SAND2015-1341PE

Cryogenic Hydrogen Release Modeling Validation – Update for Hydrogen Safety Panel

Ethan Hecht, Chris LaFleur, Isaac Ekoto

Sandia National Laboratories

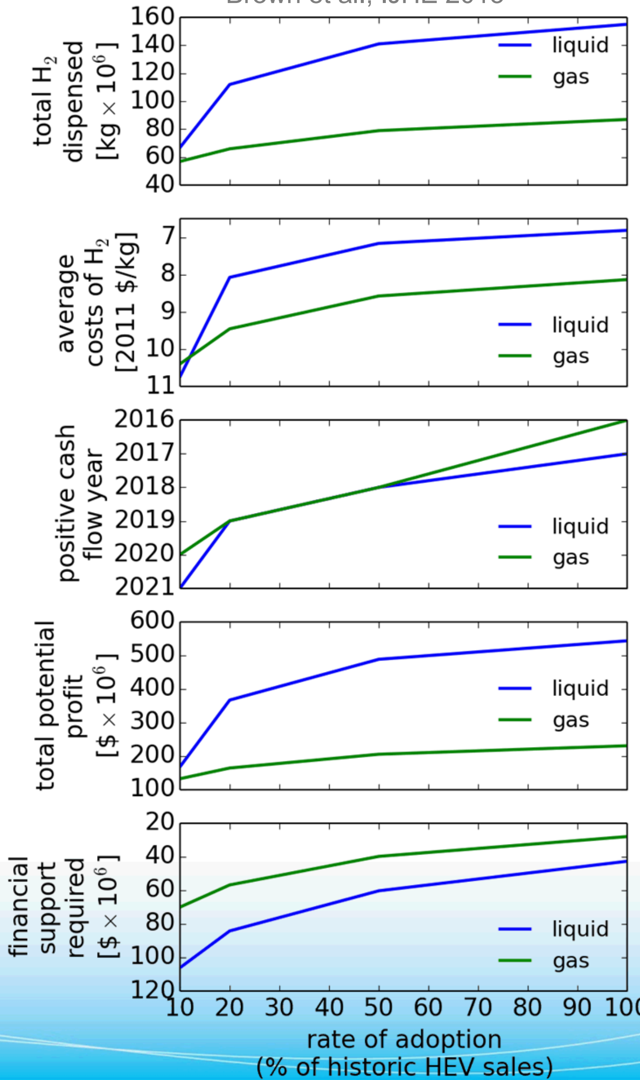
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

Liquid hydrogen stations have been found to be more economically favorable than gaseous stations

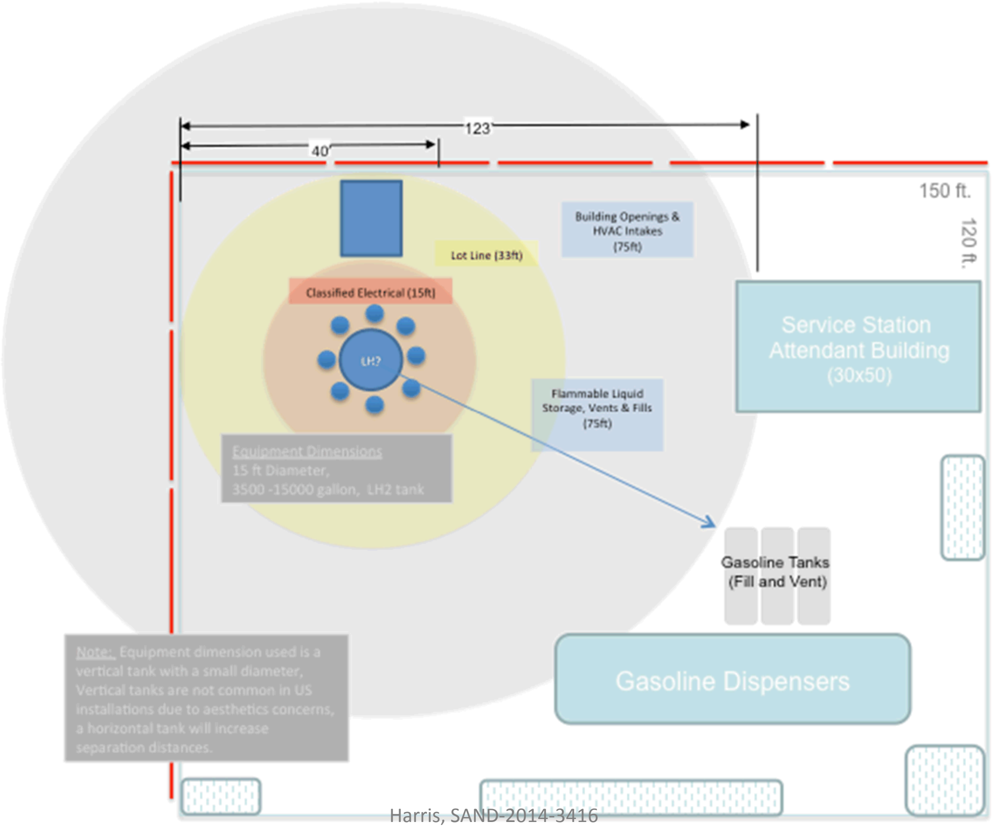
As compared to gaseous stations, liquid storage stations have:

- Larger storage capacity
- Lower costs for product
- Similar positive cash flow year
- Higher potential profit
- Larger return on investment (although more investment is required)

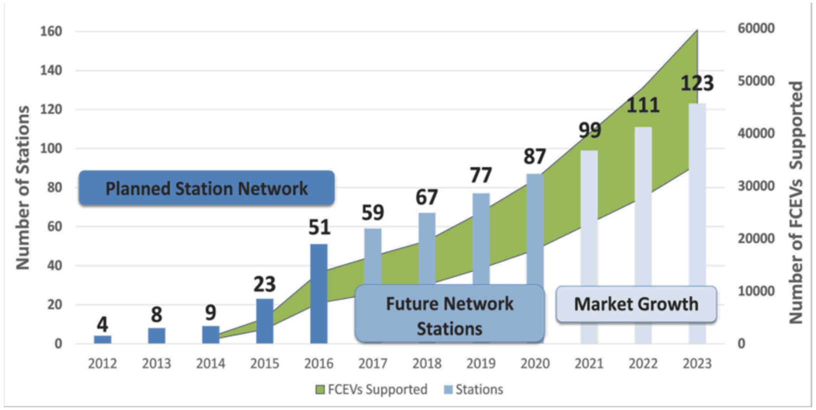
Brown et al., IJHE 2013



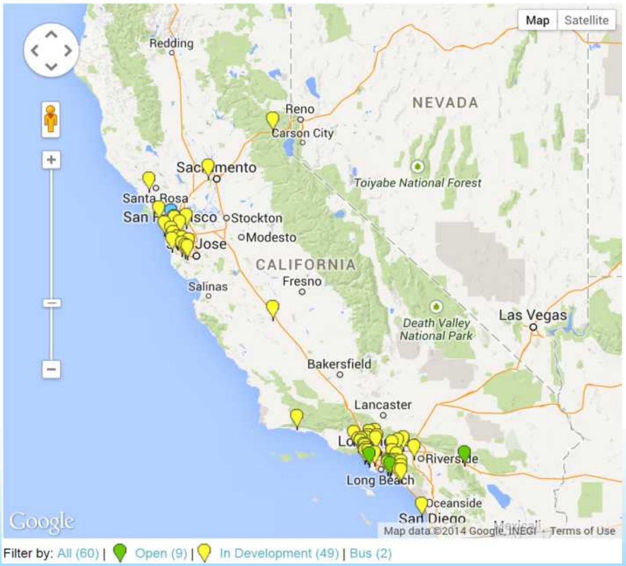
Standoff distances in NFPA 2 for liquid hydrogen stations are often prohibitively large



