



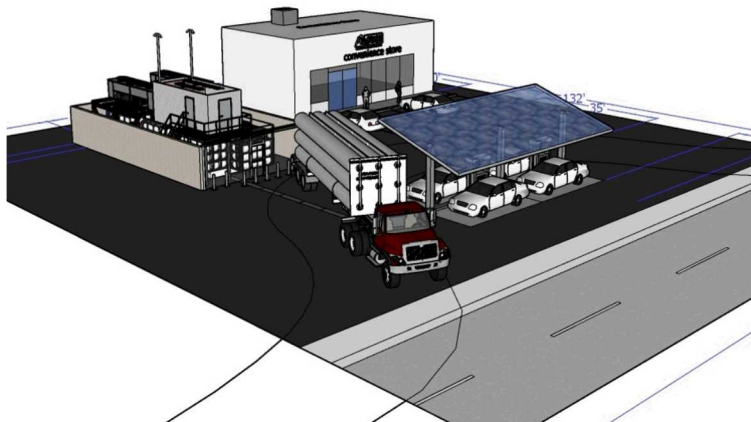
Hydrogen behavior research as a foundation for codes & standards

Ethan S. Hecht and Bikram Roy Chowdhury

Current separation distances for liquid hydrogen systems in the U.S. are based on consensus rather than a comprehensive scientific basis

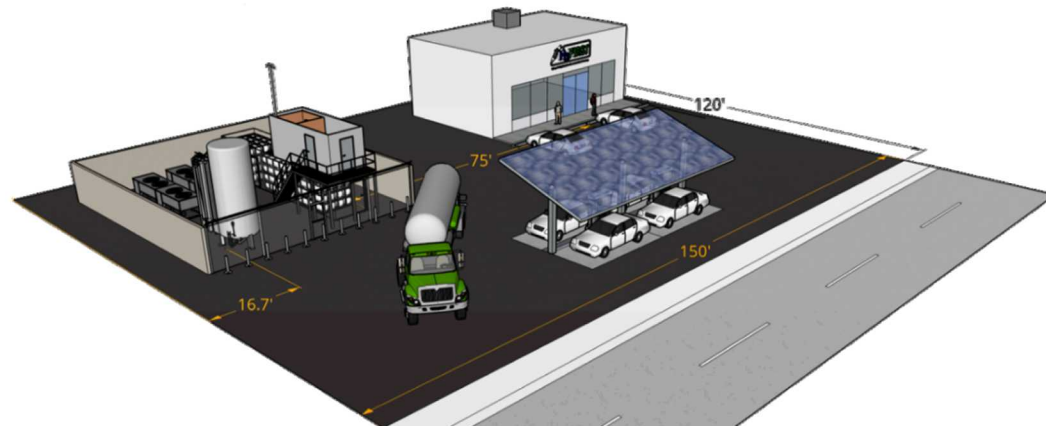
Compressed H₂ storage

- Previous work by Sandia led to science-based gaseous H₂ separation distances



Liquid H₂ storage

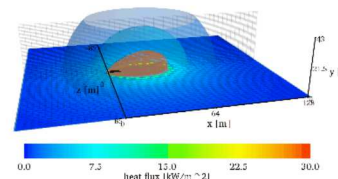
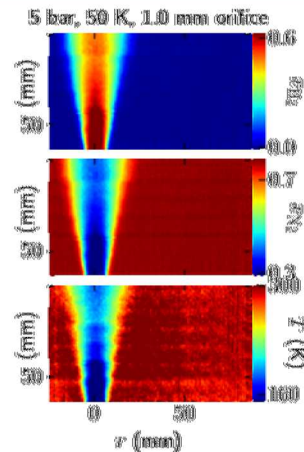
- Even with credits for insulation and fire-rated barrier wall, 75 ft. offset to building intakes and parking make footprint large



DOE goal: By September 30, 2022, identify ways to reduce the siting burdens that prohibit expansion of hydrogen fueling stations, through hydrogen research and development that enables a 40% reduction in station footprint, compared to the 2016 baseline of 18,000 square feet

