

Experimental validation of a model for cryogenic hydrogen jet dispersion

Ethan S. Hecht and Bikram Roy Chowdhury

Sandia National Laboratories

Livermore, CA 94550

255th American Chemical Society National Meeting, New Orleans, LA

March 20, 2018

As FCEV fueling stations serve higher capacity, liquid hydrogen delivery and on-site storage is the likely technology

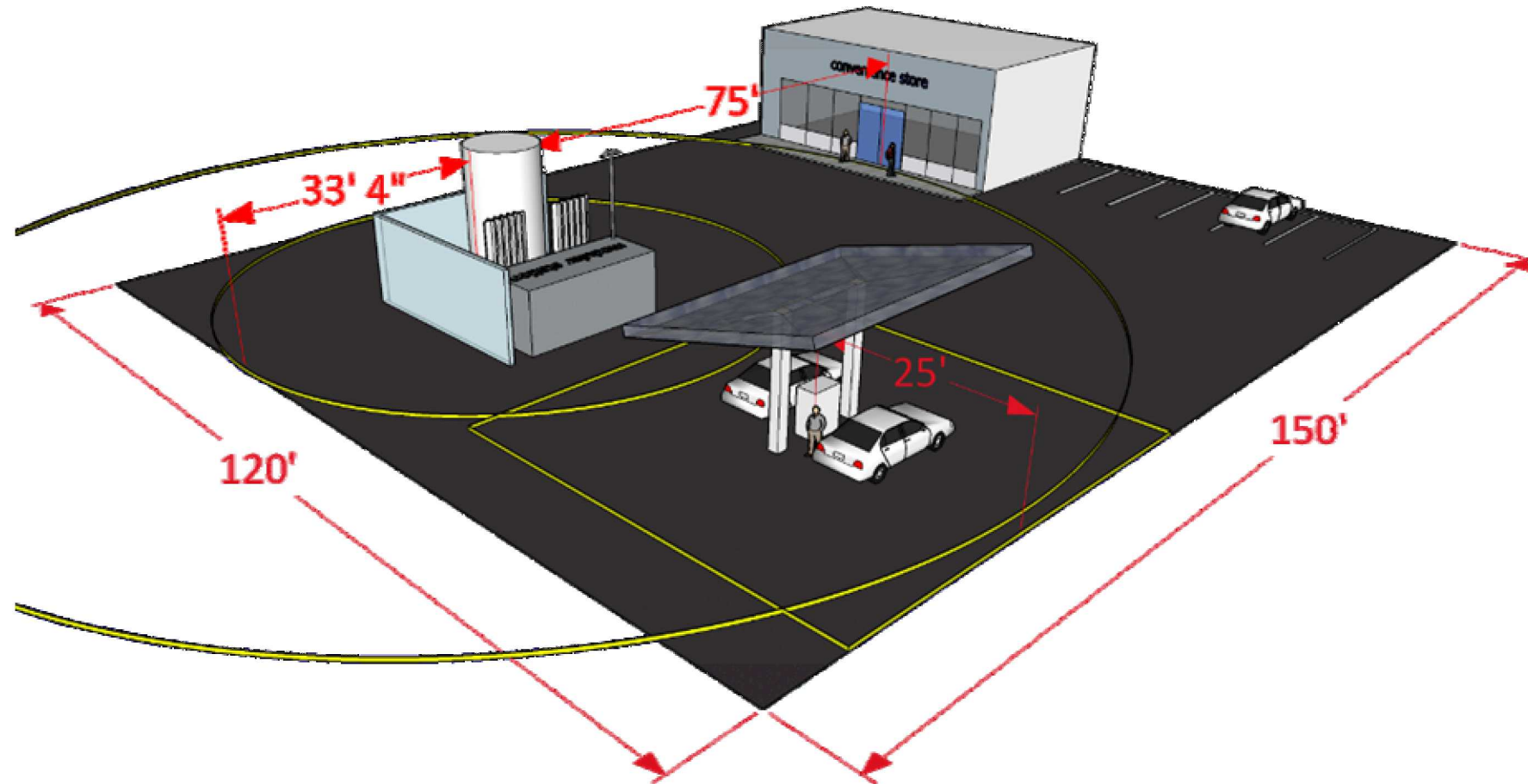
- For a similar vehicle/day capacity as gasoline, liquid H₂ tankers make sense
 - Underground gasoline stations tanks hold on the order of 10,000 gallons
 - Liquid H₂ tankers can hold up to approximately 4,000 kg
 - Compressed tube trailers hold approximately 300 kg
 - Lack of hydrogen pipelines where stations are needed
- High purity hydrogen needed for FCEVs
- Cryo pump and utilization of cold make compression and dispensing efficient and fast



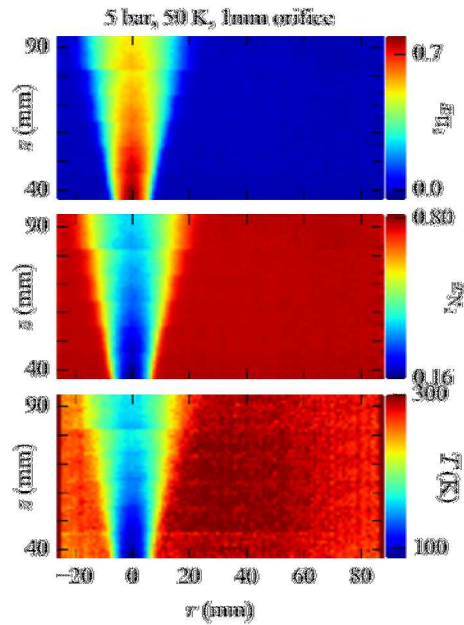
Linde's cryo pump fueling station system
<https://www.youtube.com/watch?v=Pjh639S2dek>

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 H₂ separation distances
- Higher energy density of liquid hydrogen over compressed H₂ 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



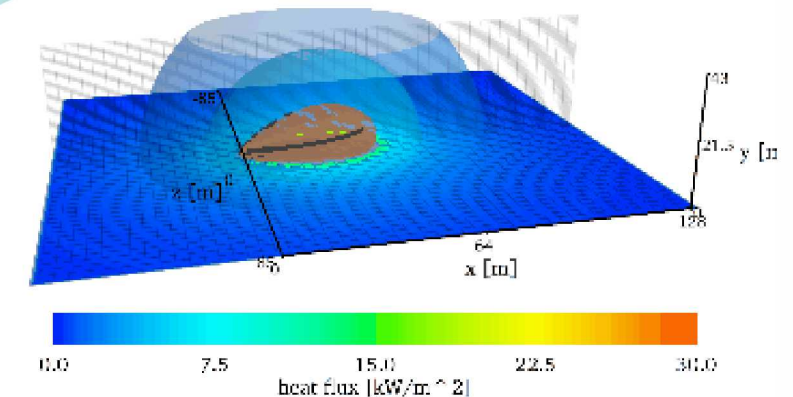
Coordinated activities at Sandia National Labs facilitate deployment of hydrogen technologies



Develop and validate scientific models to accurately predict hazards and harm from liquid releases, flames, etc.

