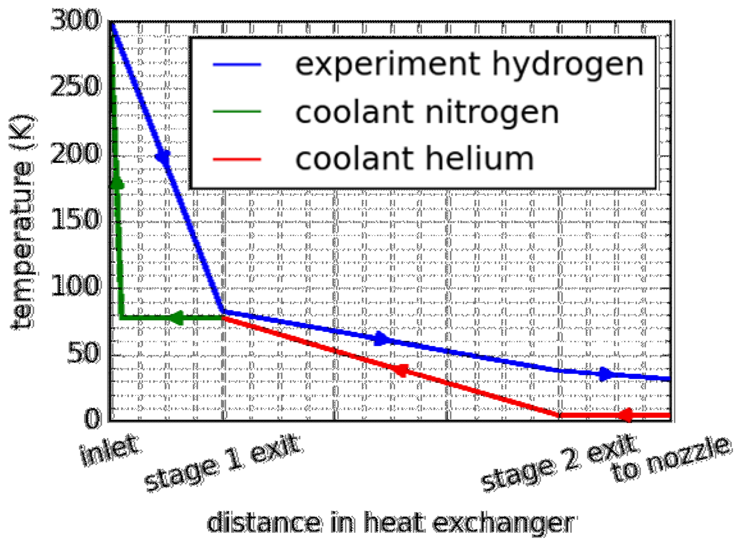


Two high priority scenarios identified by the NFPA 2 code committee are initially targeted for modeling

- ✓ 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

REVIEWER ONLY SLIDES

Critical Assumptions and Issues

- While the current laboratory low temperature jet/plume testing is a necessary part of advising the C&S community on liquid hydrogen, it is not sufficient for fire code revision. We need the larger scale tests and validated models of pooling and evaporation. We also need to be able to incorporate wind into our simulations to determine if this could cause the hydrogen to be pushed to the ground from a cold vent release.
- Assumption: the science-based approach to setback distances will be smaller than the current expert consensus numbers. It may very well be that the risk-informed, science-based setback distances are not smaller than the current values.

Publications and Presentations

- C. San Marchi, E. S. Hecht, I. W. Ekoto, K. M. Groth, C. LaFleur, B. P. Somerday, R. Mukundan, T. Rockward, J. Keller & C. W. James. "Overview of the DOE hydrogen safety, codes and standards program, part 3: Advances in Research and Development to Enhance the Scientific Basis for Hydrogen regulations, Codes and Standards." *International Journal of Hydrogen Energy,* in press. http://dx.doi.org/10.1016/j.ijhydene.2016.07.014.
- K.M. Groth & E.S. Hecht. "HyRAM: A methodology and toolkit for Quantitative Risk Assessment of hydrogen systems." *International Journal of Hydrogen Energy*. In press http://dx.doi.org/10.1016/j.ijhydene.2016.07.002.
- P.P. Panda & E.S. Hecht. "Ignition and flame characteristics of cryogenic hydrogen releases." *International Journal of Hydrogen Energy*. 62 (2017). 775-785.
- E.S. Hecht & P. Panda. "Liquid Hydrogen Behavior Studies" Presented to the LH2 Separation Distance Technical Panel. June, 2016. SAND2016-6149 PE.
- E. S. Hecht. "Cryogenic Hydrogen Plume Behavior." Prepared for the HySAFE Research Priorites Workshop, Petten, The Netherlands. Sept. 2016. SAND2016-9482 C.
- E. S. Hecht. "Accidental Hydrogen Ignition." Prepared for the HySAFE Research Priorites Workshop, Petten, The Netherlands. Sept. 2016. SAND2016-9481 C.
- E. S. Hecht. "Non-Premixed Hydrogen Combustion." Prepared for the HySAFE Research Priorites Workshop, Petten, The Netherlands. Sept. 2016. SAND2016-9480 C.
- E.S. Hecht, P. Panda. "Validation data for cryogenic hydrogen releases and flames." Presented to the Hydrogen Codes and Standards Tech Team. Oct. 2016. SAND2016-10307 PE.
- E.S. Hecht, P. Panda. "Validation data for cryogenic hydrogen releases and flames." Presented to the LH2 Separation Distance Stakeholders. Nov. 2016. SAND2016-11548 PE.
- E.S. Hecht. "Validation data for cryogenic hydrogen releases and flames." Presented to the NFPA 2 task group. Feb. 2017. SAND2017-2308 PE.
- E.S. Hecht, P. Panda "Mixing and Warming of Cryogenic Hydrogen Releases." Submitted to the International Conference on Hydrogen Safety, Hamburg, Germany, Sept. 2017. SAND2017-3301 C.

Additional References available in SCS010 & SCS025 & previous AMRs for SCS010, SCS011, & SCS025