Sandia National Laboratories

Hydrogen and Fuel Cells Program

SAND2017-12045PE

Current research and future outlook for behavior and consequence modeling

Ethan S. Hecht

Sandia National Laboratories

Livermore, CA

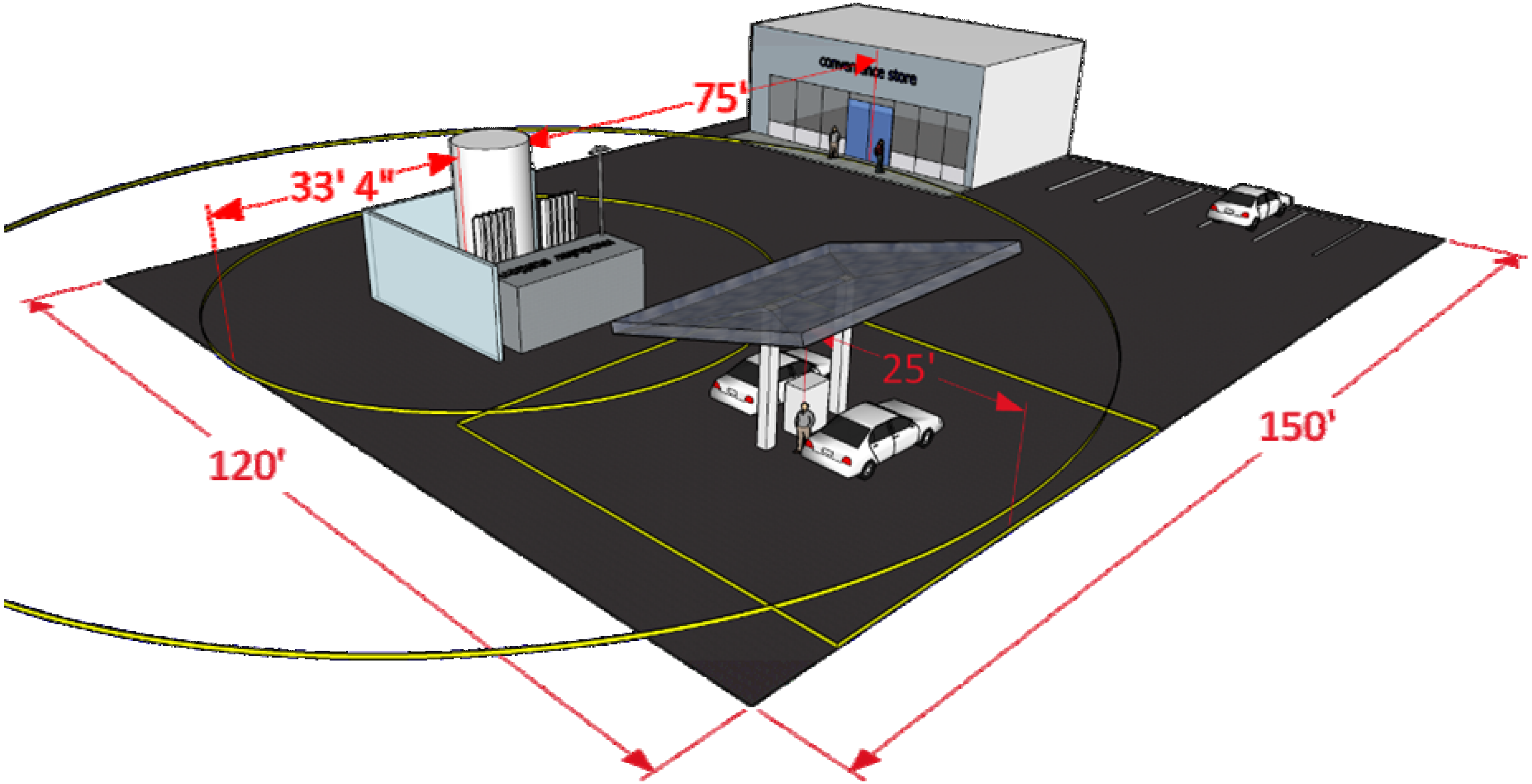
US-Korea Joint Research Meeting

November 6, 2017

Sandia National Laboratories is a multimission 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.

Current experiments are focused on understanding cryogenic hydrogen systems to provide a scientific basis for setback distances

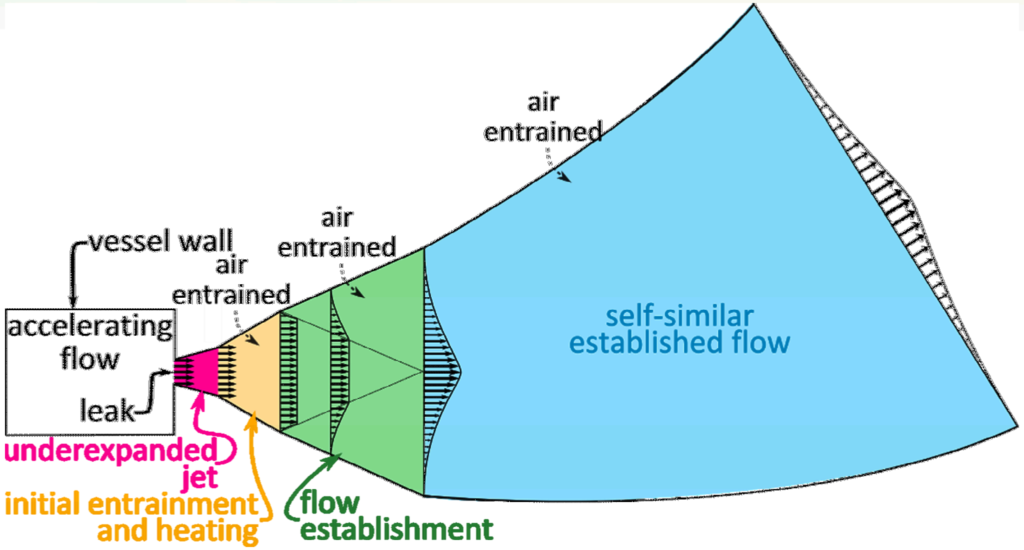
- Previous work by this group led to science-based, reduced, gaseous H_2 separation distances
- Higher energy density of liquid hydrogen over compressed H_2 makes it more economically favorable for larger fueling stations
- Even with credits for insulation and fire-rated barrier wall 75 ft. offset to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

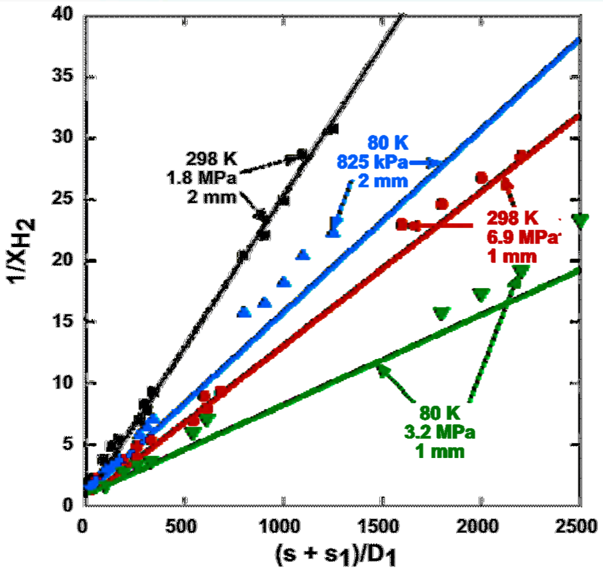


NFPA 2 code committee has identified high priority scenarios that impact separation distances