Harris, SAND-2014-3416



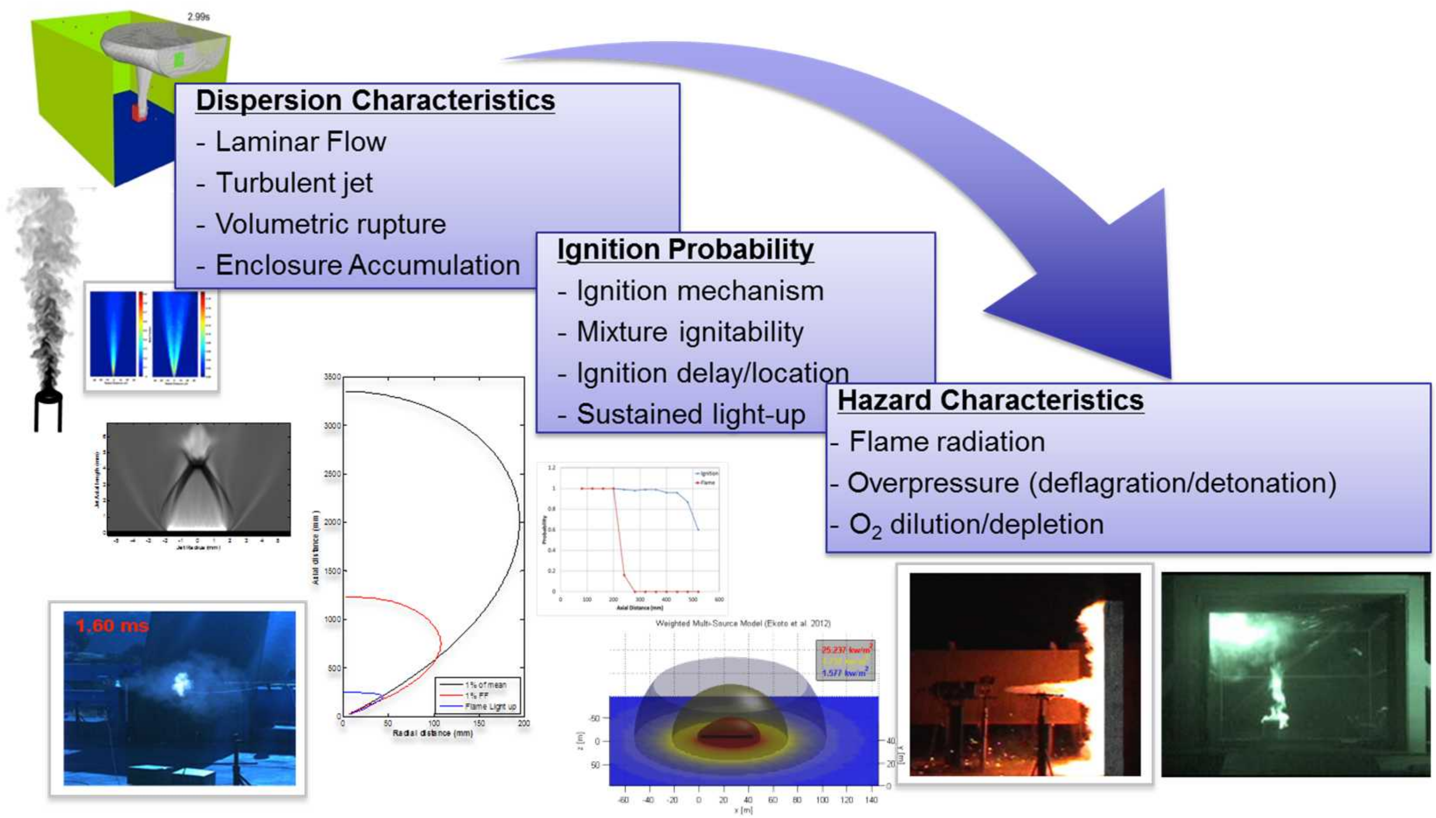
A California Road Map: The Commercialization of Hydrogen Fuel Cell Vehicles, CalFCP, July 2014



http://www.cafcp.org/stationmap

Of 70 stations surveyed (out of 343), none met the NFPA 2 Ch. 6 separation distance requirements. Harris, SAND-2014-3416

Previous modeling of releases from gaseous hydrogen storage have informed the fire code



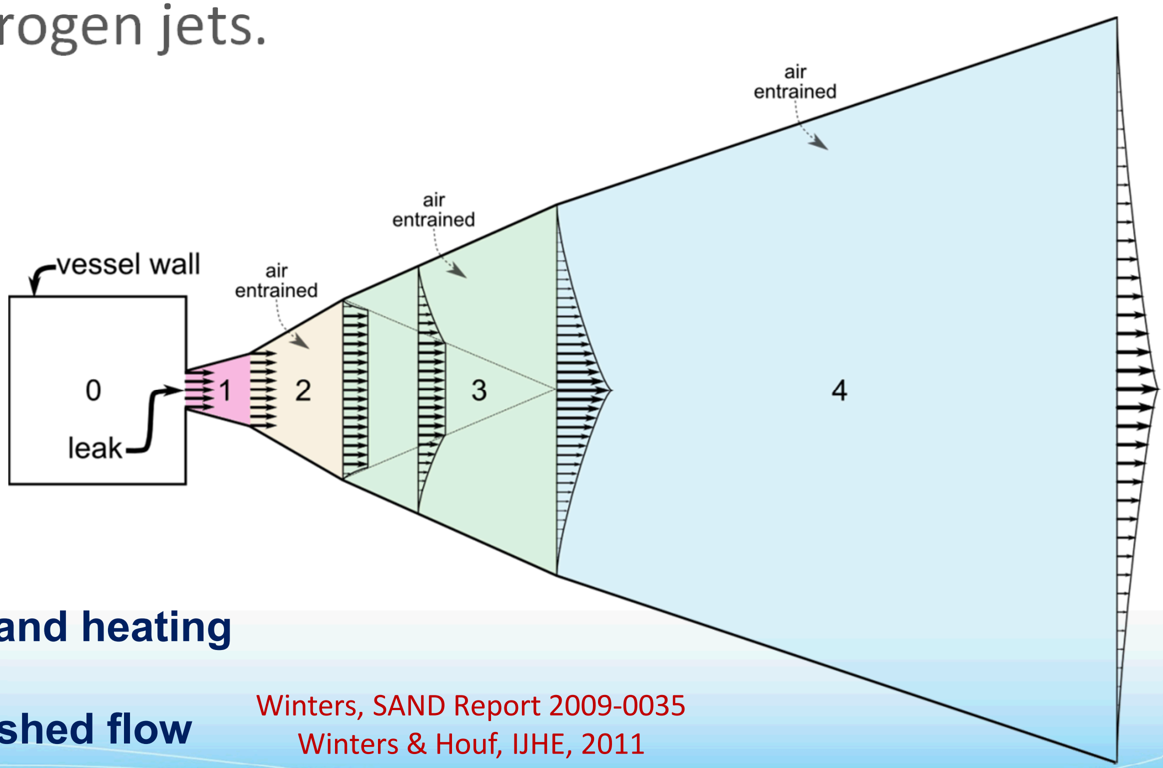
Risk requires a **Release**, then **Ignition**, forming a **Hazard**, causing **Harm**

- We ***quantify*** each of these events using models
- **Purple** events are quantified with statistical models, **Red** with behavior models

Cold hydrogen behavior experiments for model development/validation

Objective:

- The primary objective of the low-temperature H_2 delivery system is to study flow and flame characteristics that result from cryogenic hydrogen jets.