Develop integrated methods and algorithms enabling consistent, traceable, and rigorous Quantitative Risk Assessment for H₂ facilities and vehicles

Apply QRA and behavior models to real problems in hydrogen infrastructure and emerging technology



NFPA 2 code committee has identified high priority scenarios that impact separation distances, and venting LH₂ is a regular occurrence

Current focus: validated ColdPLUME model

✓ Flow from vent of ultra-cold hydrogen

- Why?
 - Trailer venting excess pressure after normal LH₂ delivery
 - Pressure relief if tank underutilized
 - Burst disk rupture
 - A (small) liquid leak vaporizes rapidly, forming a cold gas
- Outcomes
 - Are vent stacks appropriately designed?
 - Are separation distance from air intakes and overhead utilities appropriate?
 - Quantitative risk assessment for leaks of non-pooling LH₂



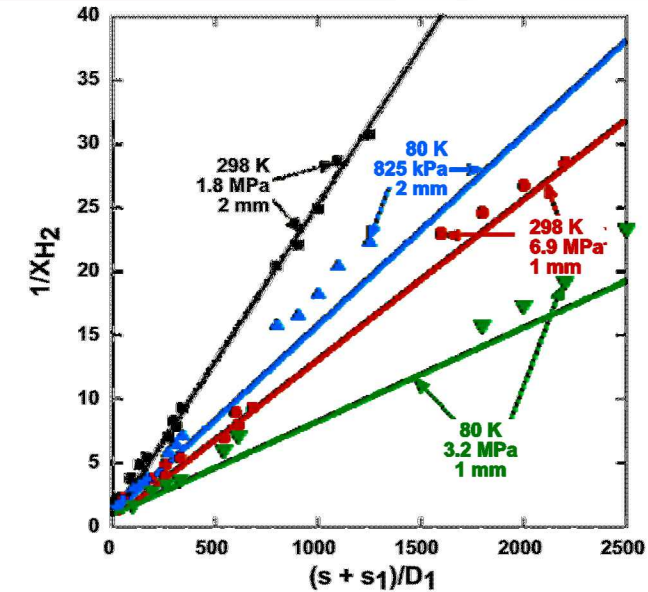
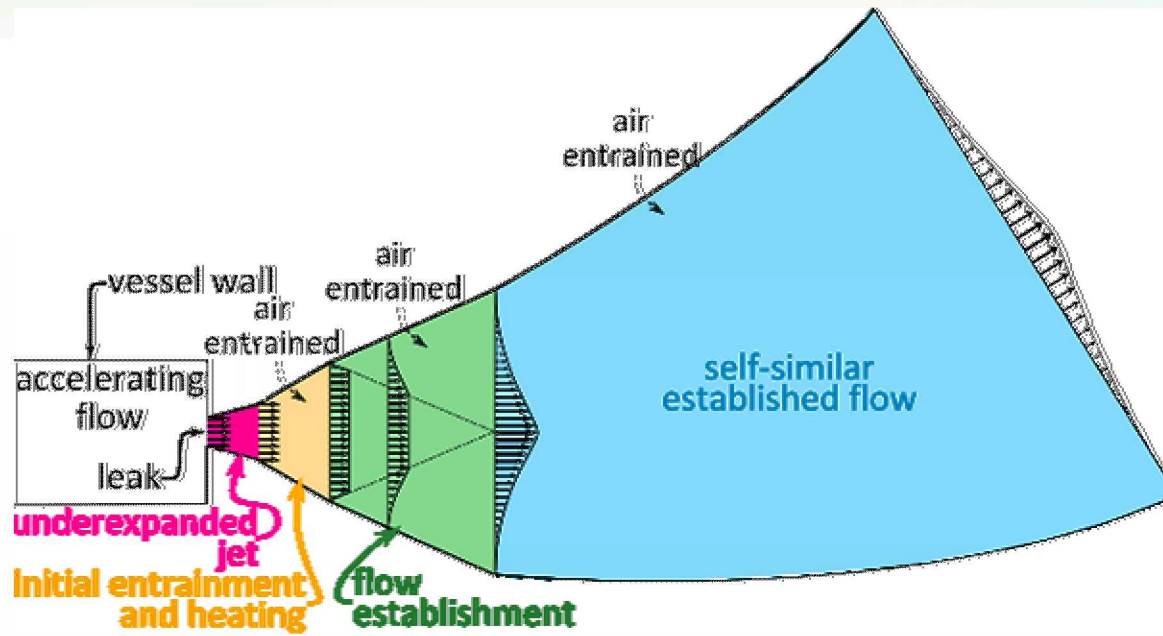
Additional experiments/modeling *and frequency data* needed

☐ Release from pipe containing liquid H₂

- Why?
 - Thermal cycles of line leading from tank to vaporizer or vaporizer itself causes leak
 - Ice falling from vaporizer shears line
- Outcomes – ability to model
 - Flashing
 - Pooling
 - Evaporation from pools
 - Heat flux from a subsequent fire
 - QRA for large, pooling leaks