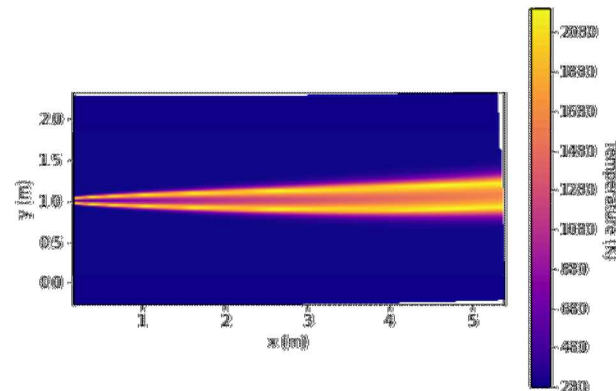
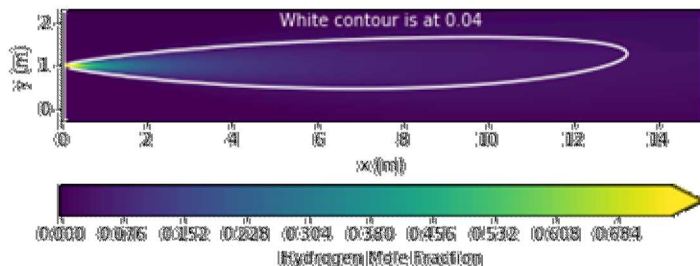
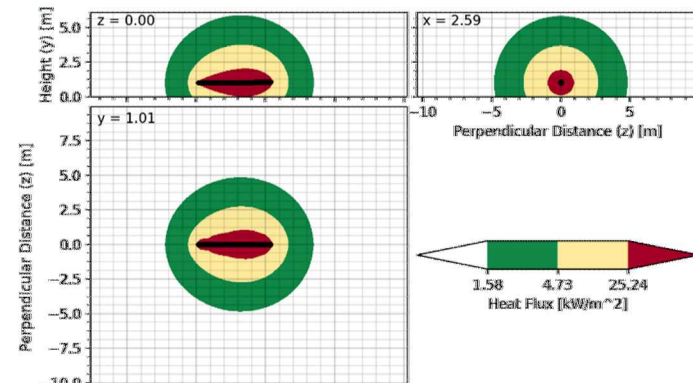
Sandia H₂ Safety Codes and Standards research includes coordinated activities that facilitate deployment of hydrogen technologies

- Hydrogen Behavior
 - **Develop and validate scientific models** to accurately predict hazards and harm from liquid releases, flames, etc.
- Quantitative Risk Assessment, tools R&D
 - **Develop integrated methods and algorithms** enabling consistent, traceable, and rigorous QRA (Quantitative Risk Assessment) for H₂ facilities and vehicles
- Enable Hydrogen Infrastructure through Science-based Codes and Standards
 - **Apply QRA and behavior models to real problems** in hydrogen infrastructure and emerging technology
 - **Facilitate updates to NFPA 2** through deep technical analyses



A variety of validated physical models are used in HyRAM – current focus on developing validated models for LH

- Unignited dispersion
 - Distance to certain concentration
- Flame model
 - Temperature field
 - Heat flux field
- Overpressure for delayed



Python modeling packages have been updated this year and include the validated ColdPLUME model

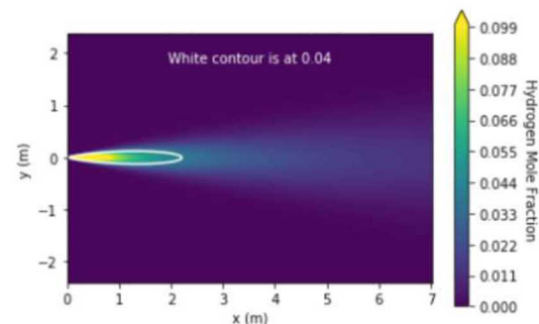
- Received open source software license for HyRAM 2.0
- Validated version of ColdPLUME included
- Intuitive object oriented structure
- Updated physics and QRA submodules
- Python package implementation with documentation

➤ Code organization, ease of use and documentation critical for outside development and use