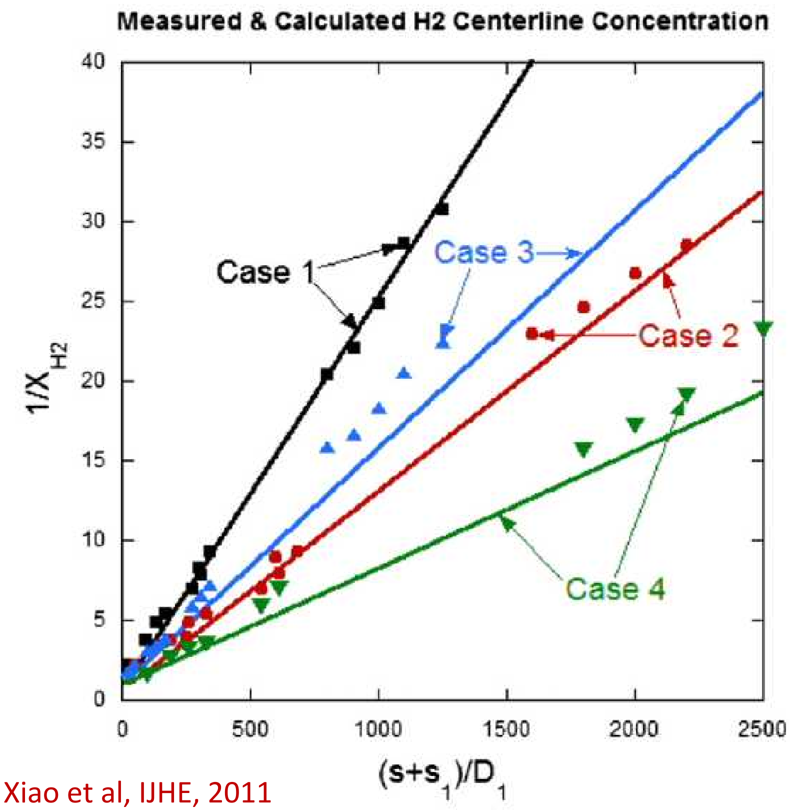


- **Zone 0: accelerating flow**
- **Zone 1: underexpanded jet**
- **Zone 2: initial entrainment and heating**
- **Zone 3: flow establishment**
- **Zone 4: self-similar, established flow**

Winters, SAND Report 2009-0035
Winters & Houf, IJHE, 2011
Houf & Winters, IJHE, 2013

Model results compare favorably to experiments from Karlsruhe Institute of Technology

Case	Reservoir pressure [MPa]	Reservoir temperature [K]	Leak diameter [mm]
1	1.7	298	2
2	6.85	298	1
3	0.825	80	2
4	3.2	80	1

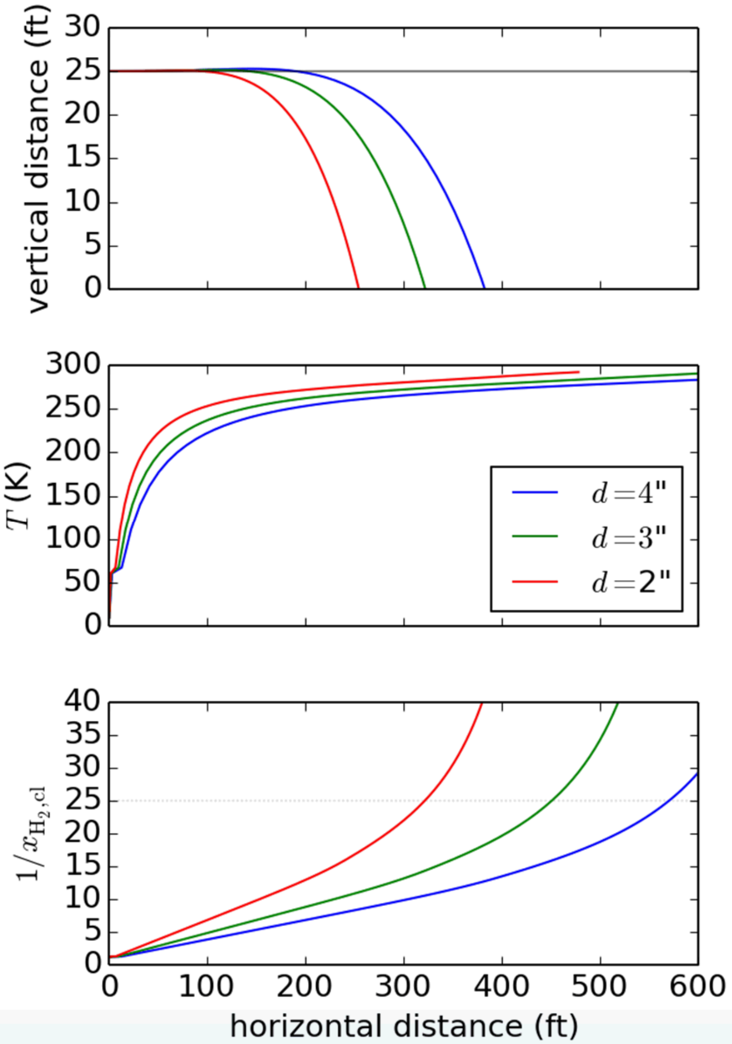


Xiao et al, IJHE, 2011
Houf & Winters, IJHE, 2013

However, no well-controlled validation data is available at lower temperatures where multi-phase flows are expected (i.e., T < 77 K)

Regardless of leak size, heavy jet falls towards the ground

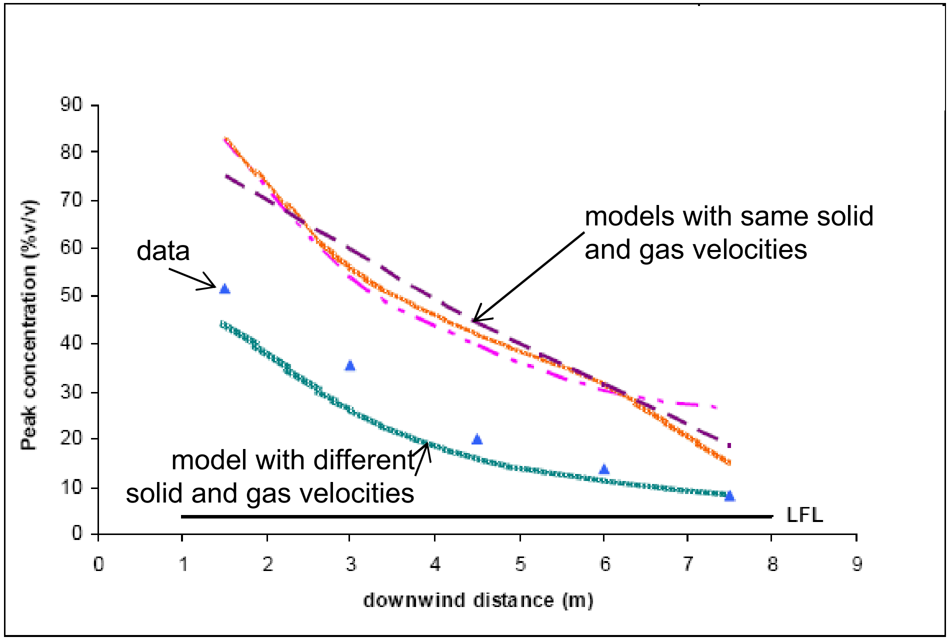
- Storage pressure = 180 psi
- Release (saturation) temperature = 20 K
- Release angle = 0º
- Release height = 25 ft



Clear need to develop jet-impingement model to account for spread along the ground

Multi-phase behavior is important—particularly for high-humidity conditions

Liquid and vapor phases have different velocities due to density differences — slip models have captured these effects in CFD simulations.