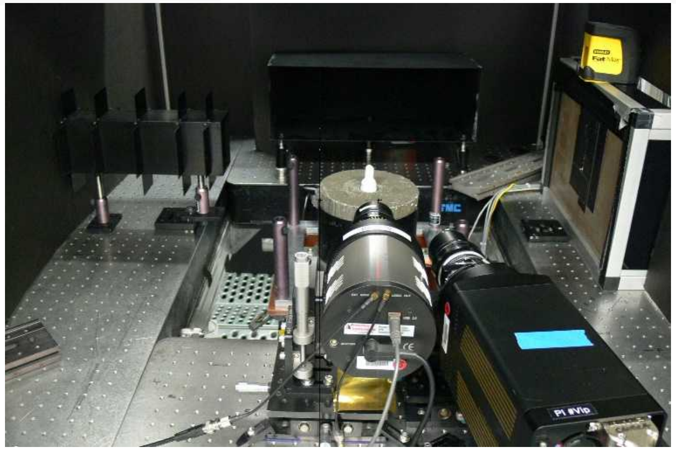
- ✓ Flow from vent of ultra-cold hydrogen (e.g. trailer venting excess pressure after normal LH_2 delivery or burst disk rupture)
  - Are vent stacks appropriately designed?
  - Separation distance from air intakes and overhead utilities
  - Vertical discharge, 3” diameter pipe, 20-140 psig
- ❑ Release 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 focusing on validating a model for cryogenic hydrogen dispersion



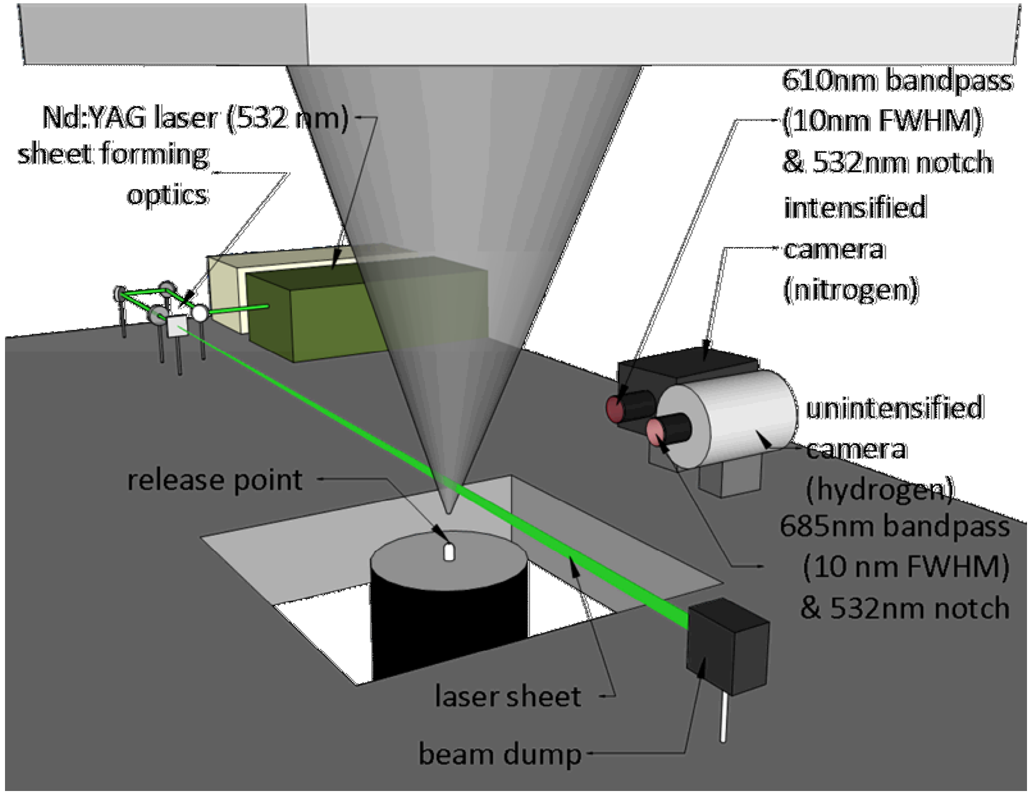


Houf & Winters, IJHE, 2013



- 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 2016 to generate cryogenic hydrogen releases

We developed and implemented a Raman imaging technique to measure cryogenic plumes



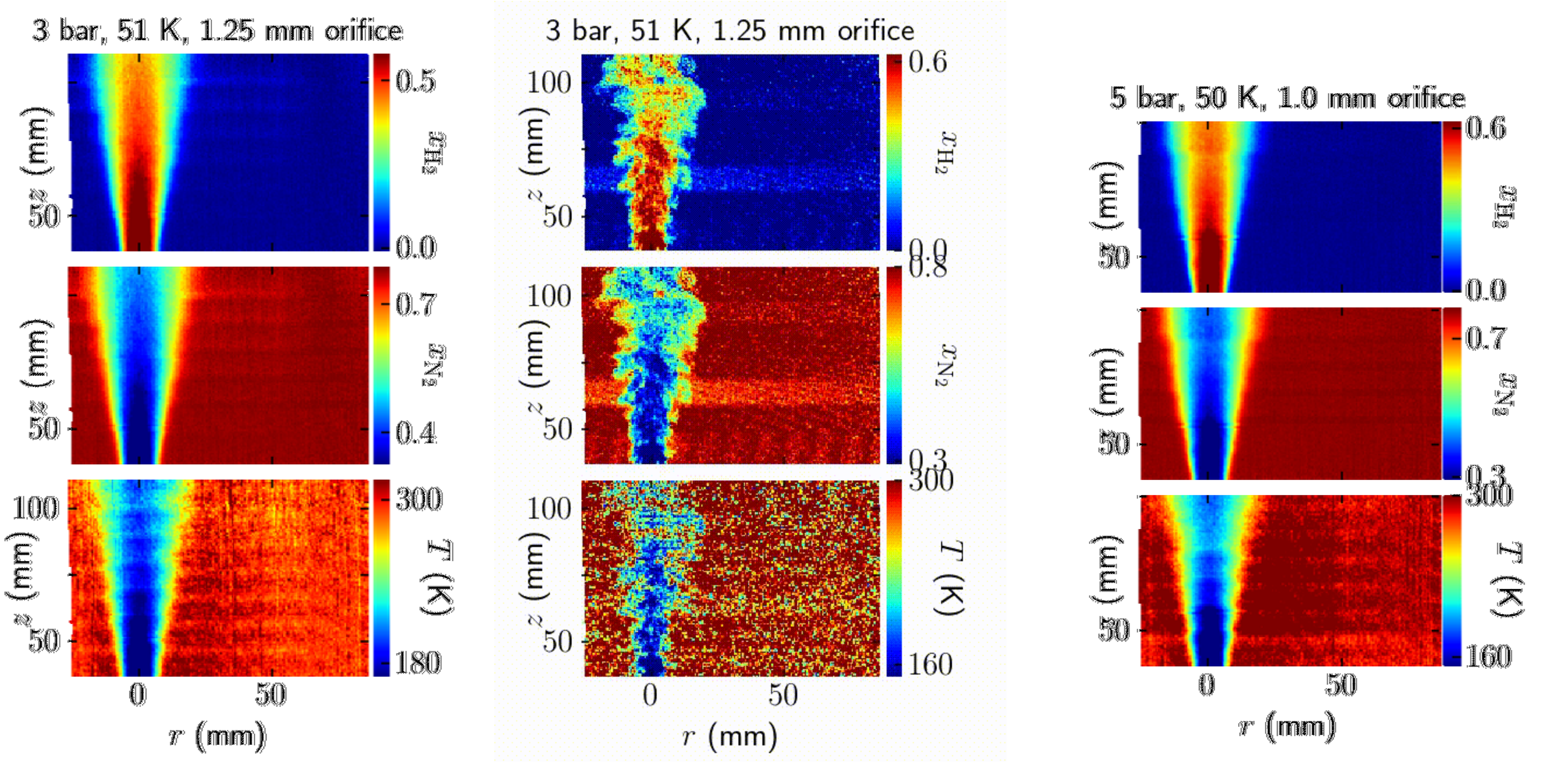
- Conventional Rayleigh signal overwhelmed by Mie scattering off of condensed water vapor in jet
- Filtered Rayleigh had insufficient Mie scattering light suppression (OD≈3)
- Raman scattering enables higher optical density filters
  - 10 nm FWHM bandpass filters at wavelengths of interest
  - OD of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