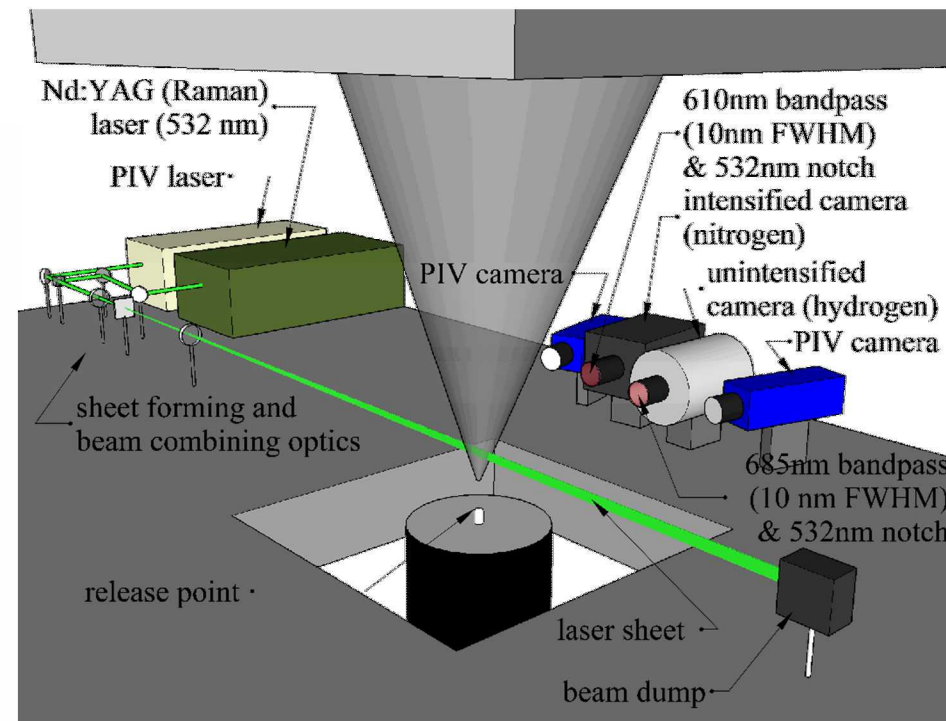
Because we couple the behavior models to risk models, we use fast-running engineering and integral models



- Previously developed model requires additional 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
- Use refined optical techniques to measure parameters of flow

Planar Raman imaging and particle imaging velocimetry off of the condensed moisture are used to measure all model parameters in 2D

- Previous lab approach of Planar Rayleigh imaging had signal overwhelmed by Mie scattering off of condensed entrained moisture in jet
- Filtered Rayleigh had insufficient Mie scattering light suppression (OD \approx 3)
- Raman scattering enables higher optical density filters to remove unwanted Mie scatter
 - 10 nm FWHM bandpass filters at wavelengths of interest
 - OD of 12 @ all wavelengths
 - OD of 18 @ 532 nm
- Condensed, entrained moisture acts as particles for stereo-PIV

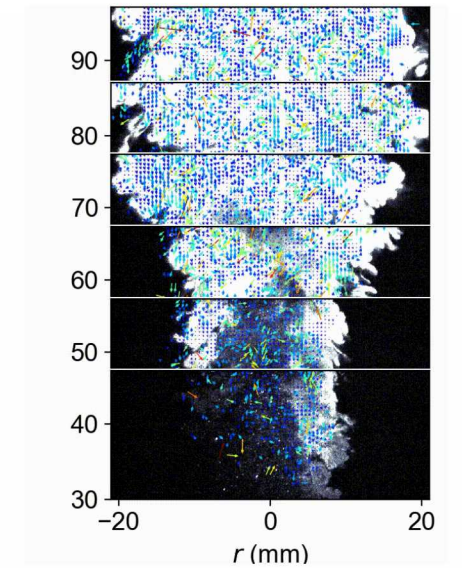
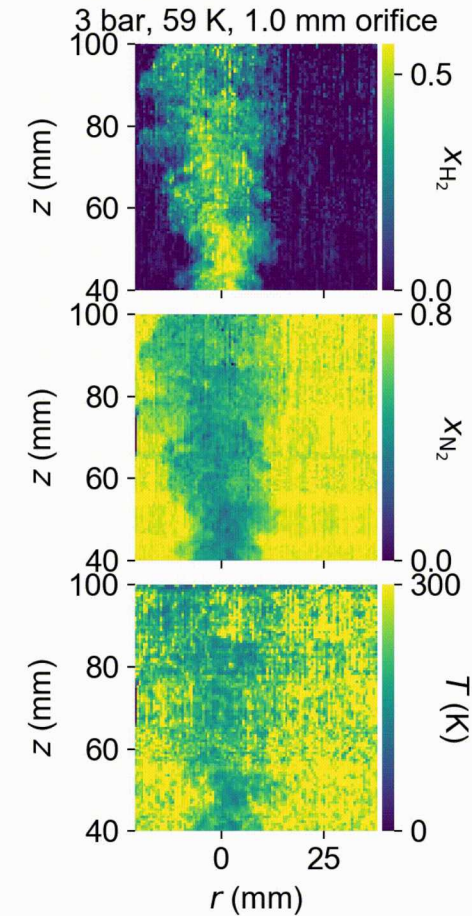
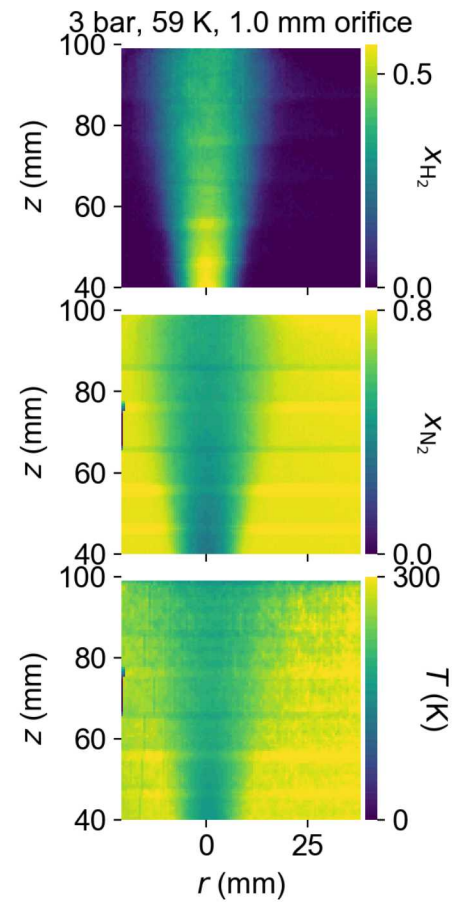


- Independent model parameters:
- ✓ T - temperature
 - ✓ x - mole fraction
 - ✓ v - velocity
 - ✓ B - halfwidth (velocity, concentration, temperature)