HSL Measurements: Sample probes

Hooker et al, ICHS, 2011

ADREA-HF CFD Simulations

Giannissi et al, ICHS, 2013

Substantial differences in model results suggest 2-phase effects cannot be neglected for LH2 releases

Experiments had poor control of release and environmental boundary conditions, which are needed for suitable benchmark data

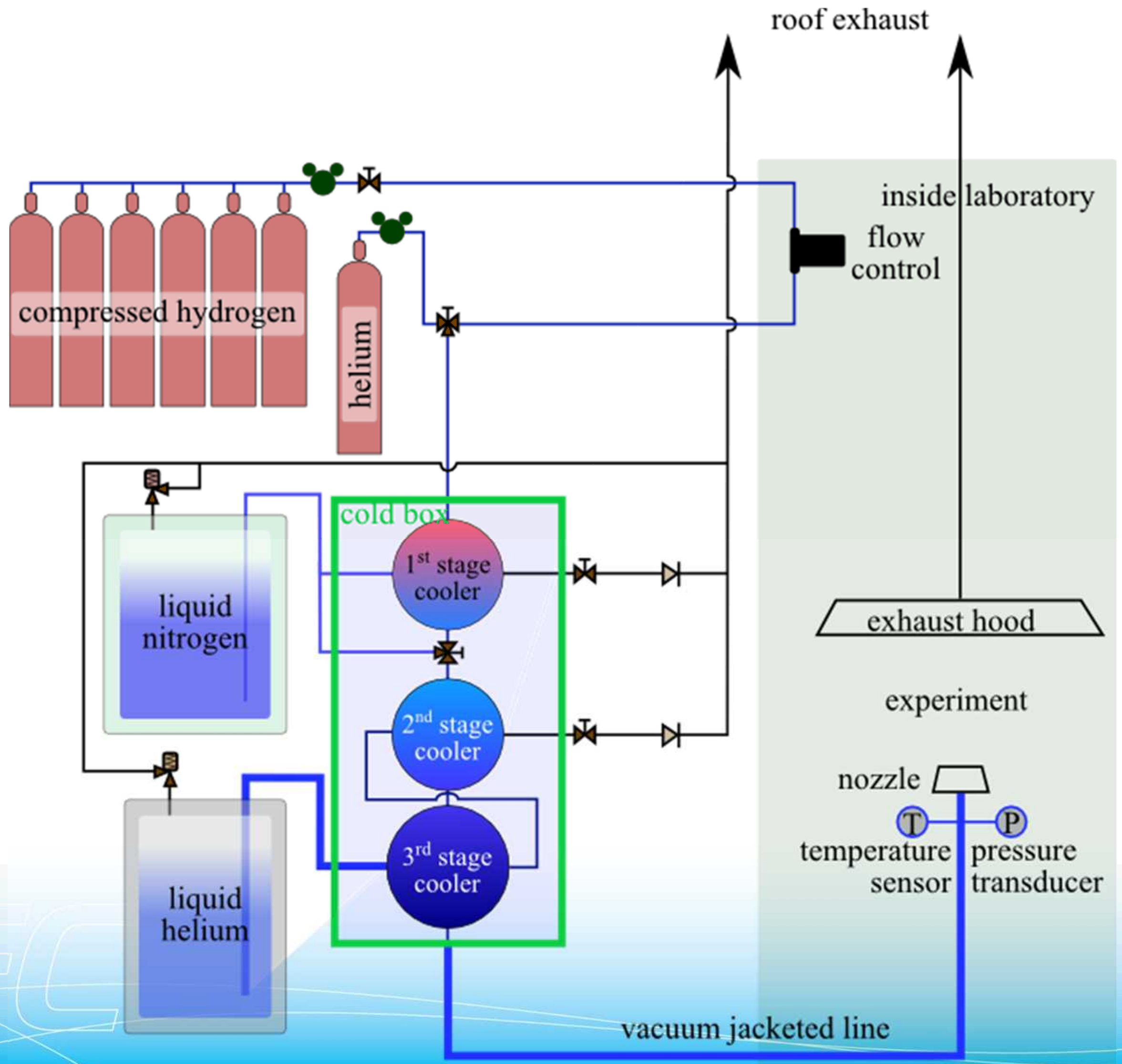
Description of Work

- Integrate a three-stage heat-exchanger into the existing Turbulent Combustion Laboratory infrastructure
- Heat-exchanger system can reduce the temperature of gaseous hydrogen to the target temperature
  - potential to generate cold gas, mixed-phase, or possibly liquid flows
  - cold hydrogen flows through a custom nozzle
- Follow the template used previously to characterize high--pressure gaseous hydrogen releases:
  - Perform Rayleigh scattering, PIV, and schlieren imaging
    - characterize concentrations and velocities of unignited plumes
  - Use well-characterized, focused laser as ignition source
    - determine light-up boundary
- Develop/validate reduced-order engineering models that can predict unintended release characteristics from liquid hydrogen storage systems due to equipment failures

Schedule

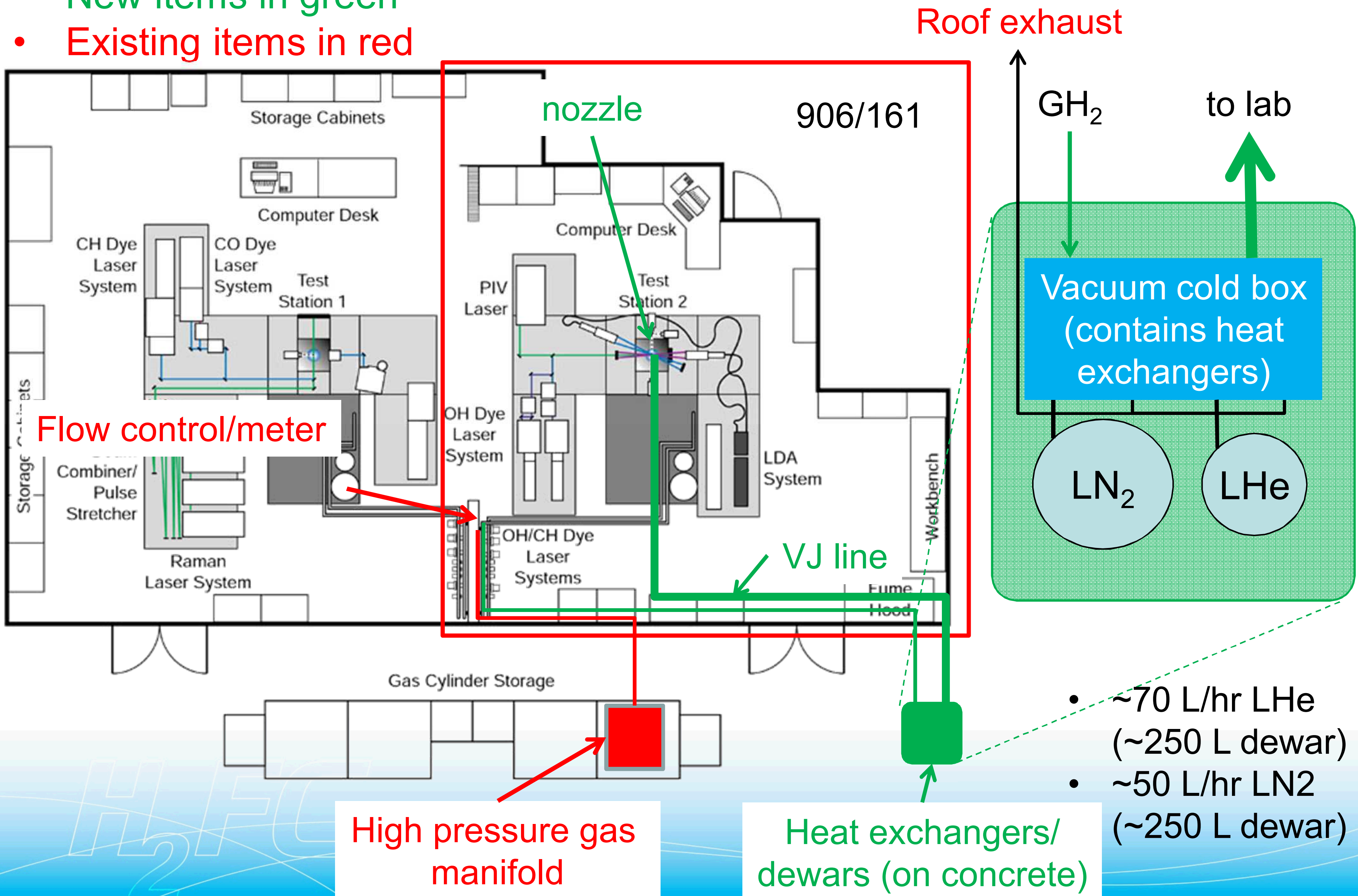
- 2015: Construct and test cold hydrogen vapor releases platform; vertical orientation (target temperature: 30 K)
- 2016:
  - Cold plume release data (2 nozzles, 6 pressures, 6 temperatures)
  - Develop/validate reduced-order cold-plume model for integration into QRA framework
- Future Work:
  - Test model performance for larger scale releases that are representative of "real-world" scenarios
  - Follow-on large-scale testing of controlled release of cryogenic vapor and liquid phase hydrogen at an outdoor test facility
  - Horizontal plume, impingement studies (plume interaction with surfaces, such as ground and barrier walls), ignition of cold plumes, bulk storage behavior in an exposure fire, large-scale validation experiments