➢ Enables simultaneous measurement of concentration and temperature in 2D

Several experimental campaigns have had variations in temperature, pressure, and nozzle size

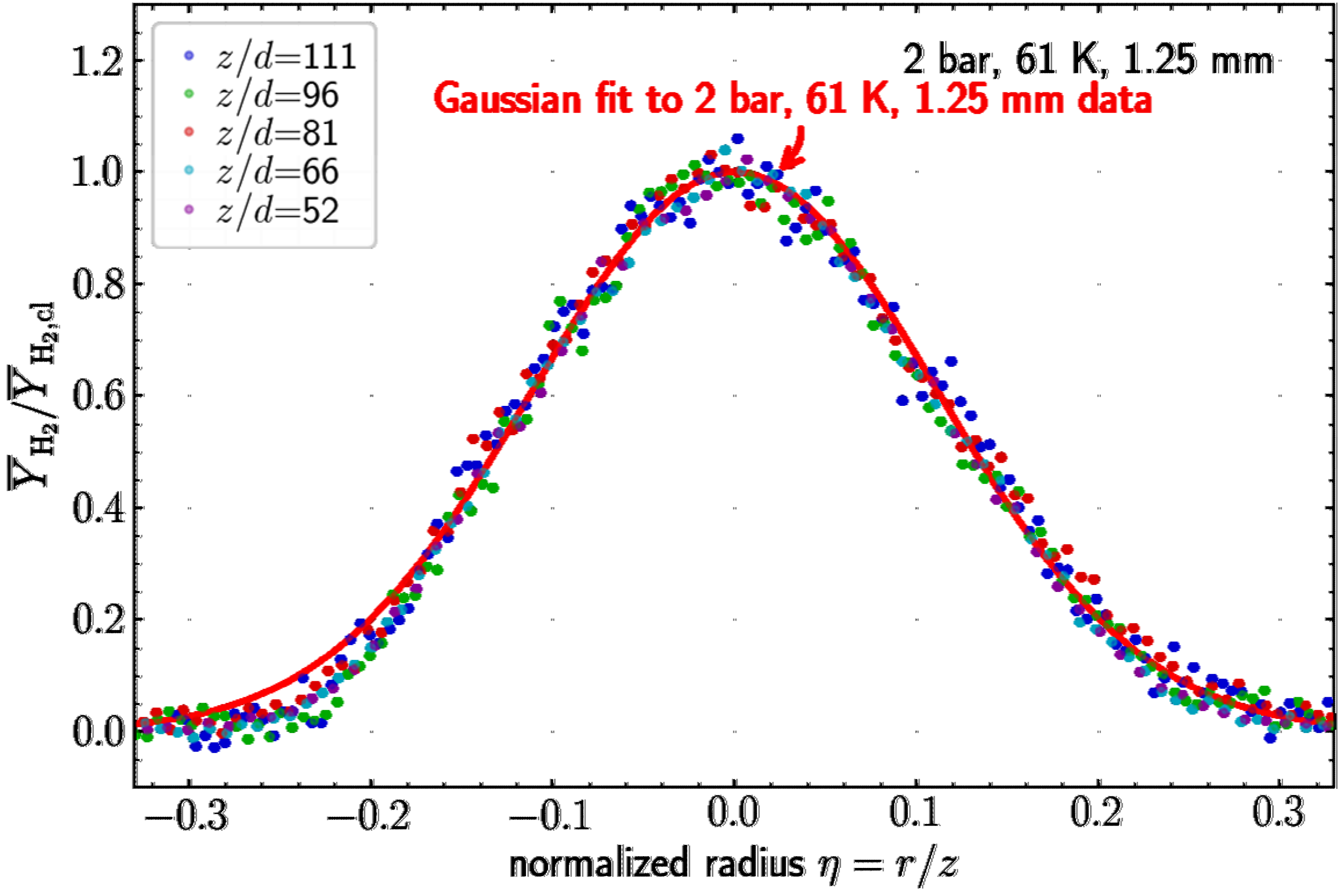
T_{noz} [K]	P_{noz} [bar_{abs}]	d [mm]	T_{throat} [K]	n_{hts}
58	2	1	43.5	4
56	3	1	41.9	4
53	4	1	39.6	4
50	5	1	37.4	5
61	2	1.25	45.7	6
51	2.5	1.25	38.2	2
51	3	1.25	38.2	6
55	3.5	1.25	41.2	3
54	4	1.25	40.4	2
43	4	1	32.1	2
59	3	1	44.2	6
56	3.5	1	41.9	1
80	3	1	60.3	5