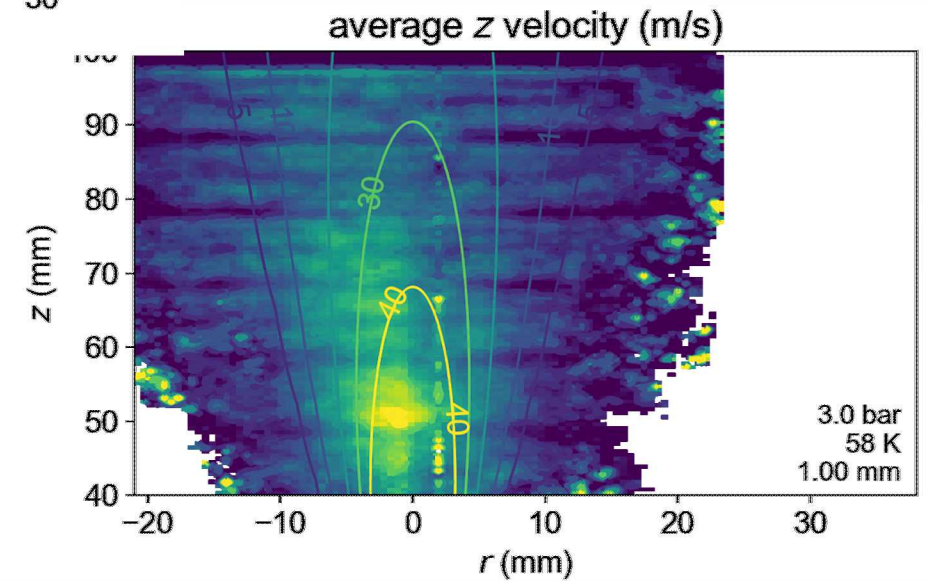
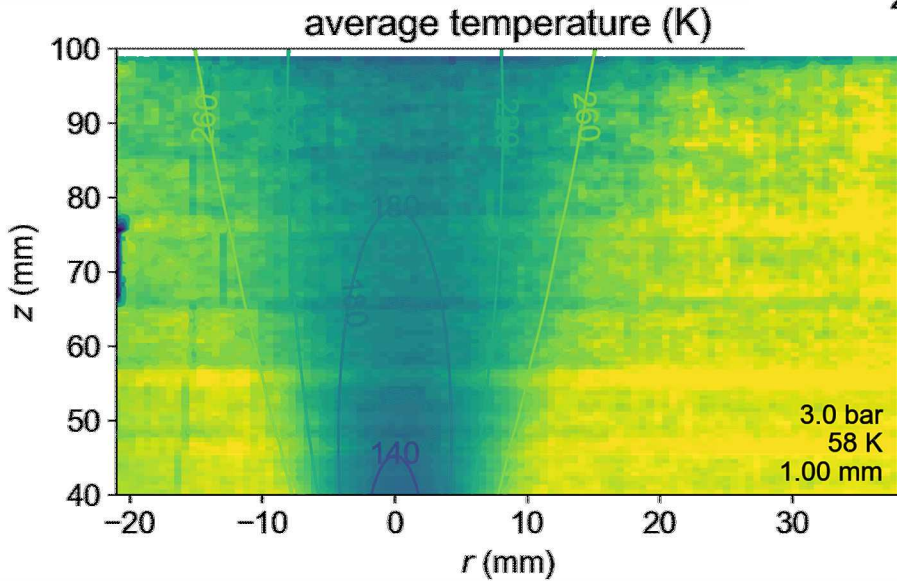
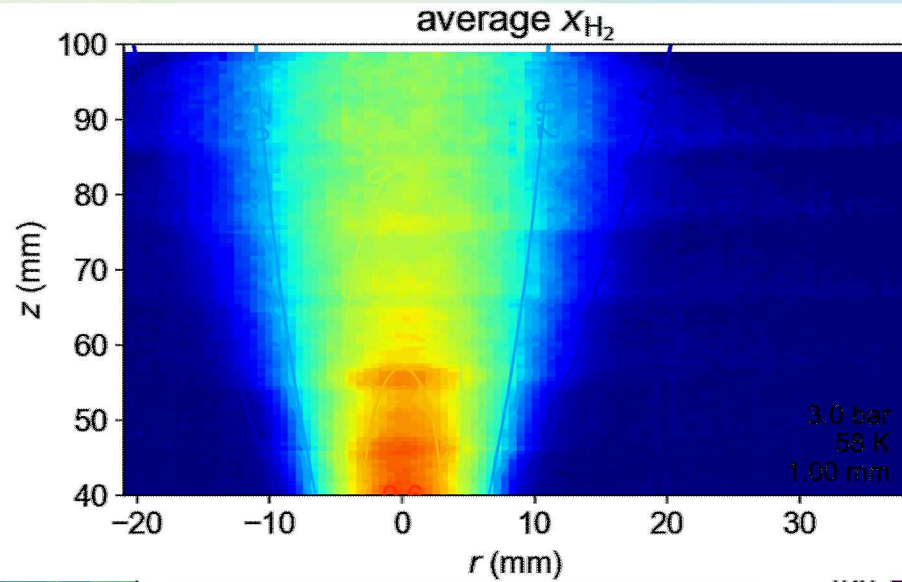
Several experimental campaigns have had variations in temperature, pressure, and nozzle size