Only a single vacuum line with a small quantity of cryogenic hydrogen penetrates into the lab



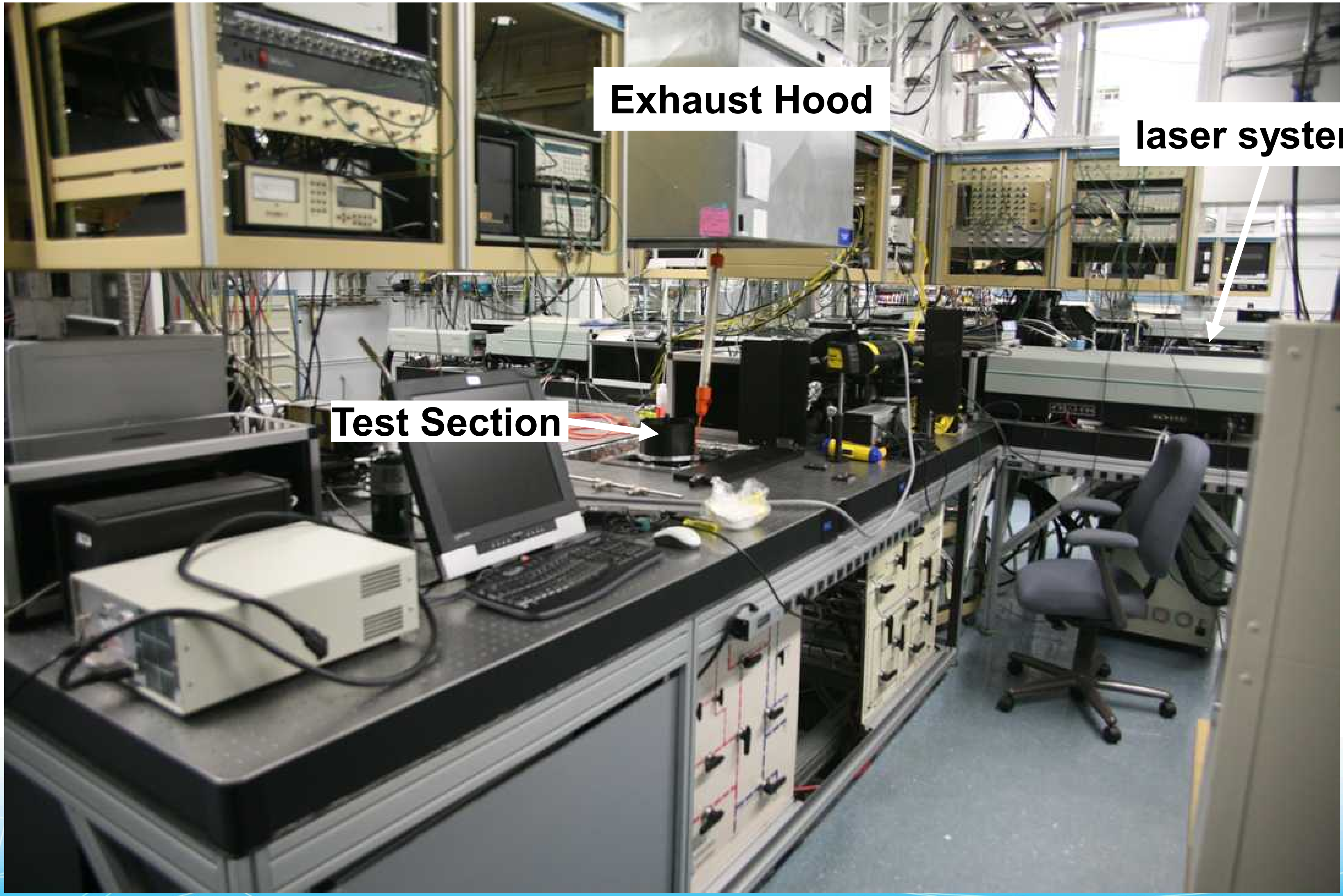
Turbulent Combustion Laboratory

- New items in green
- Existing items in red

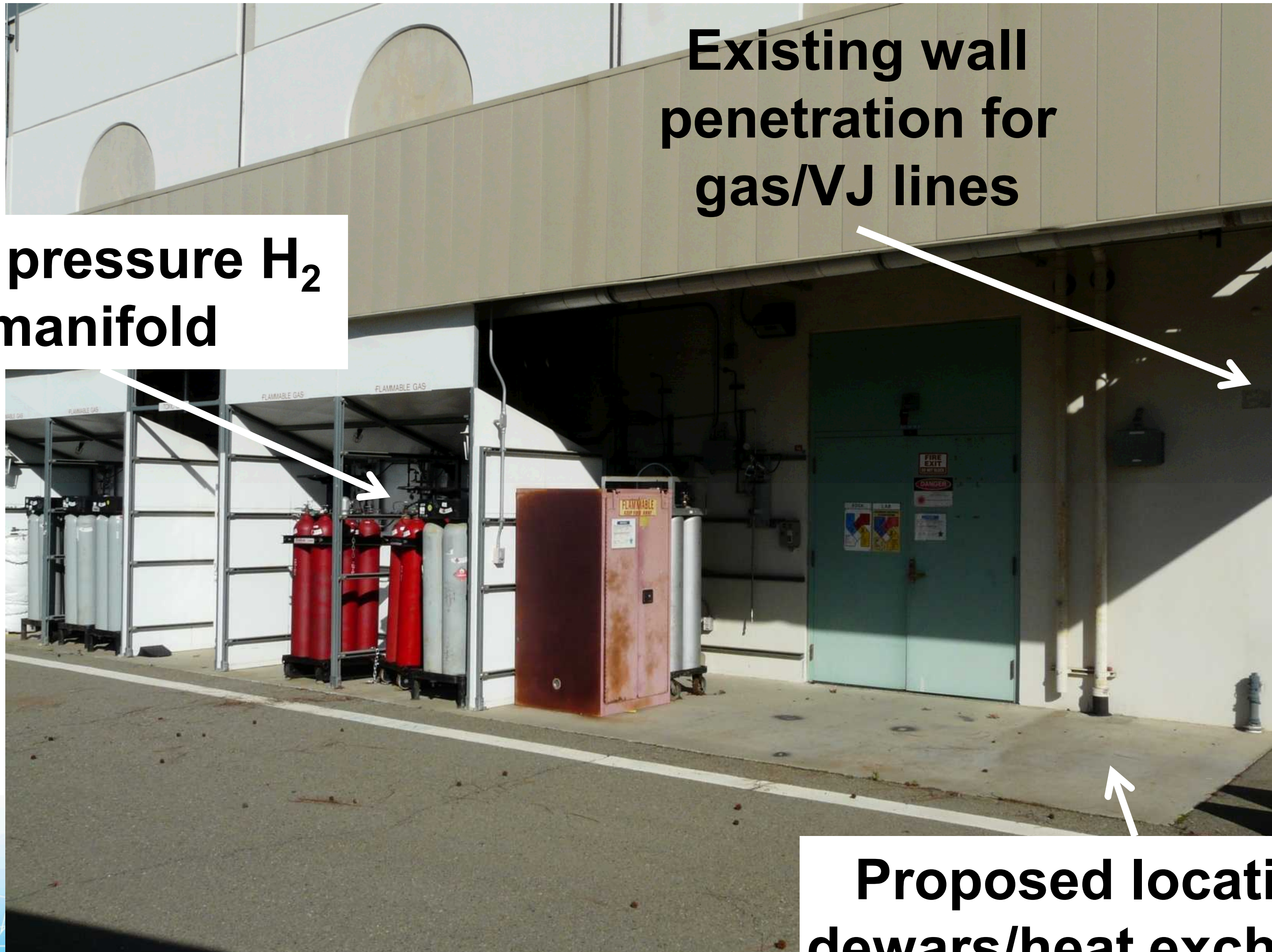


- ~70 L/hr LHe (~250 L dewar)
- ~50 L/hr LN2 (~250 L dewar)