With PIV

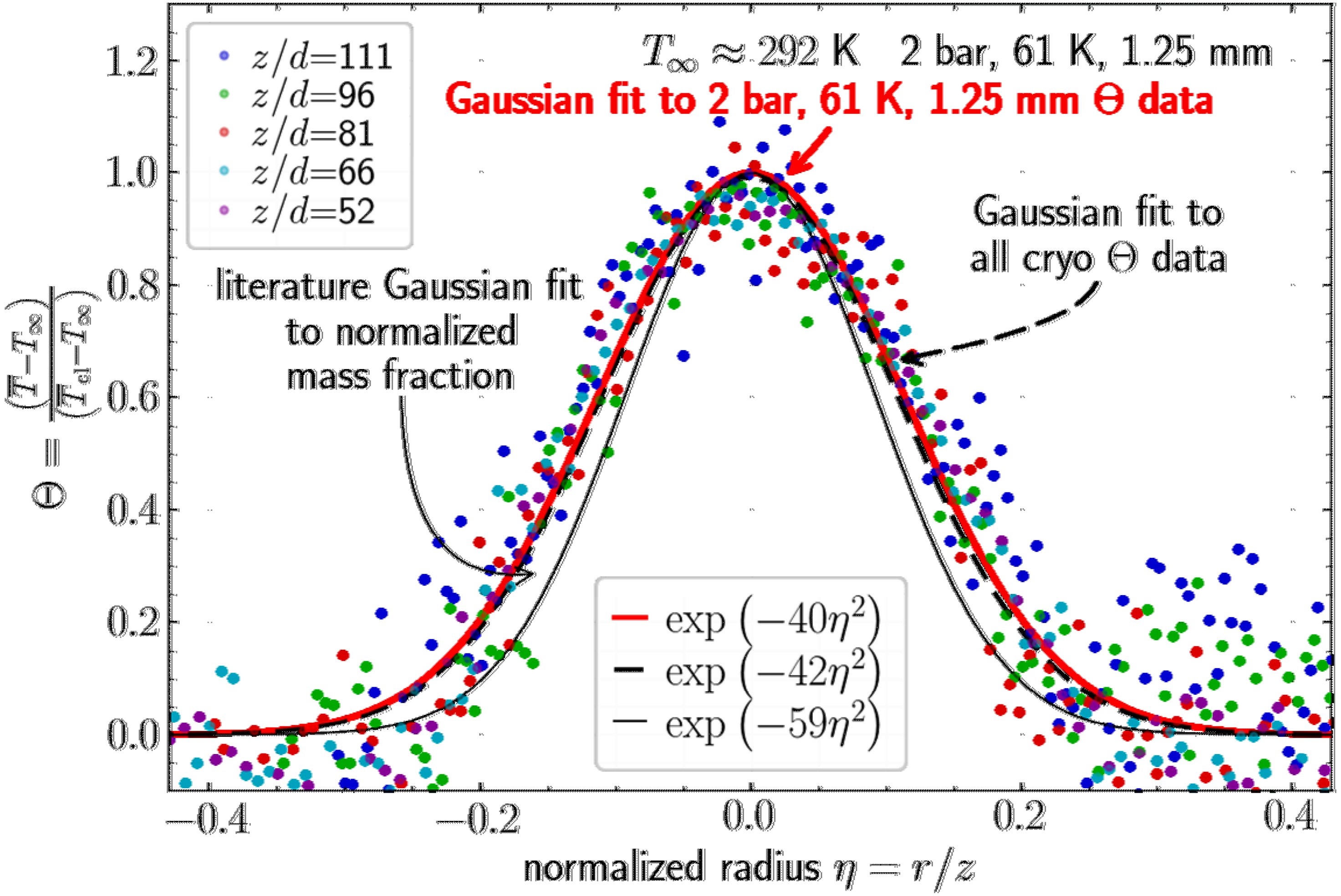


➢ Two-dimensional images are superior to centerline only measurements for model validation

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

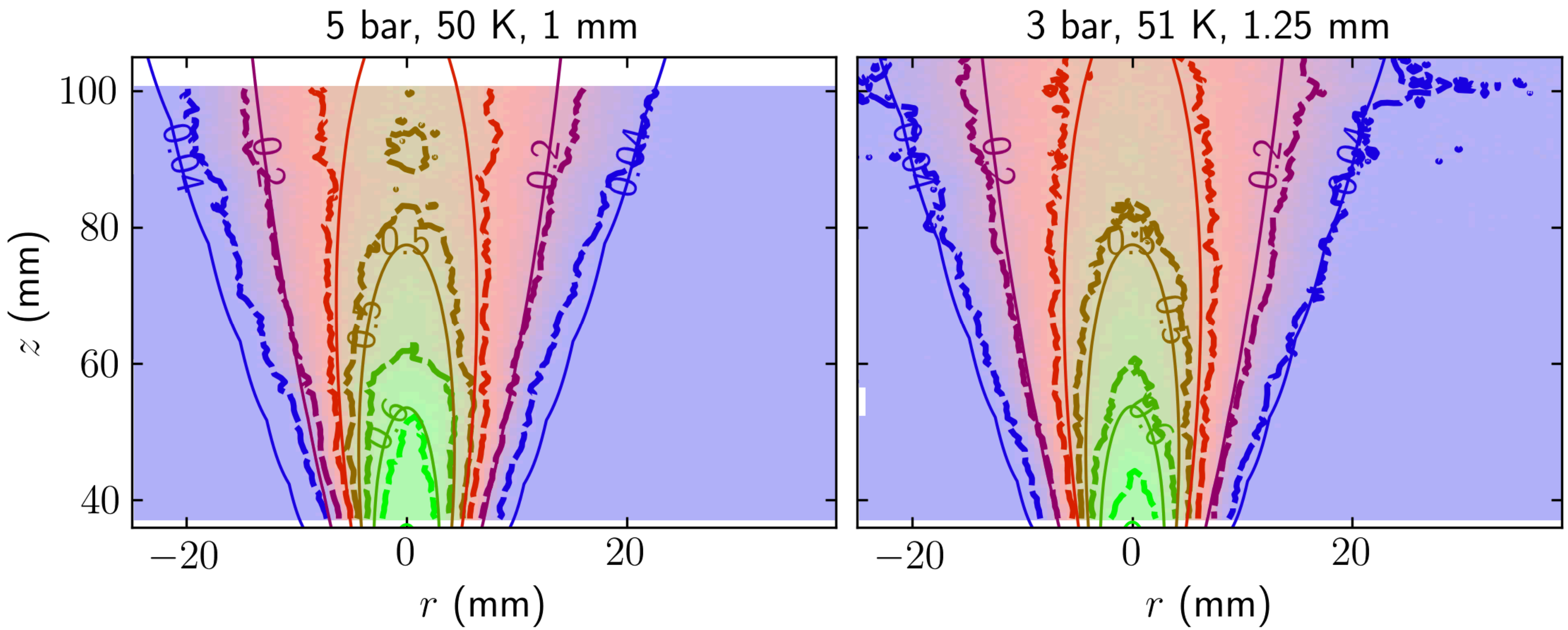


Radial profiles of temperature are also self-similar, and wider than mass fraction