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

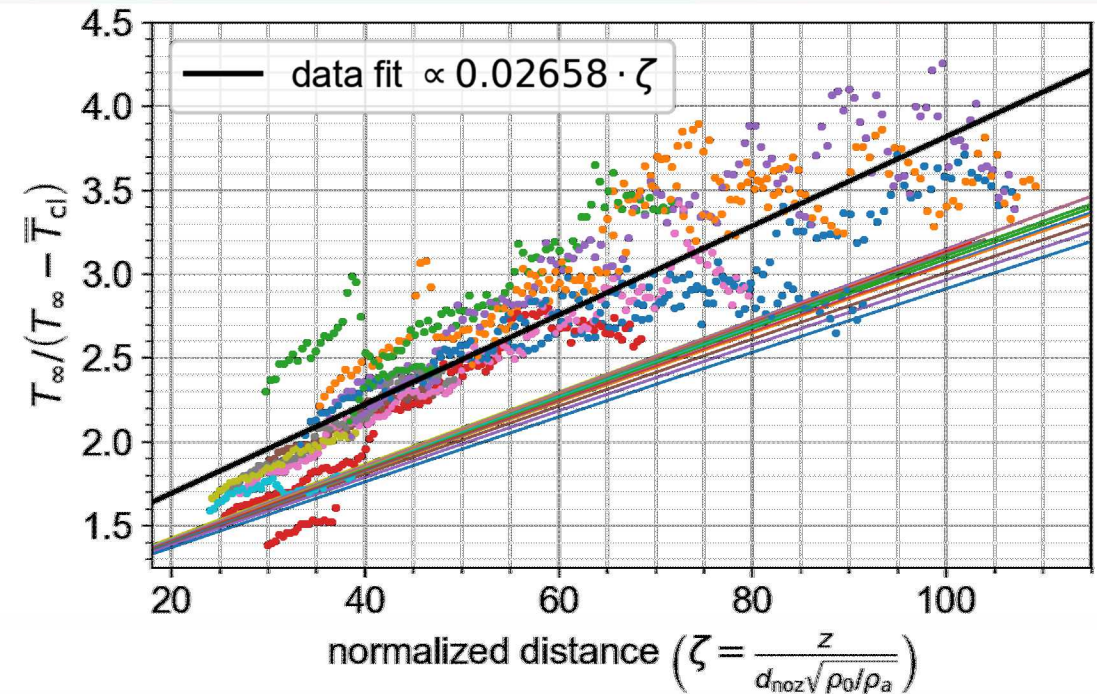
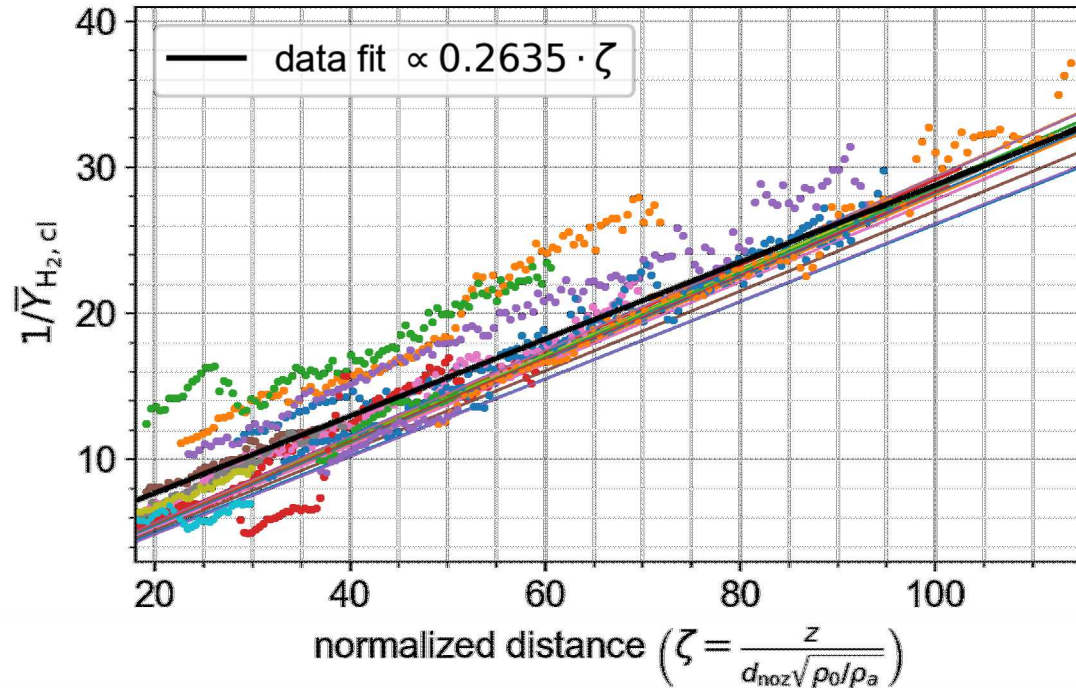
With PIV



In general, the model shows good agreement with the data



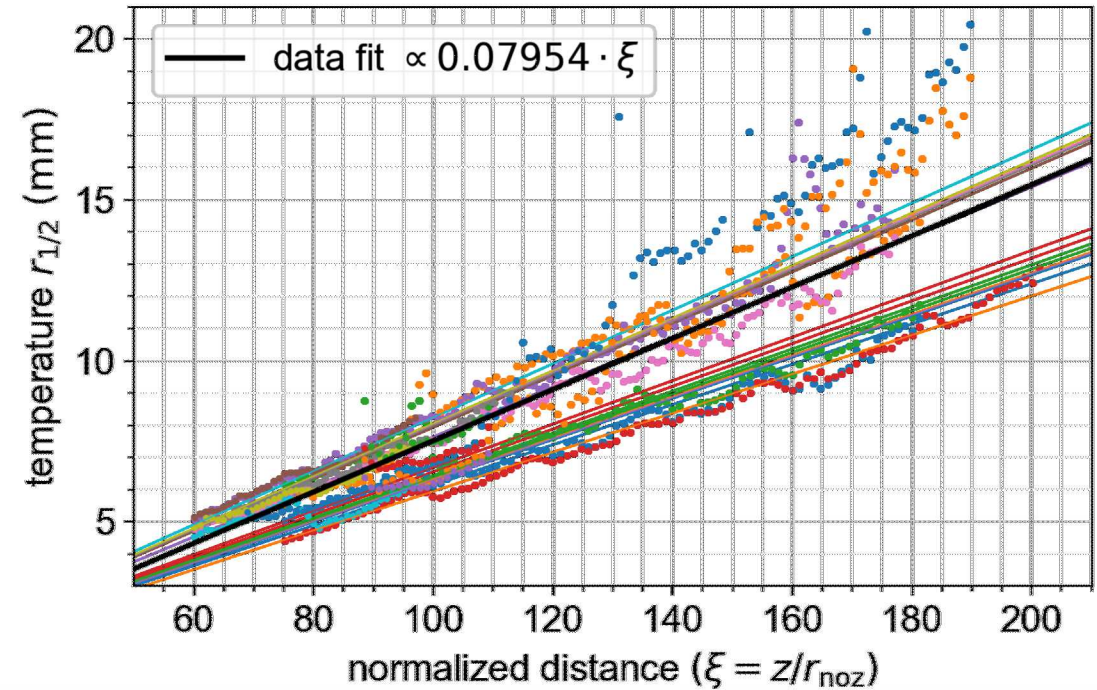
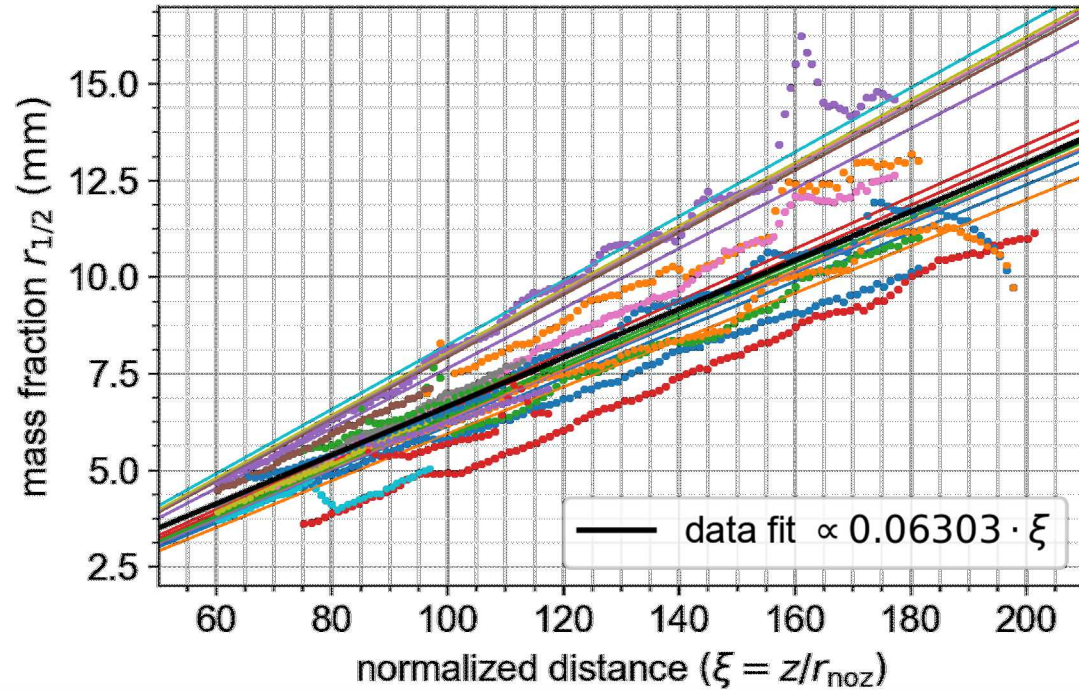
The centerline mass fraction and temperature decay linearly when plotted against the normalized distance