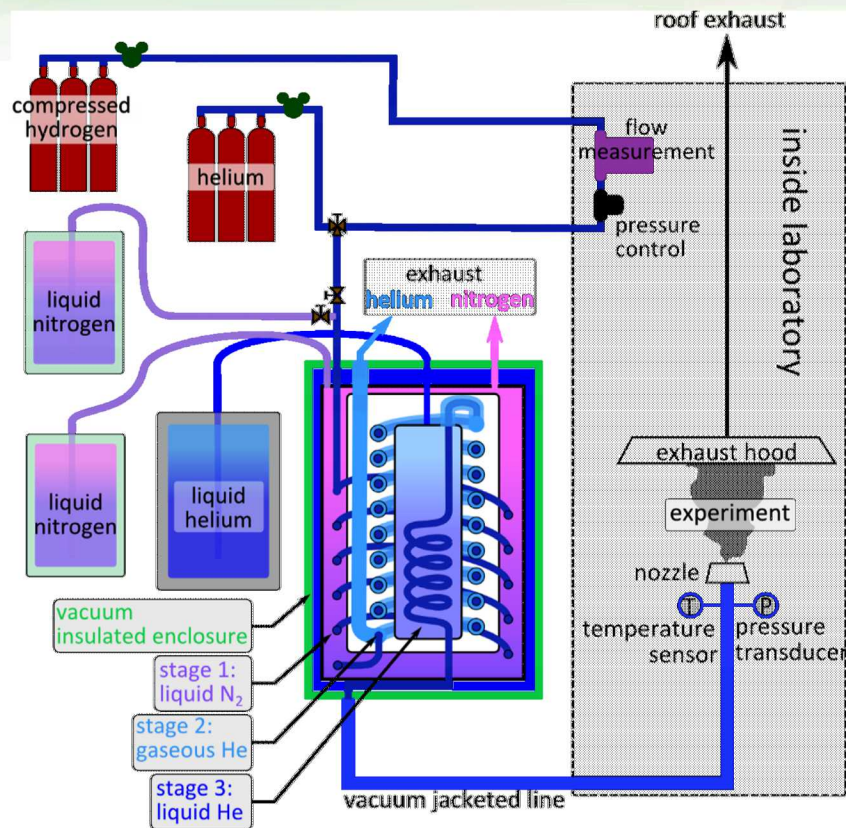
```
In [1]: from altRAM import phys
```

```
In [2]: H2 = phys.Gas(T = 40, P = 5e5);  
air = phys.Gas(T = 295, P = 101325, species =  
['air']);  
orifice = phys.Orifice(d = 0.001);  
release = phys.Jet(H2, orifice, air);  
release.solve(Ymin = .001);  
release.plot_moleFrac_Contour();
```

solving for the plume... done.



