

Cryogenic Hydrogen Release Modeling Validation – Update for Hydrogen Safety Panel

Chris LaFleur, Ethan Hecht, Isaac Ekoto

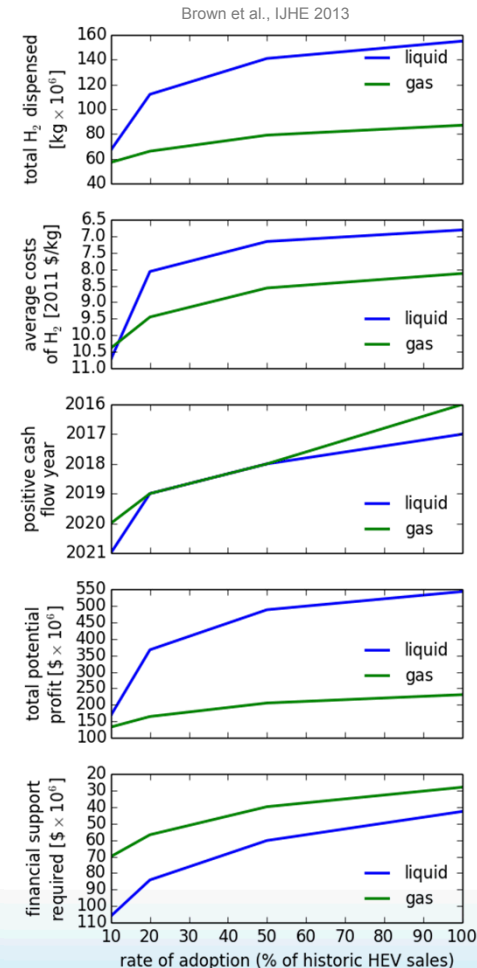
Sandia National Laboratories



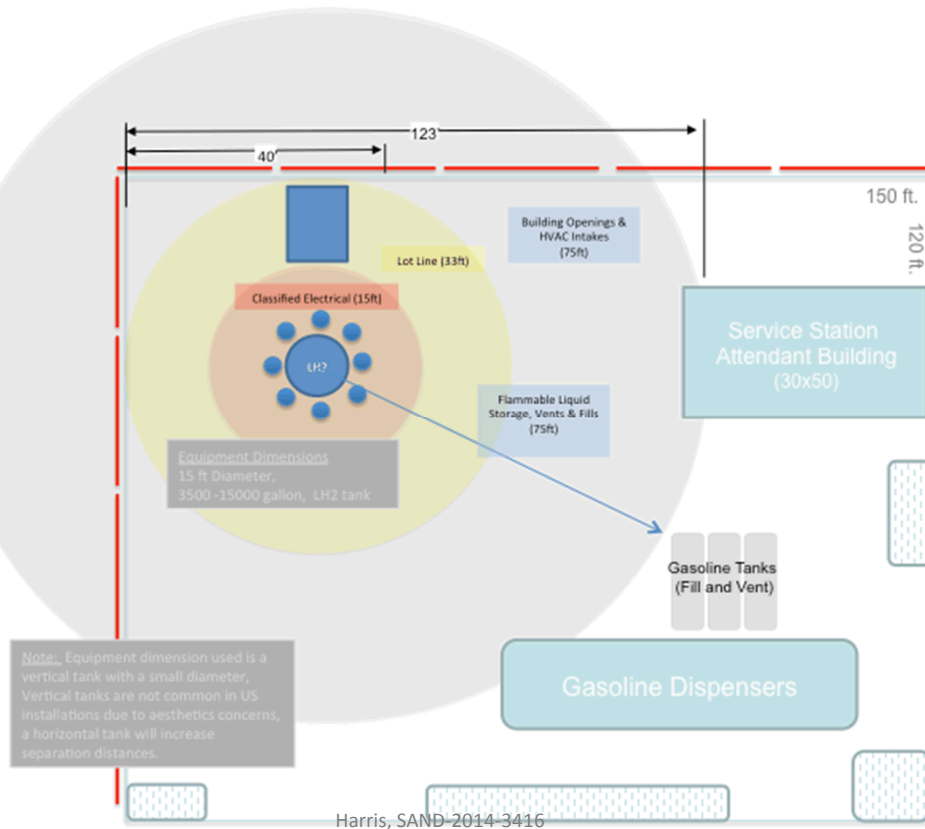
Liquid hydrogen stations have been found to be more economically favorable than gaseous stations

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)