- Literature inverse mass-fraction decay rate: 0.21–0.271
- Model does not predict perfect collapse of the data
- Virtual origin seems to be further upstream than model for both temperature and mass fraction

• 2 bar, 58 K, 1.00 mm	• 4 bar, 54 K, 1.25 mm
• 3 bar, 56 K, 1.00 mm	• 4 bar, 45 K, 1.25 mm
• 4 bar, 53 K, 1.00 mm	• 3.0 bar, 58 K, 1.00 mm
• 5 bar, 50 K, 1.00 mm	• 3.0 bar, 82 K, 1.00 mm
• 2 bar, 61 K, 1.25 mm	• 3.5 bar, 55 K, 1.00 mm
• 2.5 bar, 51 K, 1.25 mm	• 4.0 bar, 40 K, 1.00 mm
• 3 bar, 51 K, 1.25 mm	• 4.0 bar, 63 K, 1.00 mm
• 3.5 bar, 55 K, 1.25 mm	

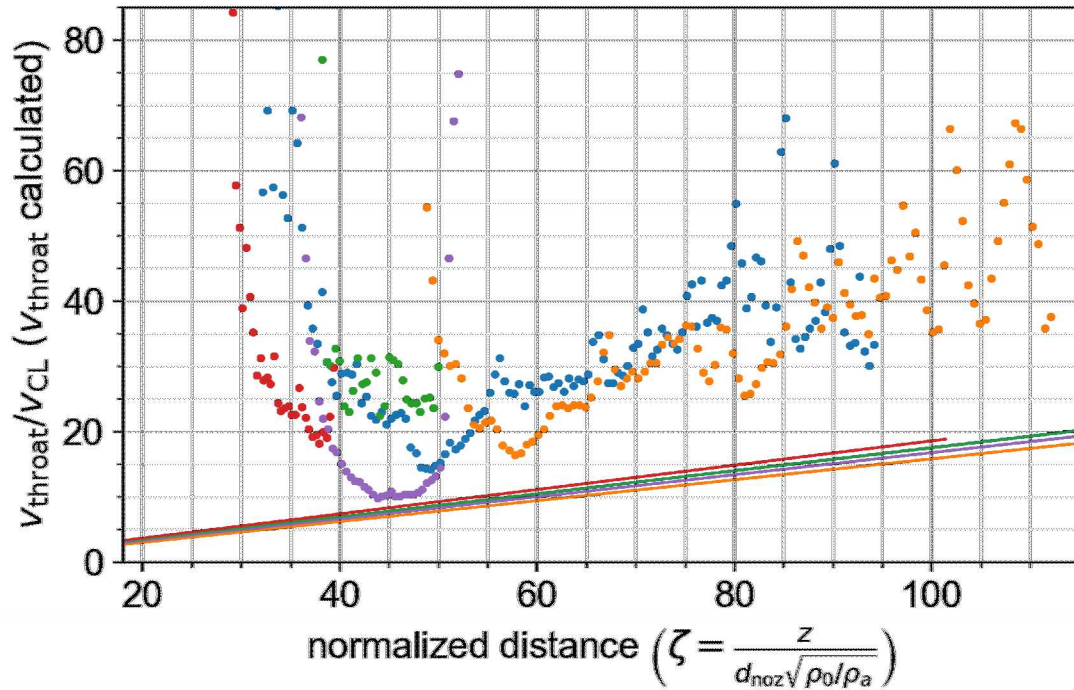
With two-dimensional images, we can also ensure that the widths of the jets are behaving as expected



- Literature mass-fraction half-width spreading rate: 0.1–0.11 mm
- Normalizing by radius of nozzle (as is done in the literature) does not allow model or experimental data to collapse

• 2 bar, 58 K, 1.00 mm	• 4 bar, 54 K, 1.25 mm
• 3 bar, 56 K, 1.00 mm	• 4 bar, 45 K, 1.25 mm
• 4 bar, 53 K, 1.00 mm	• 3.0 bar, 58 K, 1.00 mm
• 5 bar, 50 K, 1.00 mm	• 3.0 bar, 82 K, 1.00 mm
• 2 bar, 61 K, 1.25 mm	• 3.5 bar, 55 K, 1.00 mm
• 2.5 bar, 51 K, 1.25 mm	• 4.0 bar, 40 K, 1.00 mm
• 3 bar, 51 K, 1.25 mm	• 4.0 bar, 63 K, 1.00 mm
• 3.5 bar, 55 K, 1.25 mm	