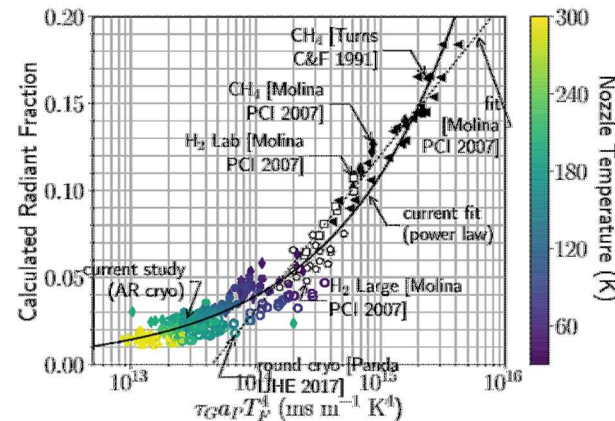
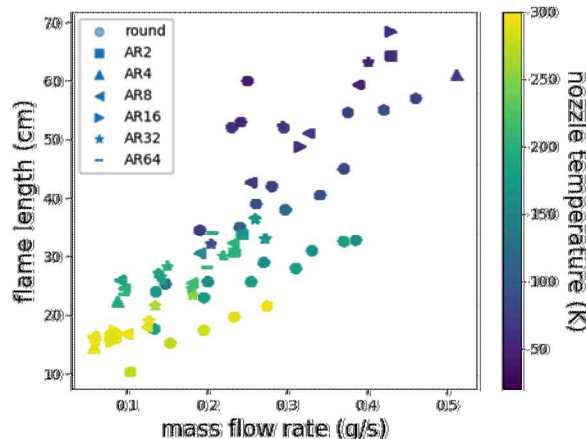
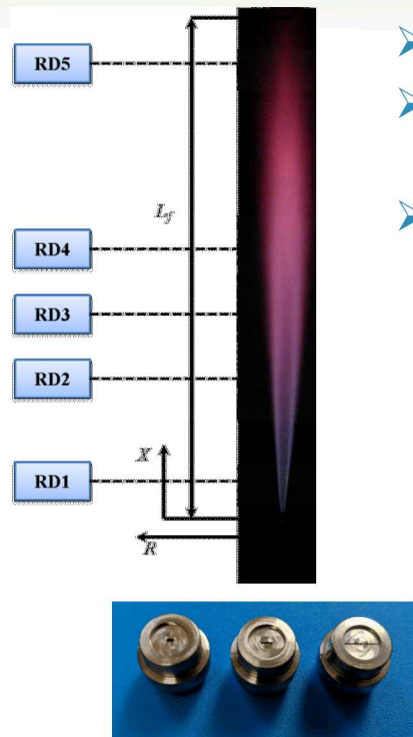
Our laboratory experiment uses a heat exchanger to liquefy hydrogen



- Gaseous hydrogen is liquefied using liquid nitrogen and liquid helium
- Flow rate is measured as a gas using a thermal mass flow meter
- Nozzle pressure is controlled upstream of heat exchanger
- Temperature at nozzle is measured
- Measurements of flames and unignited dispersion

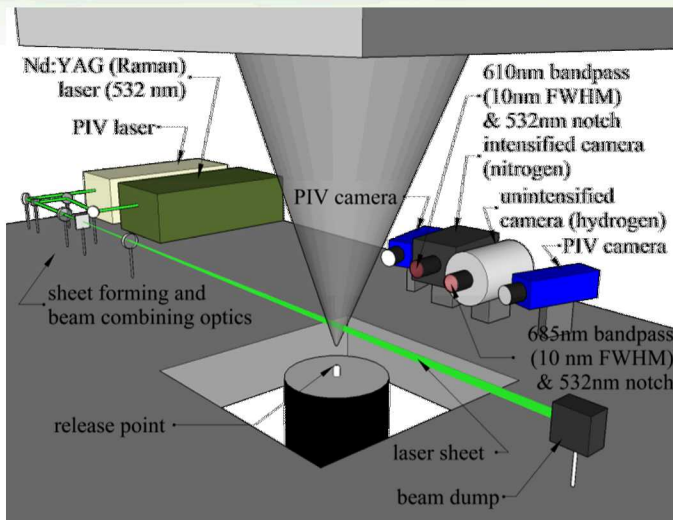
We measured and have correlations to calculate the flame length and radiant heat flux for gaseous and cryogenic hydrogen jet flames

- Hydrogen flames have lower radiant heat flux compared to hydrocarbon flames
- An increase in radiant fraction is observed for colder H₂ jets (for a given nozzle size and pressure) due to longer flame residence time (more mass flux)
- Aspect ratio does not significantly affect flame length or radiant heat flux