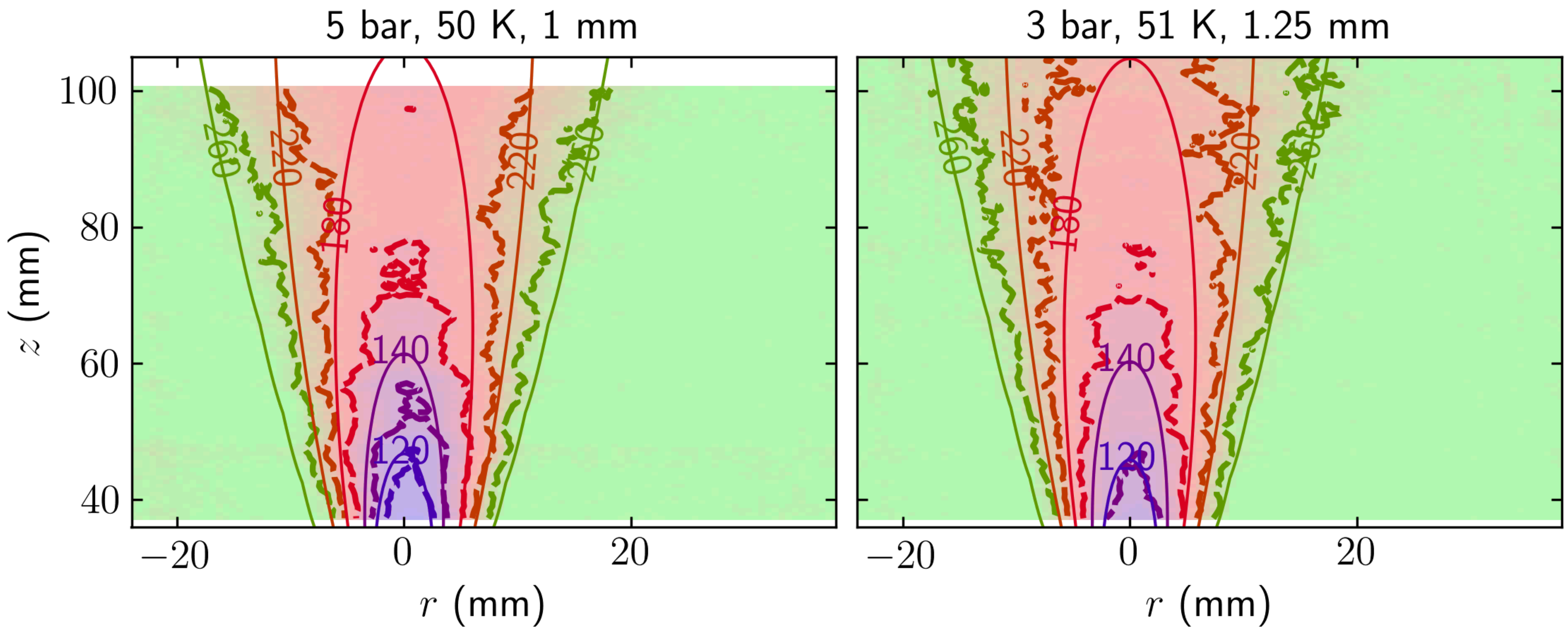
➢ Data will be used to validate relative spreading ratio in model

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



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

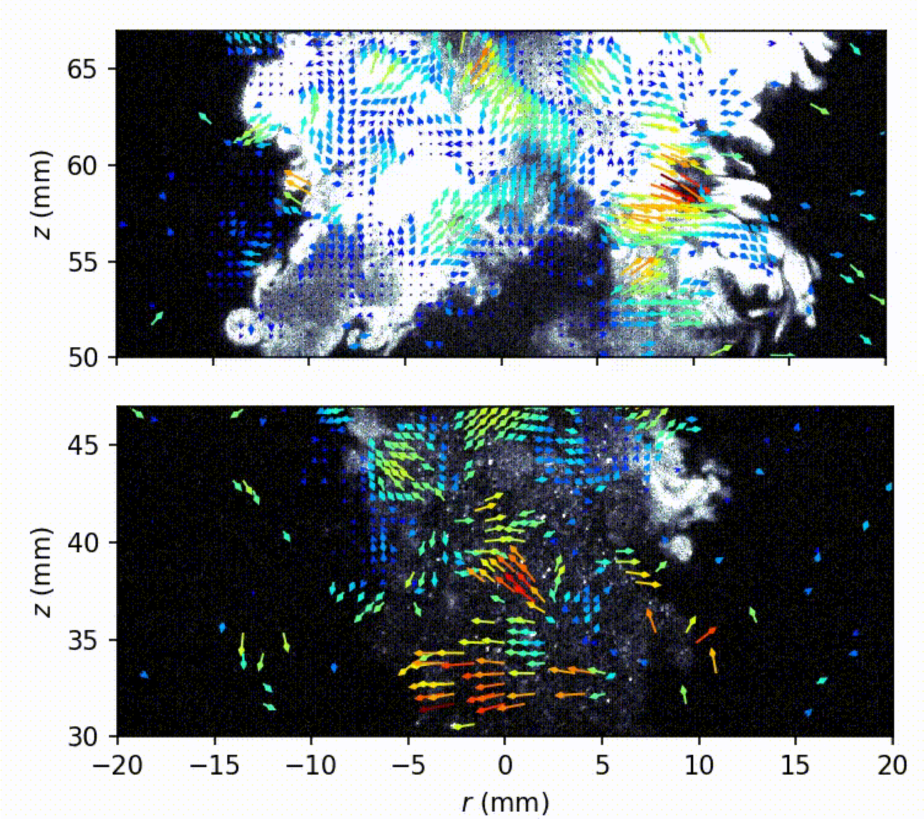
Initial comparisons to model also have minor differences in terms of temperature

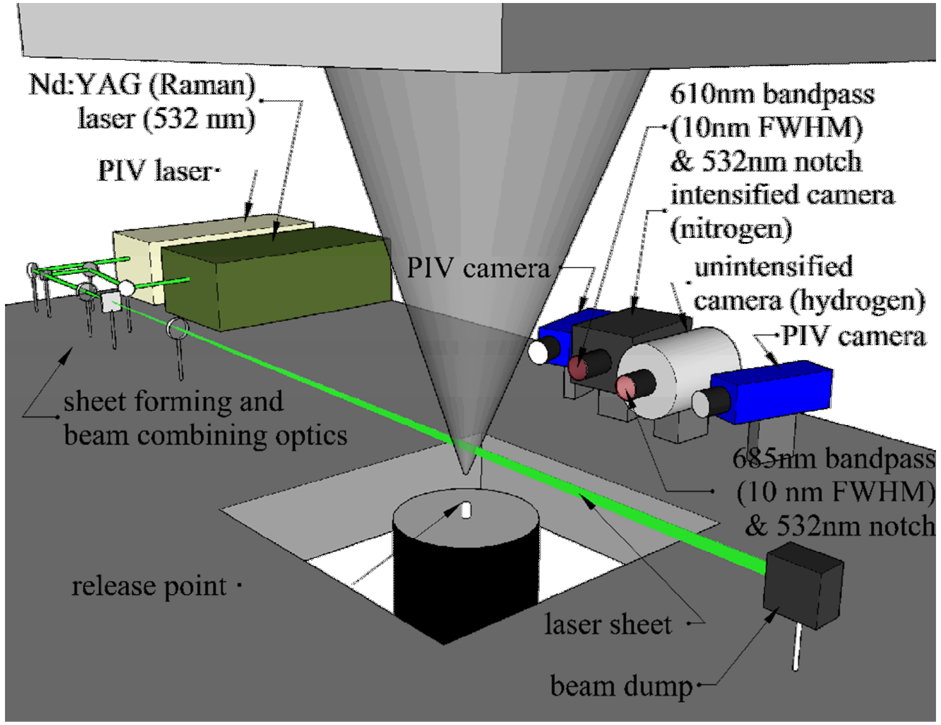


➢ Temperature measurements are noisier than mole fraction

We have recently used particle imaging velocimetry to also measure the velocity field of cryogenic hydrogen