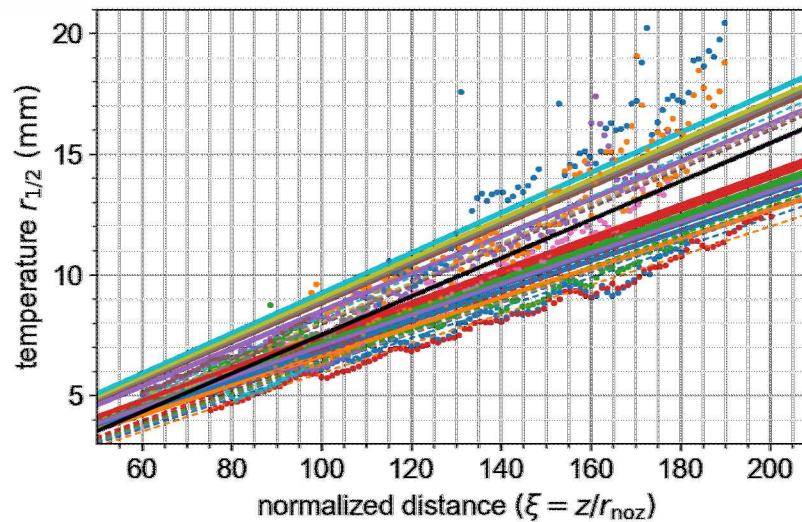
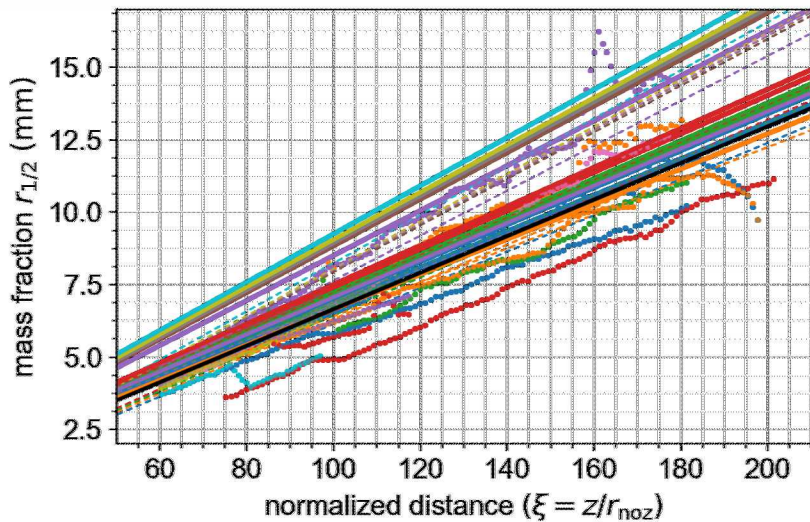
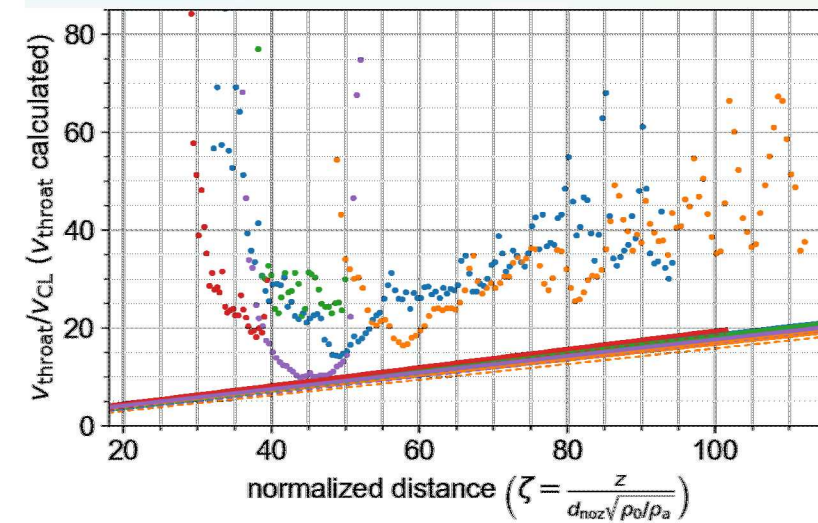
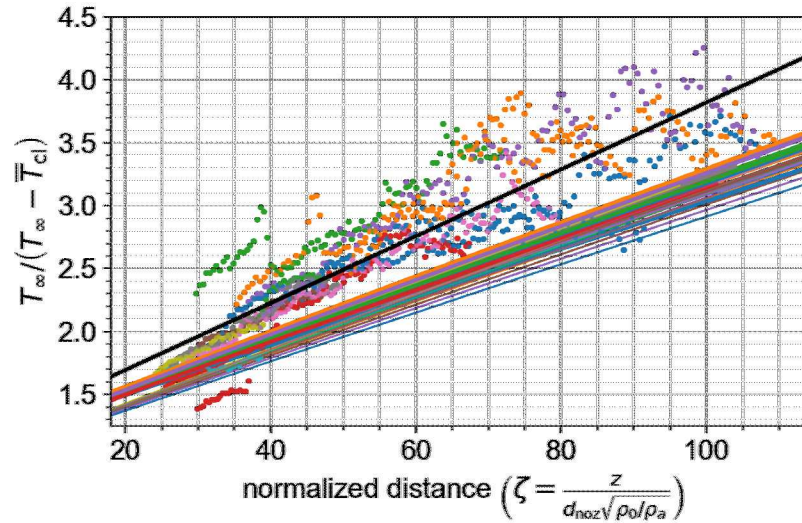
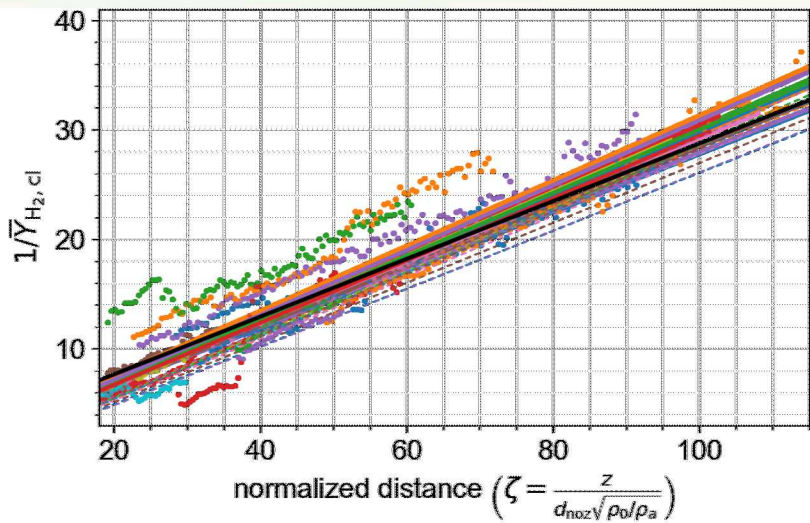
Centerline velocity data is much noisier, but also shows reasonable agreement with the model predictions