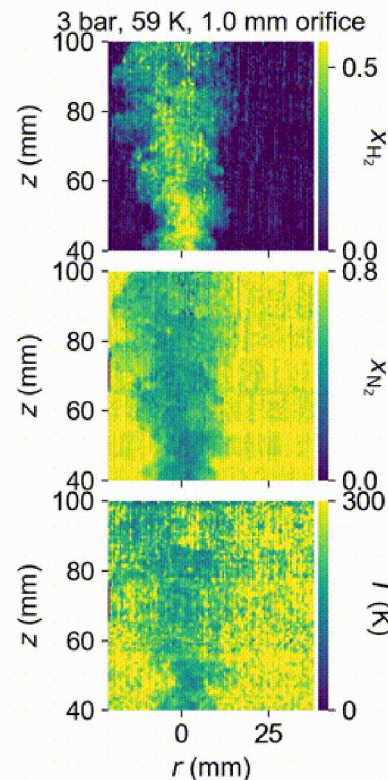
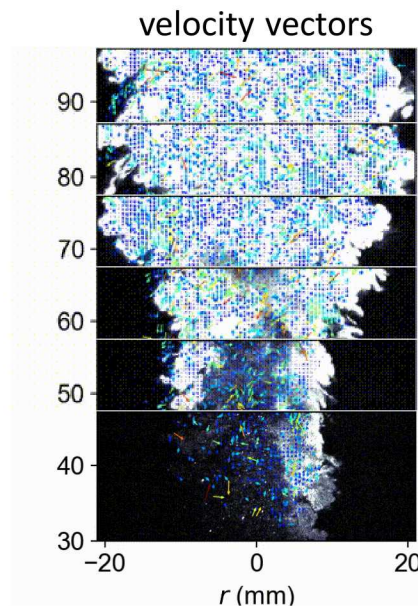
$$\text{radiant heat flux} \propto (\text{radiant fraction})(\text{mass flow})(\text{heat of combustion})(\text{transmissivity})$$

H_2 - N_2 Raman imaging and particle imaging velocimetry are used to measure concentration, temperature, and velocity of cryogenic H_2

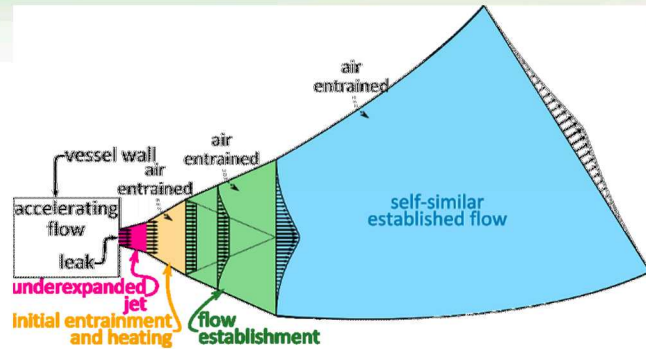


Independent model parameters:

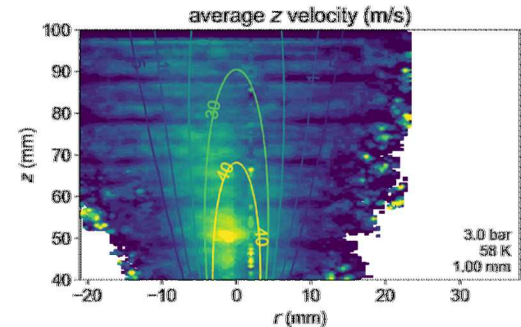
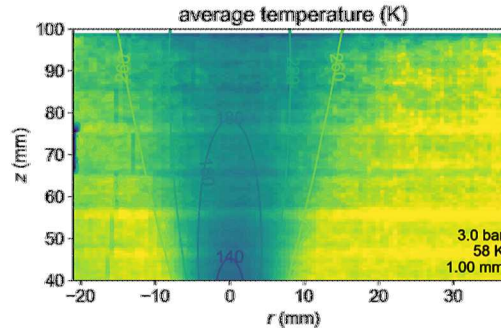
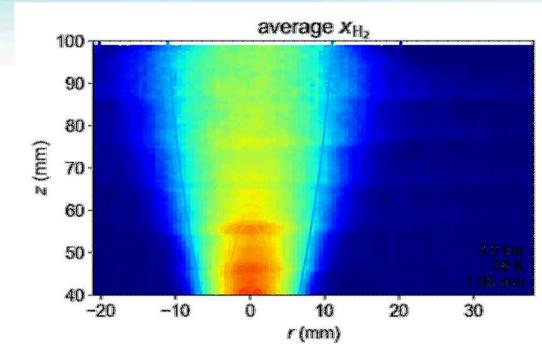
- ✓ T - temperature
- ✓ x - mole fraction
- ✓ v - velocity
- ✓ B - halfwidth (both velocity and concentration)