2 bar, 55K, 1mm orifice



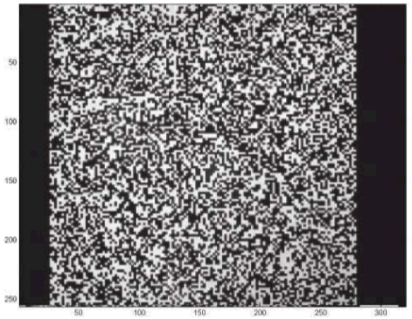


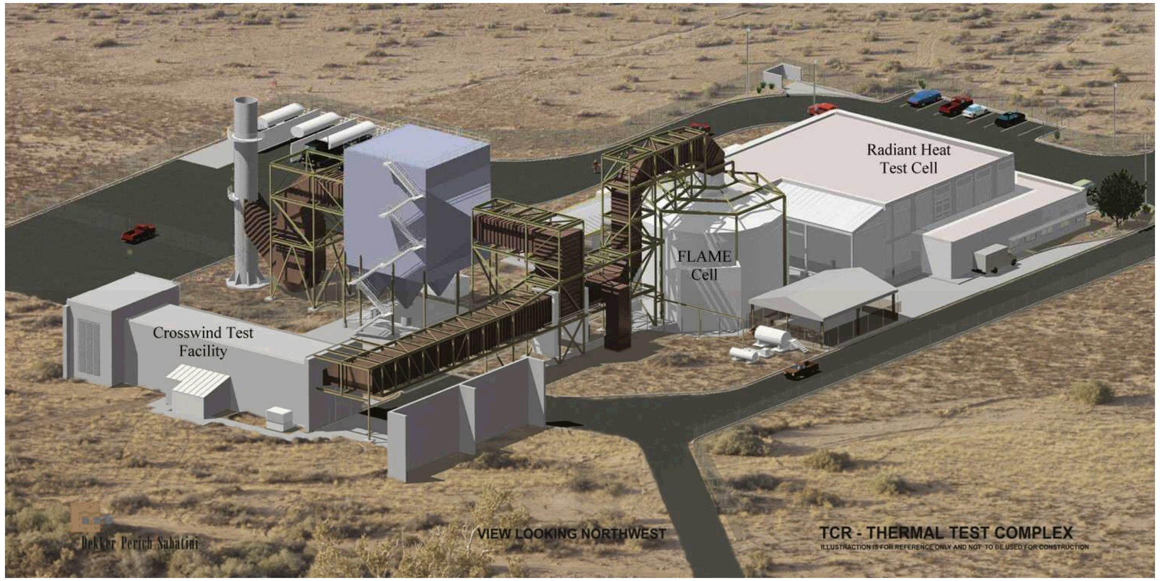
Independent model parameters:

- ✓ T - temperature
- ✓ x - mole fraction
- ✓ v - velocity
- ✓ B - halfwidth (velocity, concentration, temperature)

Future work: Characterize phenomena from large-scale releases

- Need experiments to characterize:
  - Interactions with ambient (i.e. wind)
  - Pooling
  - Evaporation from LH_2 pools
- **Currently developing an imaging diagnostic** for outdoor and large-scale experiments
- Can apply diagnostic to normally occurring outdoor releases (e.g., venting after LH2 fill) and validation experiments at well-controlled facilities