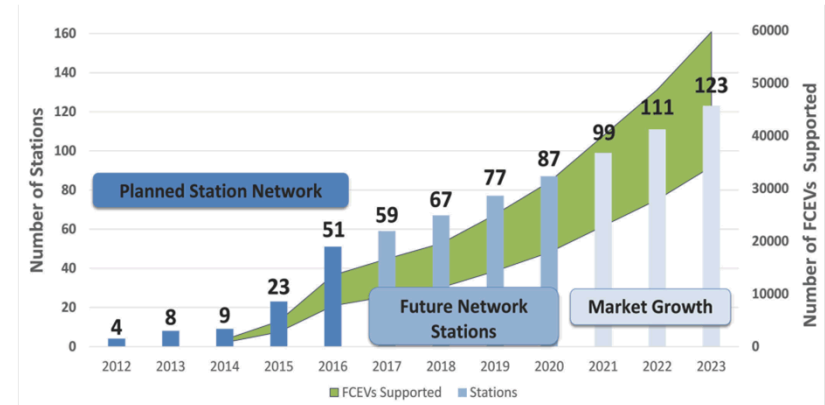


Standoff distances in NFPA 2 for liquid hydrogen stations are often prohibitively large

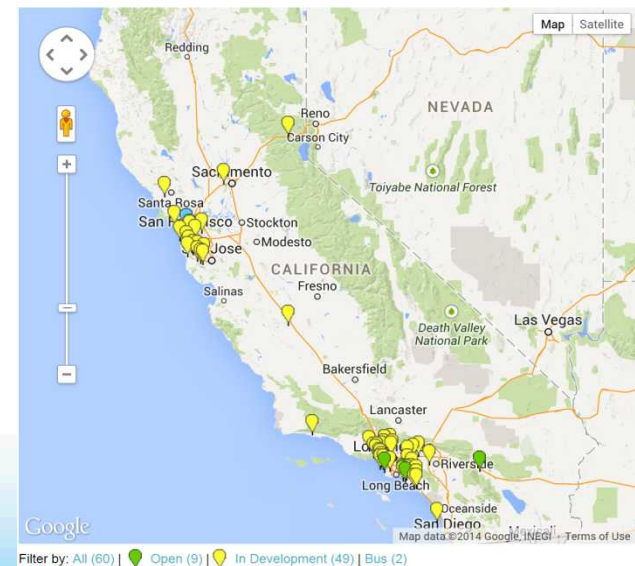


Of 70 stations surveyed (out of 343), none met the NFPA 2 Ch. 6 separation distance requirements.