The ColdPLUME model shows good agreement with the lab-scale data

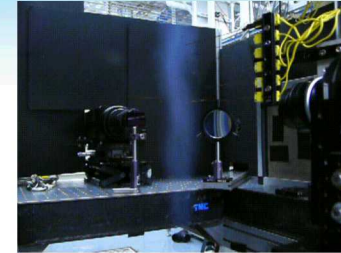
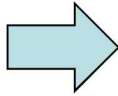


- Experimental results shown by shading and thick, dashed lines
- ColdPLUME model results are thin, solid lines

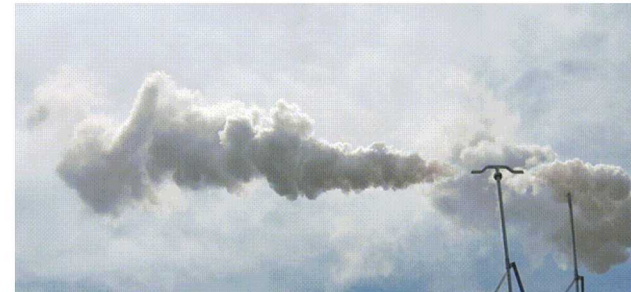


➤ Model accurately simulates mole fraction, temperature, and velocity -- can be used as a predictive tool

This fiscal year, we are planning larger outdoor experiments

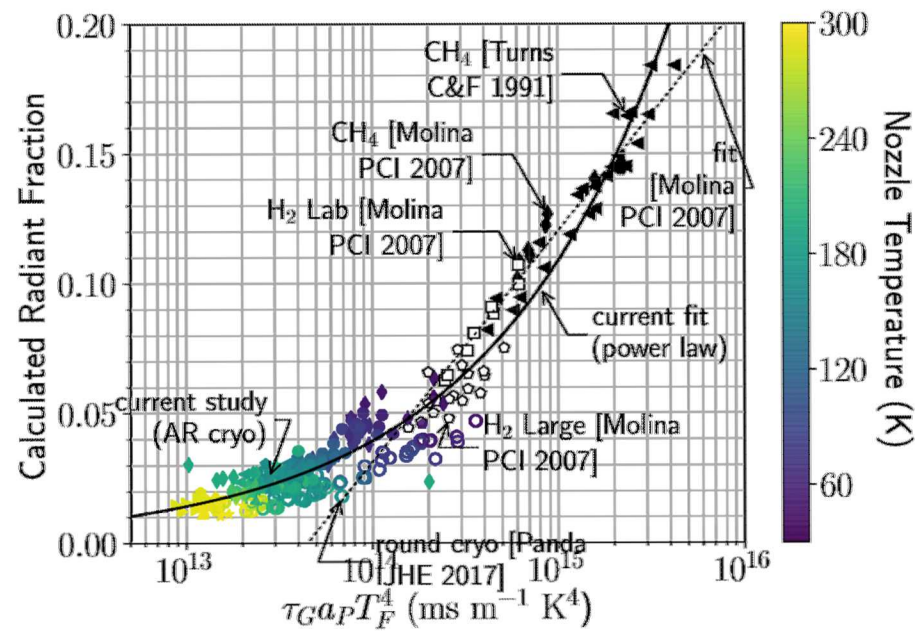


- Supporting the CGA G-5.5 testing task force measurements of LH₂ vent stack flames
- Working with colleagues at LLNL to measure dispersion from LH₂ vent stacks



Experiments coordinated by the CGA G-5.5 testing task force will determine the radiant fraction from hydrogen vent stack flames