Coded-aperture Raman imaging

dx.doi.org://10.1117/12.919292

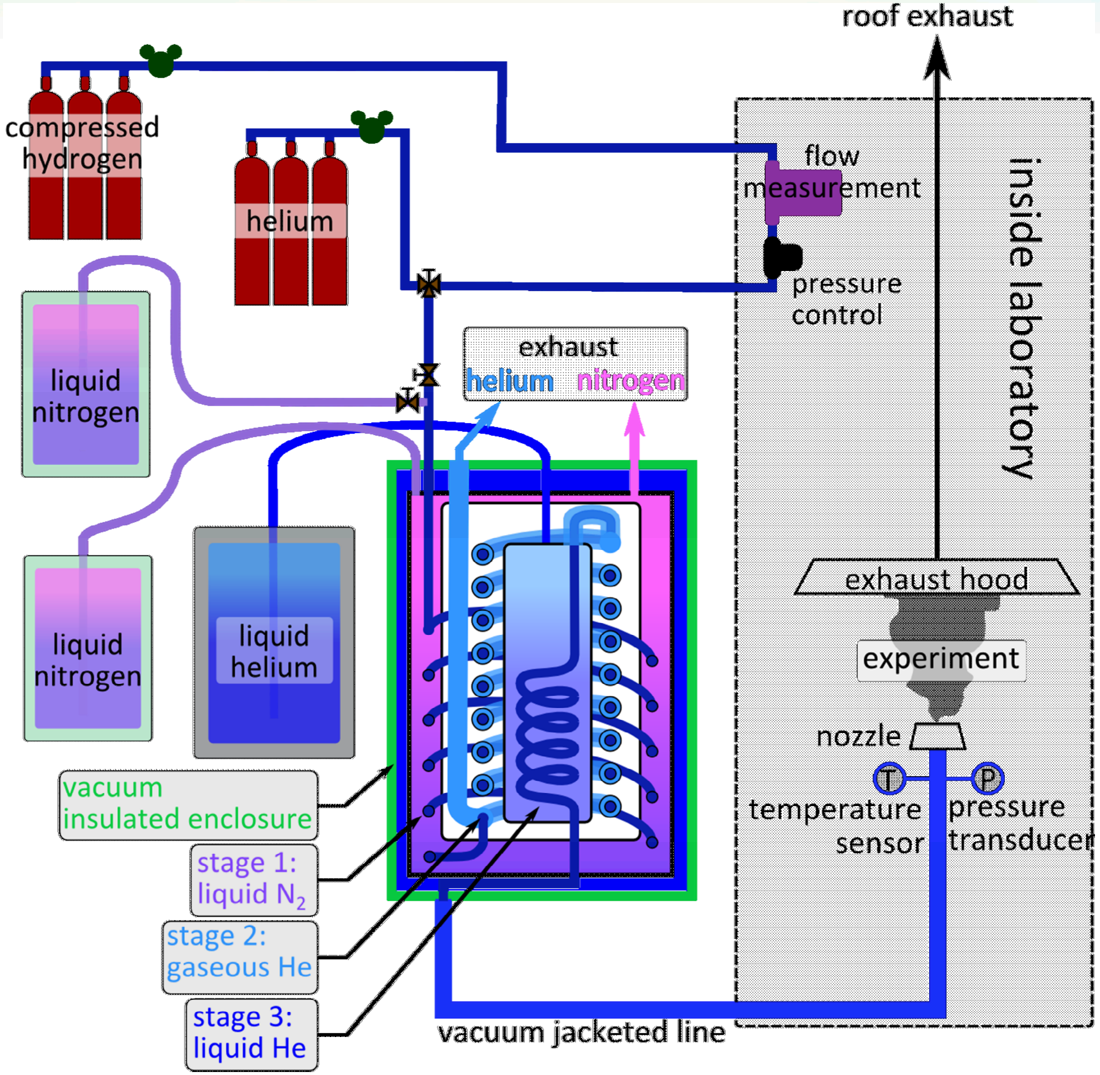
Summary

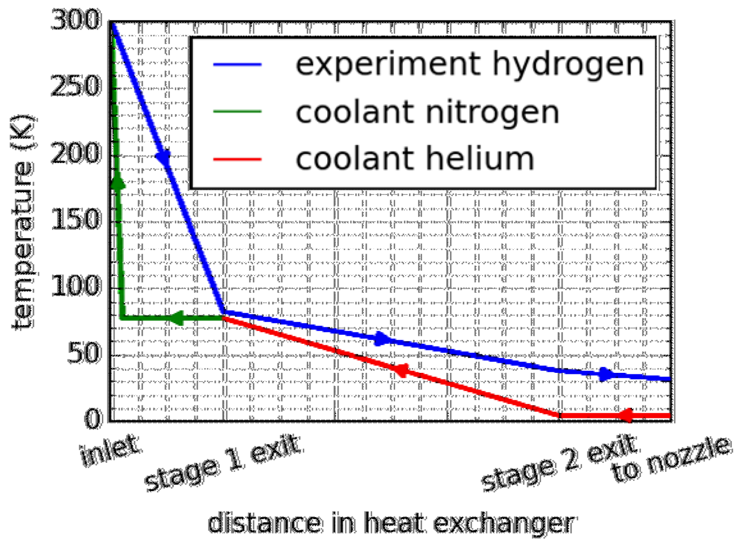
- Used advanced imaging diagnostics (planar laser Raman imaging, PIV) to measure cryogenic hydrogen mixing with air and warming
- Without modification, model is doing a reasonable job of predicting mole fraction and temperature, although improvements are possible (we have yet to compare velocity)
- Currently developing an optical diagnostic for quantitative measurements of large-scale cryogenic hydrogen dispersion phenomena
- Our diagnostics and facilities can be adapted to study other fuels (e.g. natural gas, propane)

Acknowledgements

- Funding support from:
  - United States Department of Energy, Energy Efficiency &Renewable Energy, Fuel Cell Technologies Office, Safety, Codes, and Standards subprogram managed by Will James
  - Industry support including the OEM Group at the California Fuel Cell Partnership, Linde, and Shell
- Team members:
  - Bikram Roy Chowdhury (behaviors), Anthony McDaniel (behaviors), Rad Bozinoski (modeling), Myra Blaylock (CFD), Jon Zimmerman (H2 program manager), Chris San Marchi (materials/metal interactions with H2), Chris LaFleur (Risk, Codes & Standards), John Reynolds (HyRAM), Nalini Menon (polymer interactions with H2), Alice Muna (Risk)
  - Previous researchers including: Pratikash Panda, Katrina Groth, Isaac Ekoto, Adam Ruggles, Bob Schefer, Bill Houf, Greg Evans, Bill Winters

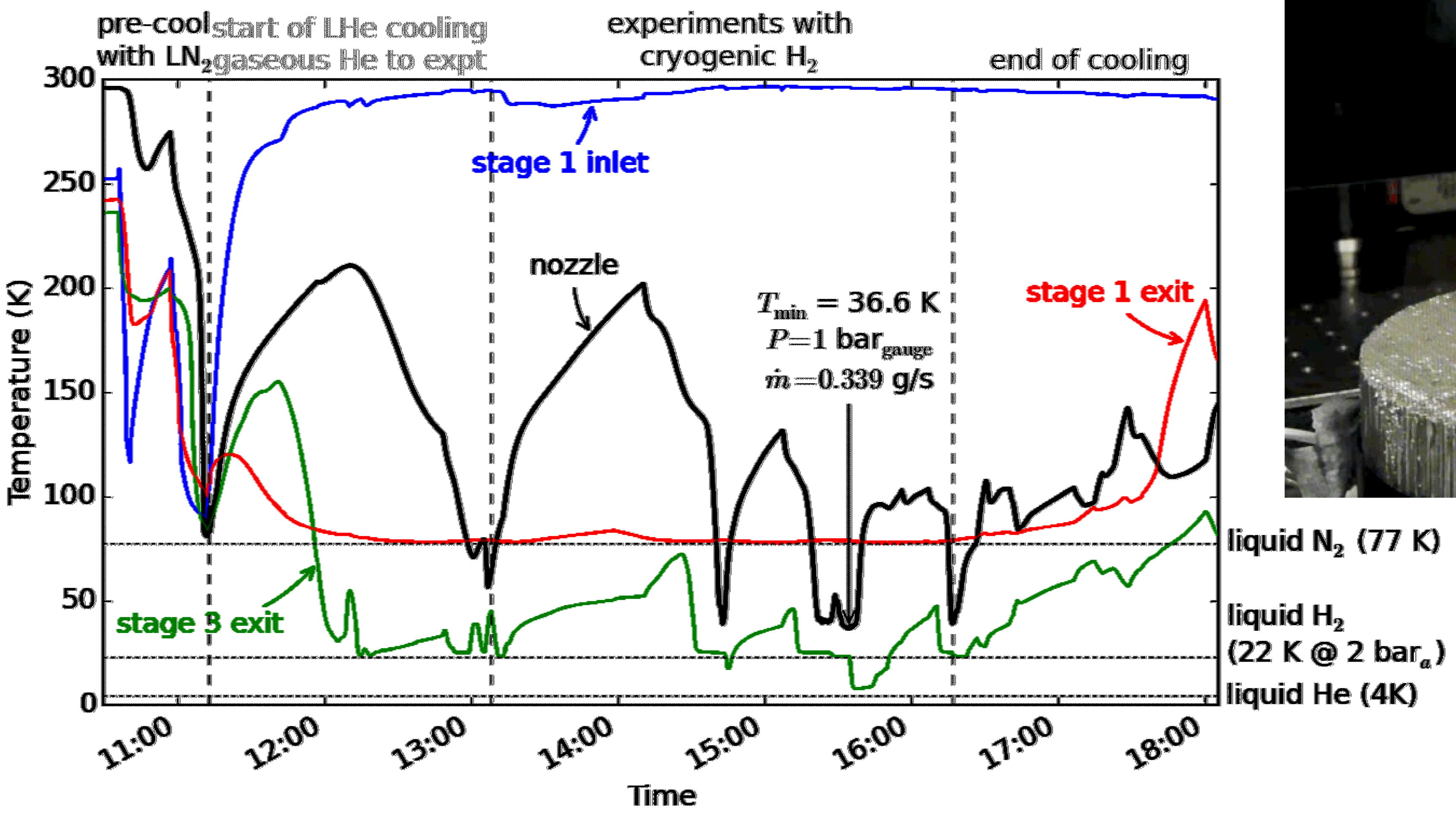
We are running an experiment, releasing ultra-cold hydrogen in the laboratory