Turbulent Combustion Laboratory: current lab setup



Turbulent Combustion Laboratory: planned modifications

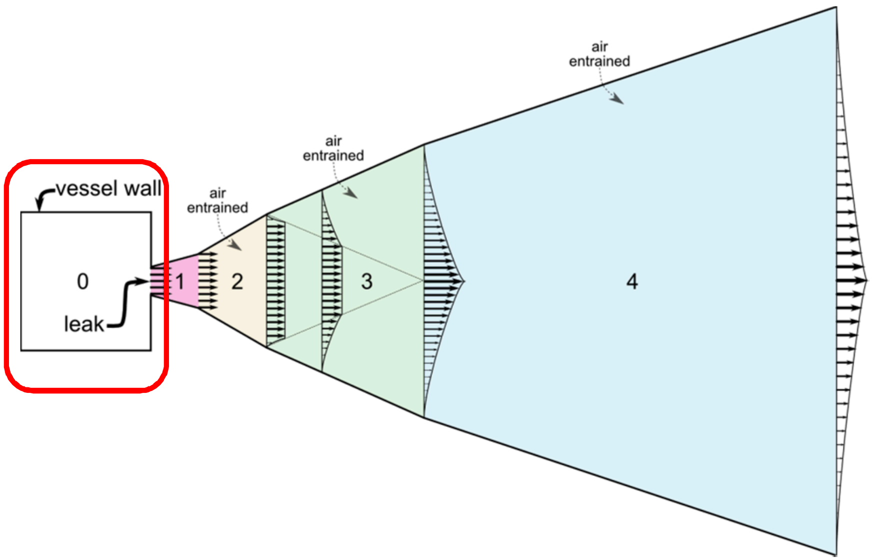


Acknowledgements

- United States Department of Energy Fuel Cell Technologies Office, under the Safety, Codes, and Standards subprogram element managed by Will James
- Thanks to the other members of the H_2 Safety, Codes, and Standards team - Daniel Dedrick, Chris San Marchi, and Katrina Groth

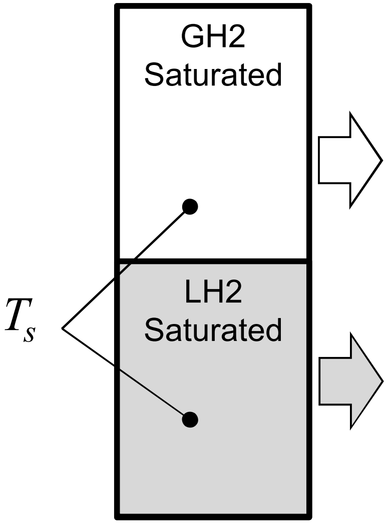
Backup

Accelerating flow (leak) develops from saturated storage conditions



- conserved energy with isentropic expansion

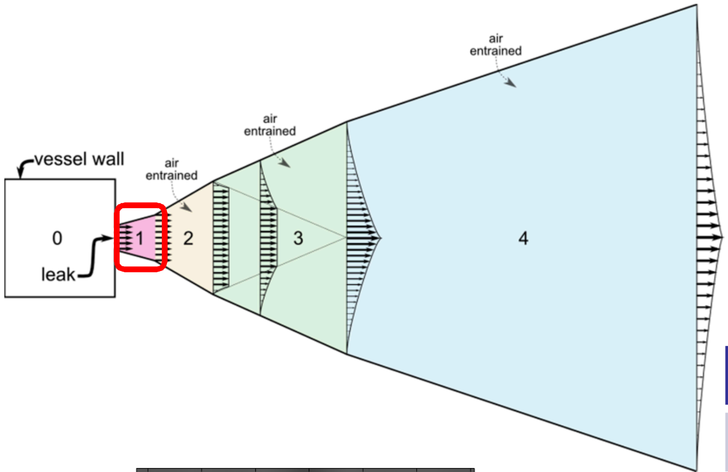
Ekoto et al., SAND2014-18776



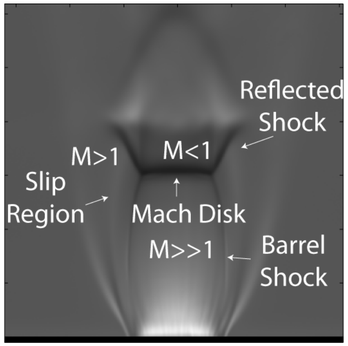
$$w_1^2 = 2(h_0 - h_1)$$
$$s_1 = s_0$$

- conditions at zone 0 capture by network flow model (requires development)
- hydrogen is stored as a pure substance
- multi-phase components have equal velocities

Pseudo source models are used to account for choked flow behavior in Zone 1 (if applicable)



Several source models have been developed to predict the mass weighted effective diameter, (i.e., the critical scaling parameter): $d^* \equiv d_{eff}\sqrt{\rho_{eff}/\rho_{amb}}$



Ruggles & Ekoto, *IJHE*, 2012

Source Model	*d** [mm]
Birch et al. (1984)	0.947
Ewan & Moodie (1986)	0.993
Birch et al. (1987)	0.790
Yuceil & Otugen (2002)	0.790
Harstad & Bellan (2006)	1.440
Molkov (2008)	0.993
SNL Data (2011)	***0.867***

***All models updated w/ Able-Noble EOS**

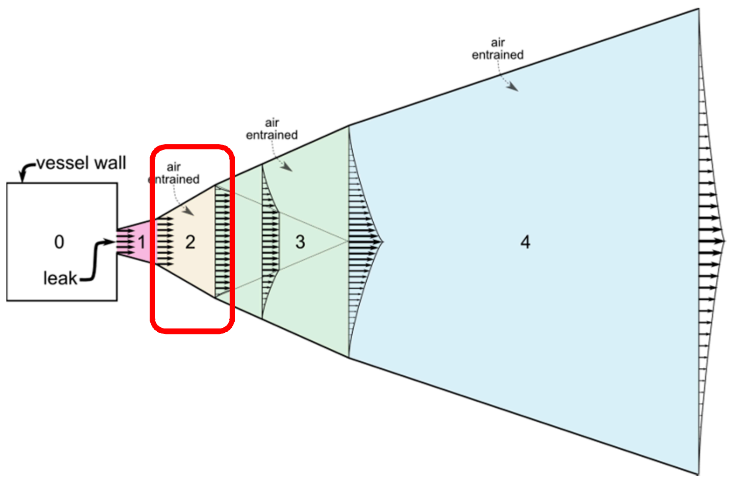
Neglects Mach Disk (i.e., fully supersonic)

All flow through Mach disk (i.e., fully subsonic)

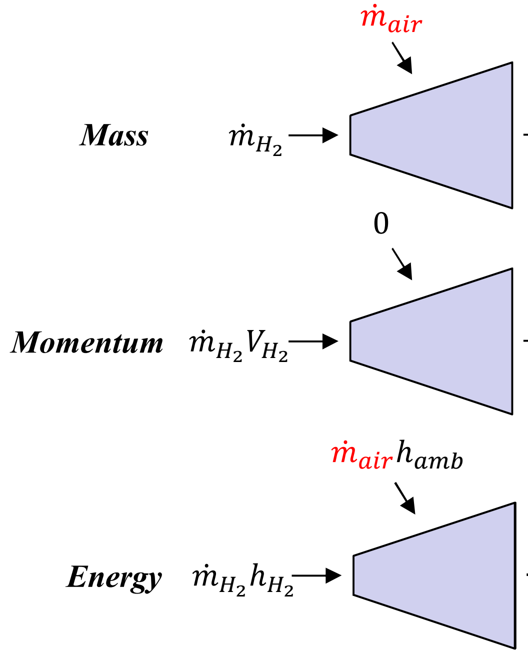
Reality is that fluid is split between the slip and Mach disk regions