- 3.0 bar, 58 K, 1.00 mm
- 3.0 bar, 82 K, 1.00 mm
- 3.5 bar, 55 K, 1.00 mm
- 4.0 bar, 40 K, 1.00 mm
- 4.0 bar, 63 K, 1.00 mm

- Moisture not an ideal ‘particle’ for PIV (causes noise)
- Delay time between images (10 μs) appropriate for 40 m/s, but not much faster (close to nozzle)

By shortening the zone of flow establishment (empirical parameter), better model/data agreement is achieved for all parameters

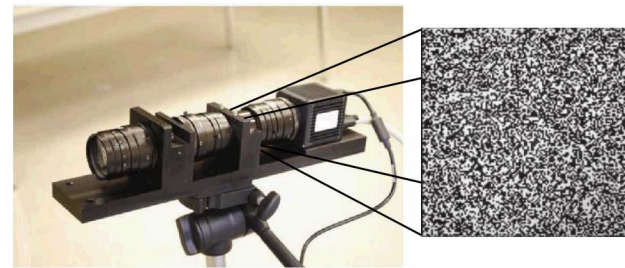


- Shortening zone of flow establishment shifts all model predictions to the left

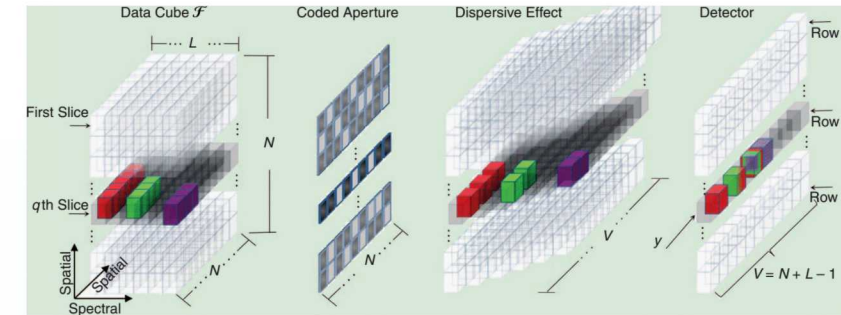
Future work: implement diagnostic to measure large-scale release dispersion

- Enable characterization and modeling of
 - Interactions with ambient (i.e. wind)
 - Pooling
 - Evaporation from LH₂ pools
- **Currently developing an imaging diagnostic** for outdoor and large-scale experiments
 - Quantitative concentration measurements
 - 2- or 3-dimensions
 - Video frame rates
 - Portable
- Will apply diagnostic to normally occurring outdoor releases (e.g., venting after LH₂ fill)
- Dedicated validation experiments at well-controlled facilities next fiscal year (FY19)

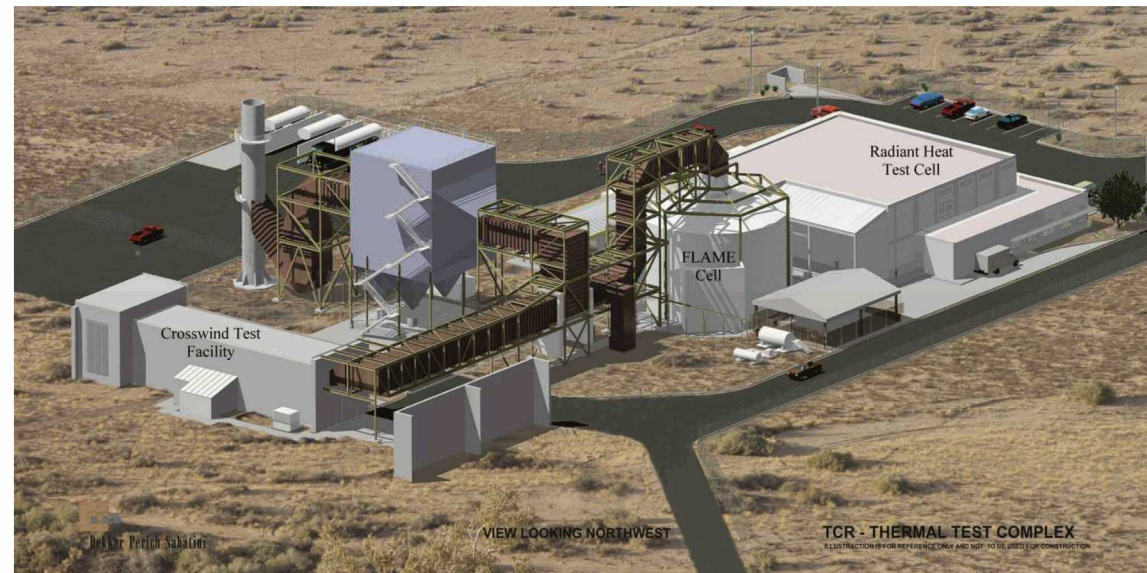
Pursuing coded-aperture Raman imaging



[dx.doi.org://10.1117/12.919292](https://dx.doi.org/10.1117/12.919292)



[dx.doi.org://10.1109/MSP.2013.2278763](https://dx.doi.org/10.1109/MSP.2013.2278763)



Summary

- Used advanced imaging diagnostics (planar laser Raman imaging, PIV) to measure cryogenic hydrogen mixing with air and warming
- Centerline mass fraction decay rate for cryogenic hydrogen similar to warm hydrogen
- Centerline temperature also increases linearly against normalized distance
- Mass-fraction, temperature, and velocity profiles are self-similar, Gaussian, and match model predictions with reasonable accuracy
- Virtual origin is further upstream than original model prediction – model was adjusted
- Model can be used to predict cryogenic hydrogen dispersion with good confidence

Future Work:

- Implement model into risk assessment toolkit HyRAM
- Perform truly simultaneous Raman/PIV experiments using different laser wavelengths for each diagnostic to give further insight into turbulent entrainment
- Develop diagnostic for outdoor and large-scale experiments
- 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)

Acknowledgements

- Funding support from:
 - United States Department of Energy, Energy Efficiency & Renewable Energy, Fuel Cell Technologies Office, Safety, Codes, and Standards subprogram managed by Laura Hill
 - Industry support including the OEM Group at the California Fuel Cell Partnership, Linde, and Shell
- Team members:
 - 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