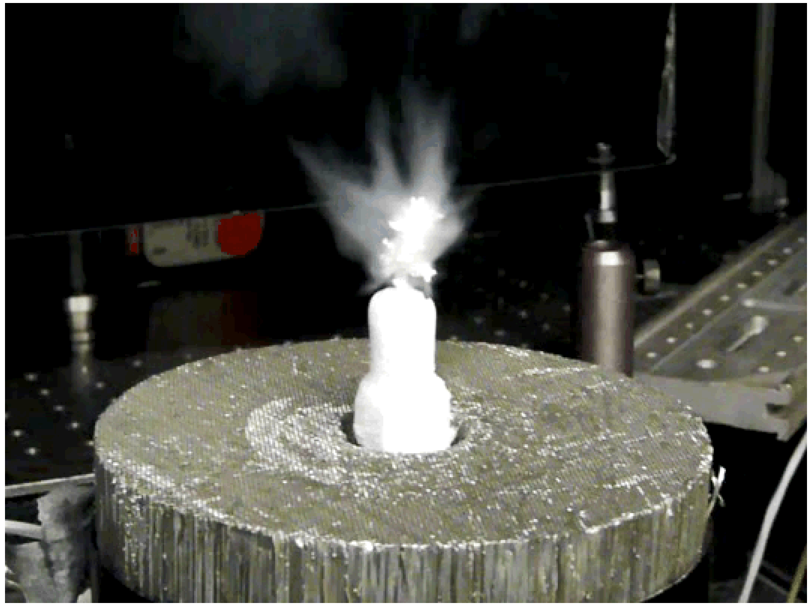




- Accurate control/measurement of boundary conditions

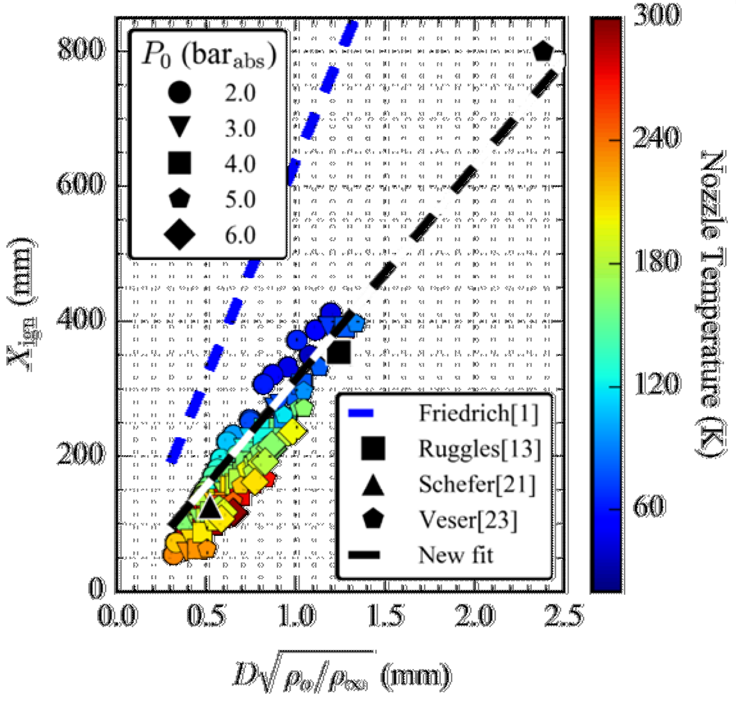
Experimental challenges include avoiding the freezing of air and hydrogen

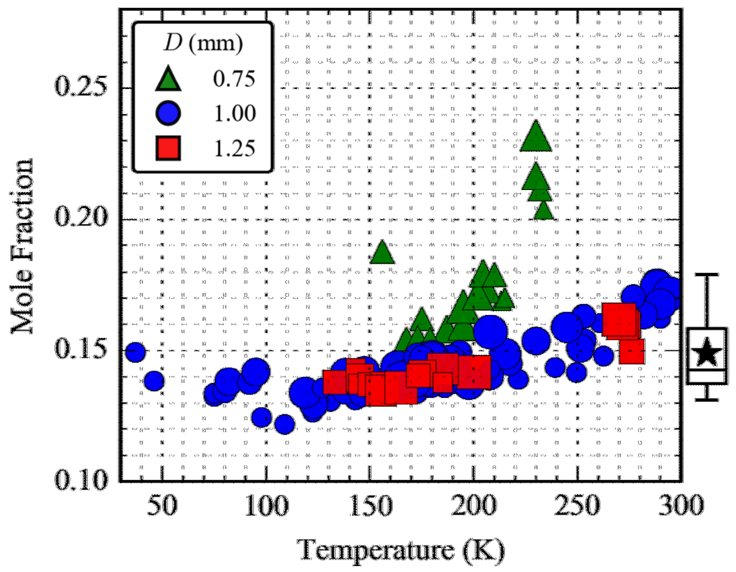


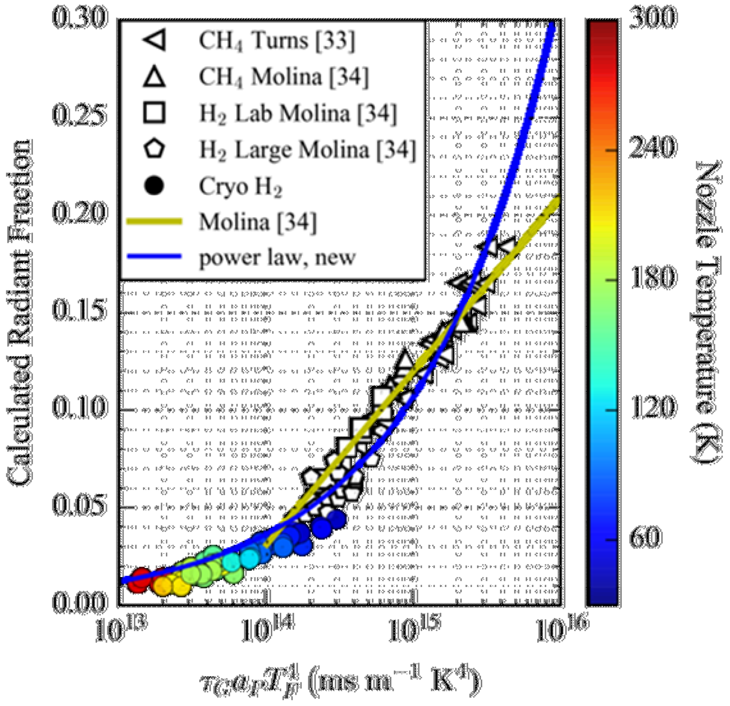


(air, moisture?) icing around liq. H_2 jet column

Ignition distance and radiant fraction for cryogenic hydrogen were mapped out last FY







- Maximum ignition distance linearly varies as a function of effective diameter (same as room temperature releases)
- Simulated H_2 mole fraction at the point of ignition is much greater than the 4% LFL
- An increase in radiant fraction is observed for the colder H_2 jets due to longer flame residence time

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