Ongoing work to develop validated two-zone source model that accounts for the fluid split ratio between the slip region & Mach disk regions

Plug flow assumption invoked for Zone 2 as the jet begins to warm



Winters, SAND Report 2009-0035



Mass: $\dot{m}_{H_2}$, $\dot{m}_{air}$ →
$$\dot{m}_3 = \dot{m}_{H_2} + \dot{m}_{air}$$

Momentum: $\dot{m}_{H_2} V_{H_2}$, 0 →
$$\dot{m}_3 V_3 = \dot{m}_{H_2} V_{H_2}$$

Energy: $\dot{m}_{H_2} h_{H_2}$, $\dot{m}_{air} h_{amb}$ →
$$\dot{m}_3 h_3 = \dot{m}_{H_2} h_{H_2} + \dot{m}_{air} h_{amb}$$

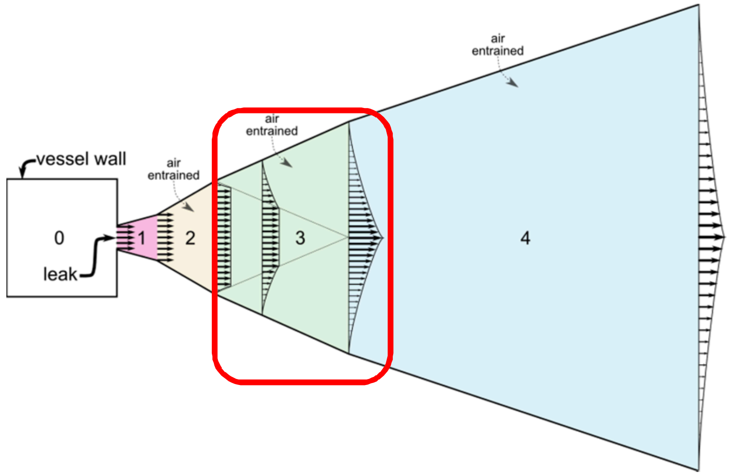
unknowns (red)
assumed value (green)

State modeling by NIST H_2 EOS:
$$h_3 = f(Y_{H_2,3}, p_{amb}, T_3)$$

Species conservation used to close system of equations:
$$\dot{m}_{air} = \dot{m}_{H_2} \frac{1 - Y_{H_2,3}}{Y_{H_2,3}}$$

Turbulent jet entrainment rate used to estimate zone length:
$$E_{mom} \equiv \frac{1}{\rho_{amb}} \frac{d\dot{m}}{dS} \approx \frac{1}{\rho_{amb}} \frac{\dot{m}_{air}}{S_3} \Rightarrow S_3 = \frac{\dot{m}_{air}}{E_{mom}\rho_{amb}}, \text{ where } E_{mom} = \alpha_m \left(\frac{\pi D_{H_2}^2}{4} \frac{\rho_{H_2} V_{H_2}^2}{\rho_{amb}} \right)^{\frac{1}{2}}$$

Flow develops to the assumed self-similar profile in Zone 3



Winters, SAND Report 2009-0035

unknowns
assumed value

$$V_{CL,4} = V_3$$

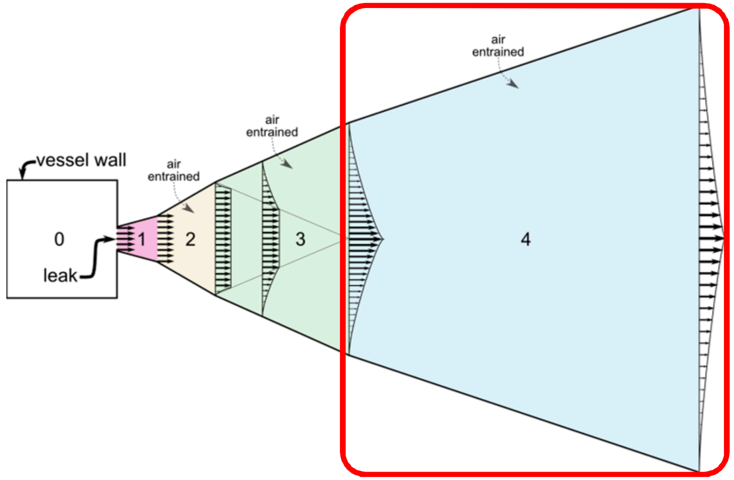
Mass

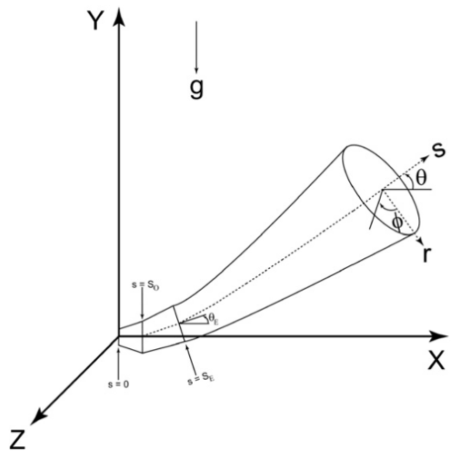
$$\rho_3 \frac{D_3^2}{4} = B_4^2 \left[\rho_{amb} - \frac{\lambda^2}{\lambda^2+1}\left(\rho_{amb} - \rho_{CL,4}\right)\right]$$

Momentum

$$\underbrace{\left(\rho_{amb} - \rho_3\right)\frac{D_3^2}{4}}_{s_3} = \underbrace{B_4^2 \left[\frac{\rho_{amb}}{2} - \frac{\lambda^2}{2\lambda^2+1}\left(\rho_{amb} - \rho_{CL,4}\right)\right]}_{s_4}$$

Zone 4 modeled with previous SNL 1D integral jet/plume models that invoke self-similarity – FY08





Entrainment due to buoyancy & momentum

F_{rL}: Jet Froude length
α_b: Buoyancy entrainment coefficient
α_m: Momentum entrainment coefficient
g: Gravity constant

$$E_{buoy} = \frac{\alpha_b}{F_{r_L}}(2\pi V_{CL} B)\sin\theta$$

$$E_{mom} = \alpha_m \left(\frac{\pi D^2}{4}\frac{\rho V^2}{\rho_{amb}}\right)^{\frac{1}{2}}$$

$$F_{r_L} = \frac{V_{CL}^2 \rho_{exit}}{gB(\rho_{amb} - \rho_{CL})}$$

Mass $$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho V r dr d\phi = \rho_{amb} E$$

x-Mom $$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho V^2 \cos\theta\, r dr d\phi = 0$$

y-Mom $$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho V^2 \sin\theta\, r dr d\phi = \int_0^{2\pi}\int_0^{\infty}(\rho_{amb} - \rho) g r dr d\phi$$

Species $$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho V Y r dr d\phi = 0$$