Harris, SAND-2014-3416

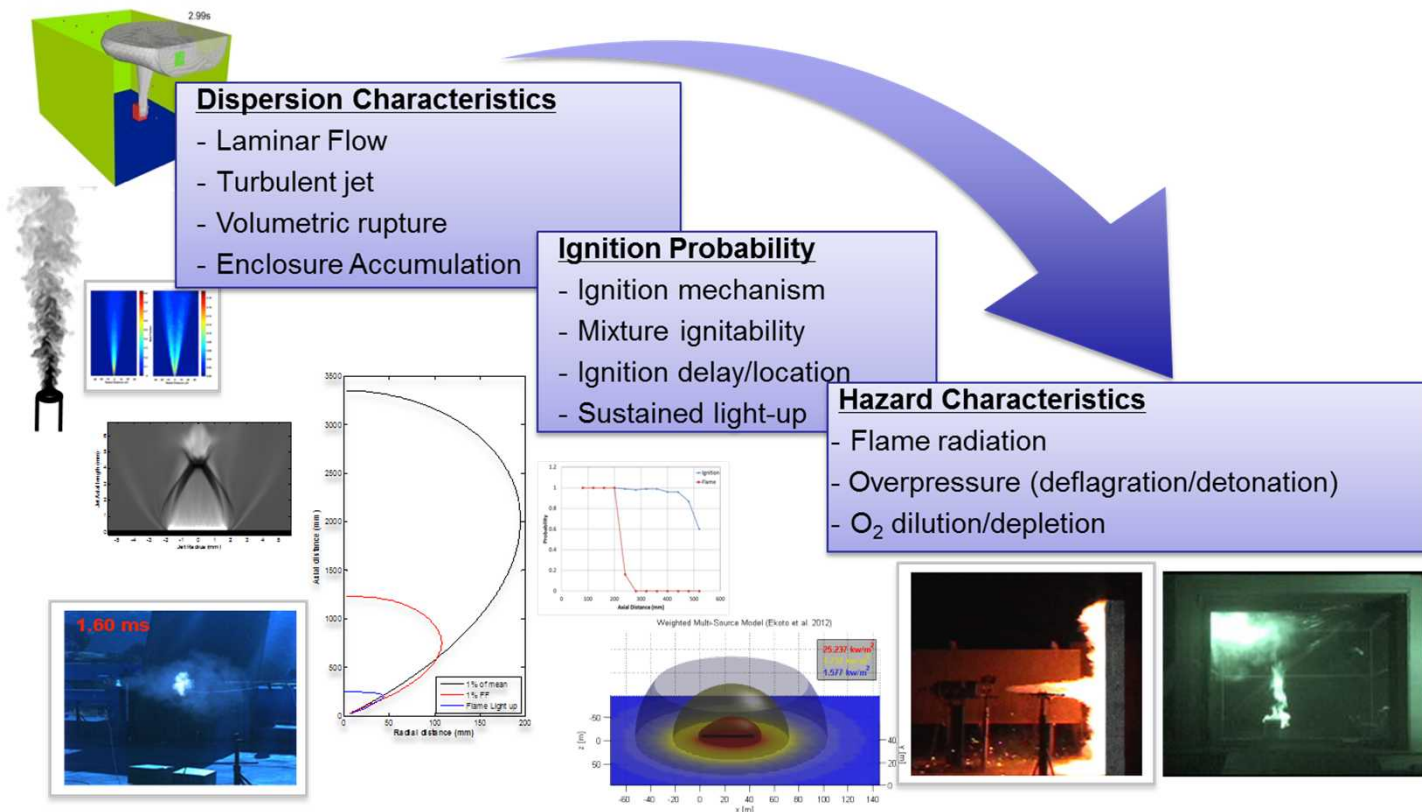


A California Road Map: The Commercialization of Hydrogen Fuel Cell Vehicles, CalFCP, July 2014



<http://www.caftp.org/stationmap>

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

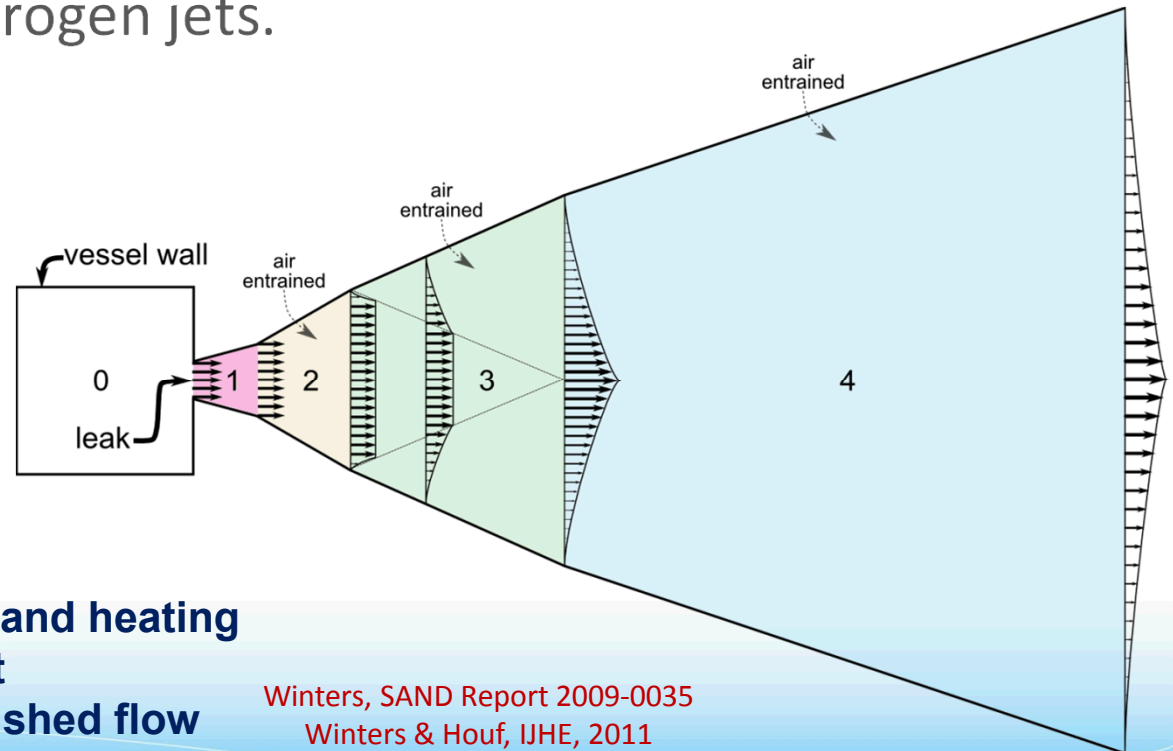


$$Risk \propto \sum_{i,j,k} P(\text{Release}_i) P(\text{Ignition}_j | \text{Release}_i) P(\text{Hazard}_k | \text{Ignition}_j \cap \text{Release}_i) P(\text{Harm} | \text{Hazard}_k)$$

Cold hydrogen behavior experiments for model development/validation

Objective:

- The primary objective of the low-temperature H₂ delivery system is to study flow and flame characteristics that result from cryogenic hydrogen jets.