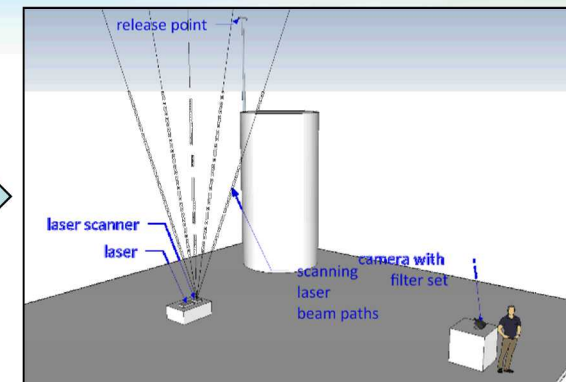
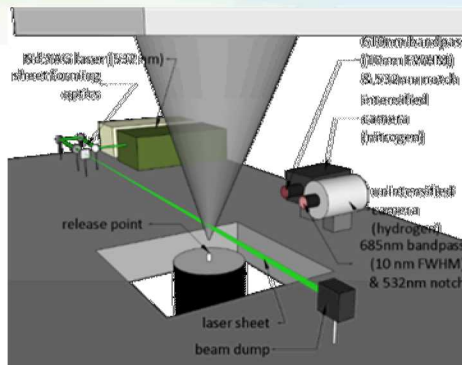
- Intended to inform CGA G-5.5 specifications for truck vent stacks
- Vertical flames from LH₂ vent stack similar to truck vent
- Variations in flow rate and wind conditions
- Radiant fraction for hydrogen much lower than other gases (no carbon that makes soot)
- Sandia providing hardware and data analysis support



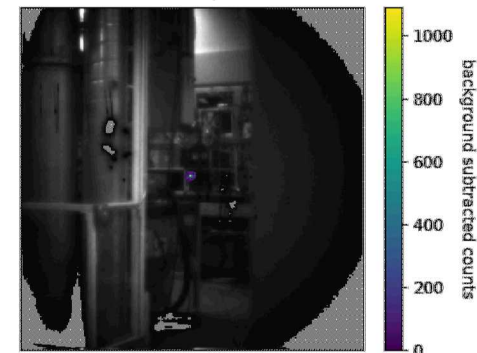
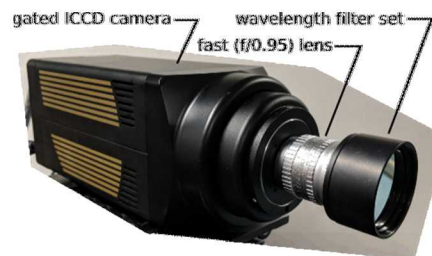
$$\text{radiant heat flux} \propto (\text{radiant fraction})(\text{mass flow})(\text{heat of combustion})(\text{transmissivity})$$

Our lab-scale diagnostic is being modified to study LH_2 vents and large-scale experiments

- Uniquely fast optics enable collection of small Raman signal
- Imaged hydrogen from 40 foot standoff distance in the laboratory
- Demonstrated acceptable signal to noise for large-scale diagnostic
- Observed nearly 30 degree field of view (20 ft scene from 40 ft distance)