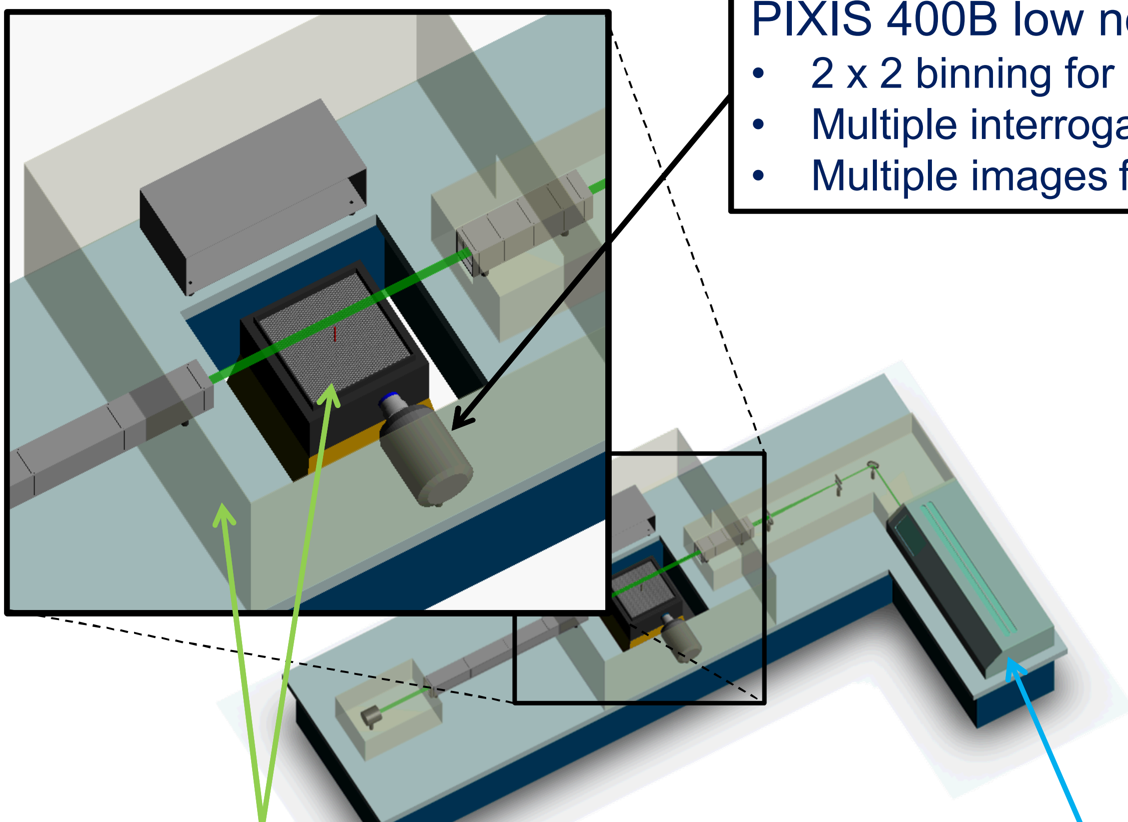
Energy $$\frac{\partial}{\partial S}\int_0^{2\pi}\int_0^{\infty}\rho V (h - h_{amb}) r dr d\phi = 0$$

Houf & Schefer, IJHE, 2008

Scalar field to be measured via Rayleigh scatter imaging in established flow zone to validate LH2 release model

PIXIS 400B low noise CCD Camera

- 2 x 2 binning for high signal-to-noise (~400:1)
- Multiple interrogation regions to image full jet
- Multiple images for converged statistics



Air co-flow & barriers to minimize impact of room currents

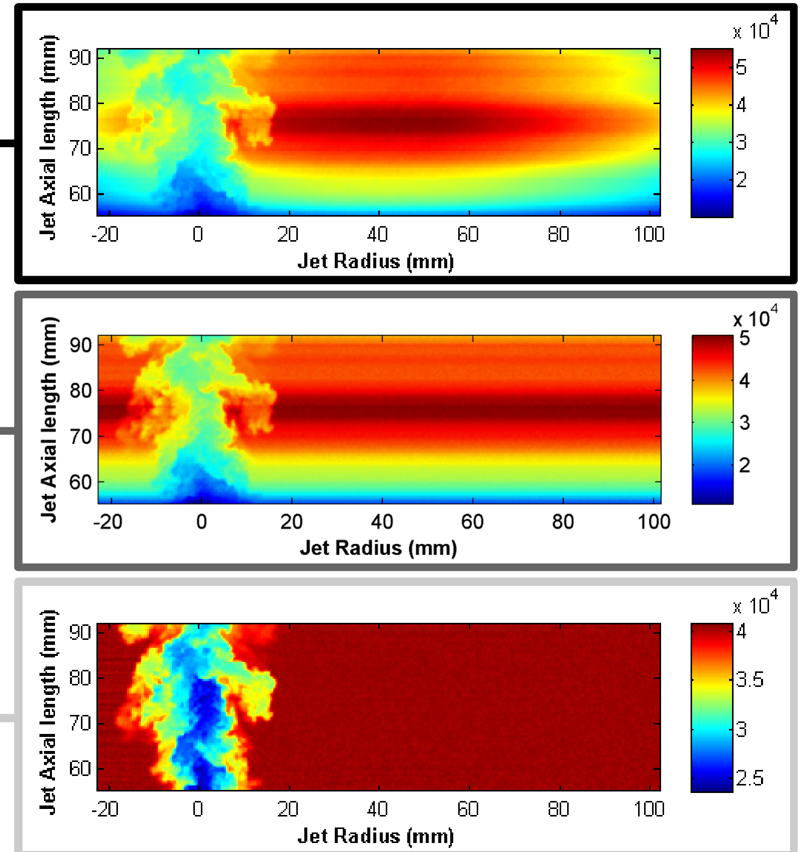
Nd:YAG injection seeded laser (1 J/pulse @ 532 nm)

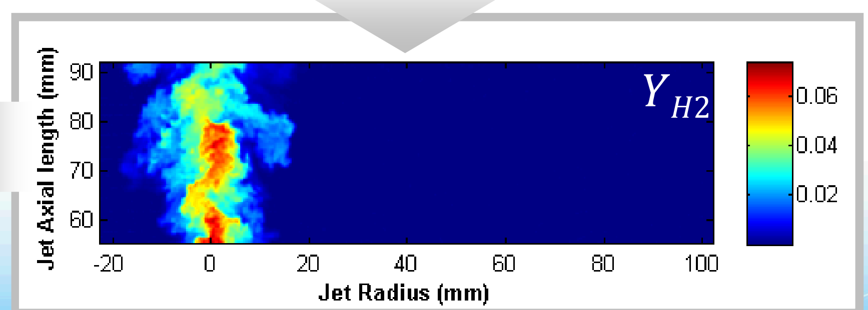
Opportunity for additional upstream measurements using complementary Raman diagnostics in an adjacent lab

Quantitative measurement w/ good accuracy

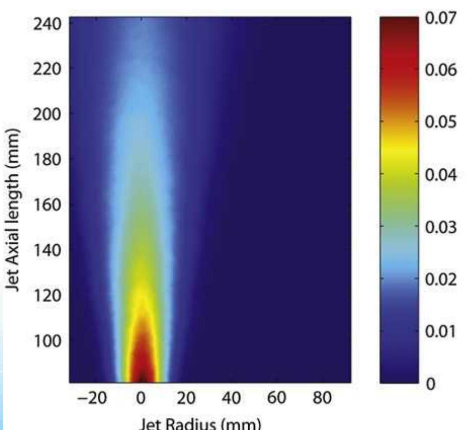
R:	Raw image
E_B:	Electronic bias
B_G:	Background luminosity
p_F:	Laser power fluctuation
O_R:	Camera/lens optical response
S_B:	Background scatter
S_t:	Laser sheet profile variation
I:	Corrected intensity

$$R = p_F \cdot O_R \cdot (I \cdot S_t + S_B) + E_B + B_G$$

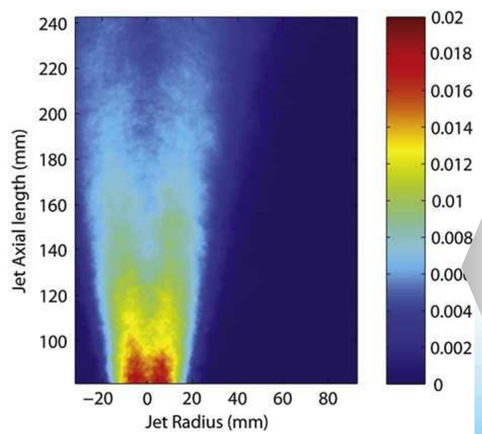




Mean mole fraction



RMS Error



Current network flow model (NETFLOW) must be updated for use near saturation conditions

- Models 1-D flow networks (e.g. piping, valves, tanks) by solving conservation and state modeling equations with local corrections for wall friction, heat transfer, and pressure loss
- Conventional state equations invalid near saturation conditions
- Important to capture phase-change behavior
- Must model compressible and incompressible flows