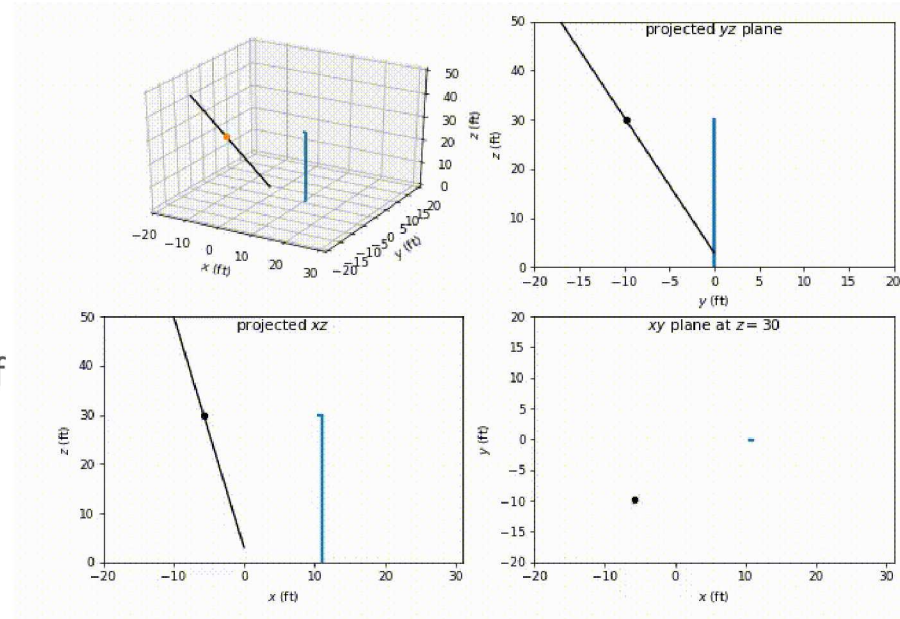


Raman signal overlaid on laboratory scene



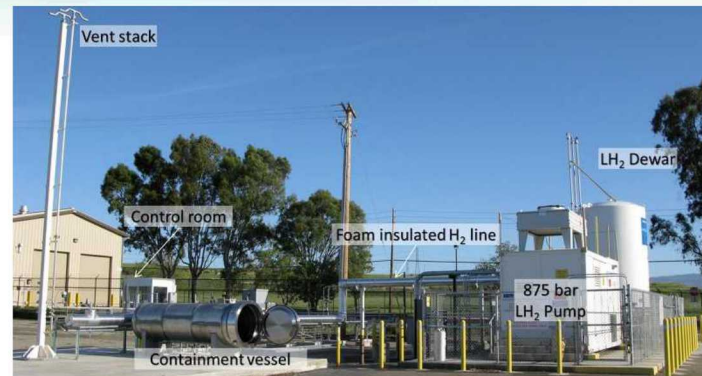
We are finalizing the method of illuminating the large-scale scene

- On-camera accumulation will provide a complete snapshot of the plume with reasonable resolution
- Effective background light suppression is key (both sunlight and illumination source that reflects off of condensed water vapor)
 - Time gating
 - Spectral gating
- High-powered light source required to excite as many molecules as possible
 - High-power laser scanning in space
 - Concentrations measured along a series of lines
 - 1st generation: galvanometer scanning a 10 Hz laser
 - 2nd generation: high speed polygonal scanning using pulse-burst laser



We are working with our colleagues at LLNL to perform LH₂ vent stack releases

- Additional temperature sensors along vent stack to validate internal flow model
- Replacing bull-horn with single outlet to enable model comparisons
- Variations in temperature, flow-rate, and external conditions (e.g. wind) in experiments
- Comparison to NREL sensor approach for some tests
- Late summer 2019



[Petitpas & Aceves, IJHE 43: 18403-18420:
https://doi.org/10.1016/j.ijhydene.2018.08.097](https://doi.org/10.1016/j.ijhydene.2018.08.097)

- Heaters and pump enable a wide range of flow rates and temperatures at vent stack
- Proximity to SNL enables experiments to be run on short notice (when weather is right – for a range of conditions)



Remaining challenges this FY: Executing outdoor experiments

Get approvals to perform experiments at LLNL

- Modification of vent stack
- Install additional instrumentation

Ensure safety when operating laser outdoors

- follow ANSI Z136 standard
- Non-visible (UV light) helps

Perform experiments during a range of weather conditions

- High- and low-wind conditions
- Humidity differences



Future work: Additional large-scale experiments

Need experiments to characterize:

- Pooling
- Evaporation from LH_2 pools
- Details of plume interactions with ambient air
- Impact of barrier walls as a mitigation

Solutions:

- Well-controlled experiments at Sandia facilities
- Partner with others, applying diagnostic at remote locations (e.g. European colleagues involved with the PreSLHy project)





Summary

- **Relevance:** Address lack of safety data, technical information relevant to development of safety codes & standards.
- **Approach:** Develop and validate scientific models to accurately predict hazards and harm from hydrogen (with a focus on liquid hydrogen) releases and subsequent combustion. Generate validation data where it is lacking. Provide a scientific foundation enabling the development/revision of codes & standards.
- **Technical Accomplishments (FY19):**
 - Updated Python modeling packages (including ColdPLUME) for ease of use
 - Measured radiative heat flux and flame properties for non-circular nozzles
 - Demonstrated good signal to noise for large-scale diagnostic
 - Planned illumination and data collection strategy for large-scale diagnostic
- **Future work:**
 - Perform vent-stack dispersion experiments at LLNL LH₂ pad
 - Support CGA G-5.5 testing task force measurements of vent stack flames
 - 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)