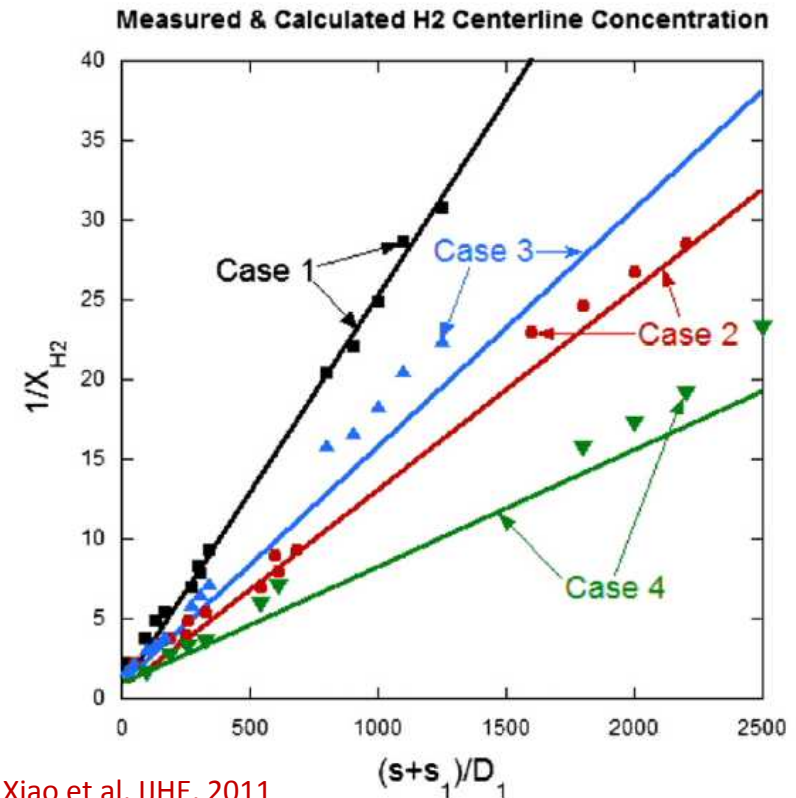


- Zone 0:** accelerating flow
- Zone 1:** underexpanded jet
- Zone 2:** initial entrainment and heating
- Zone 3:** flow establishment
- Zone 4:** self-similar, established flow

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



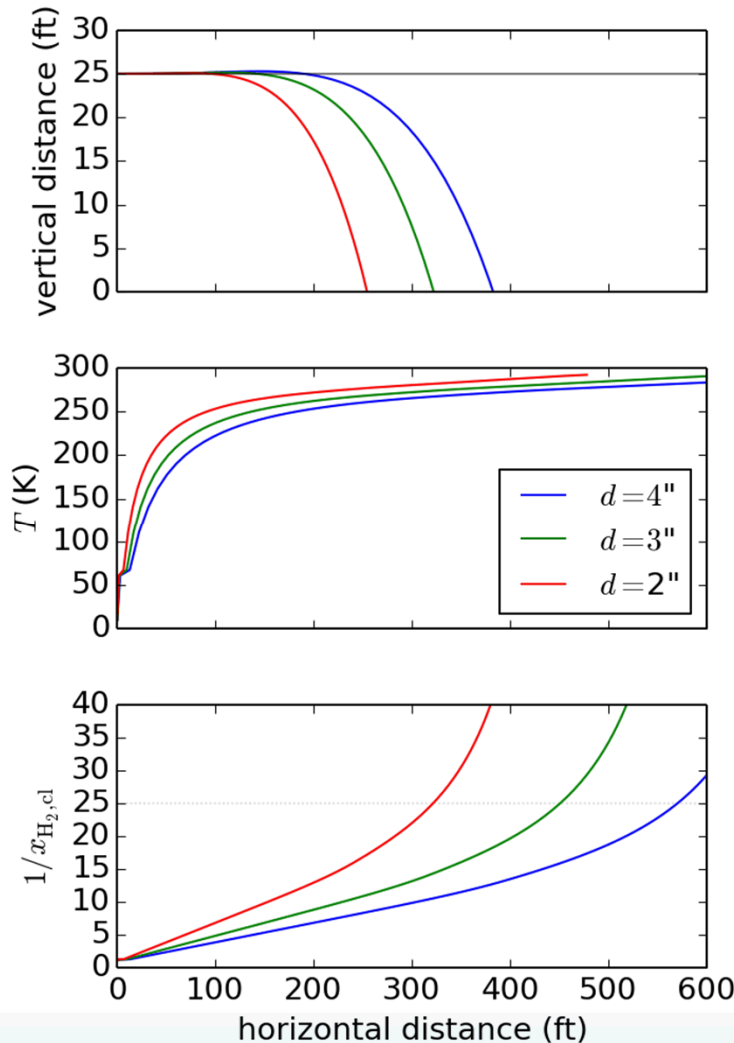
Xiao et al, IJHE, 2011

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

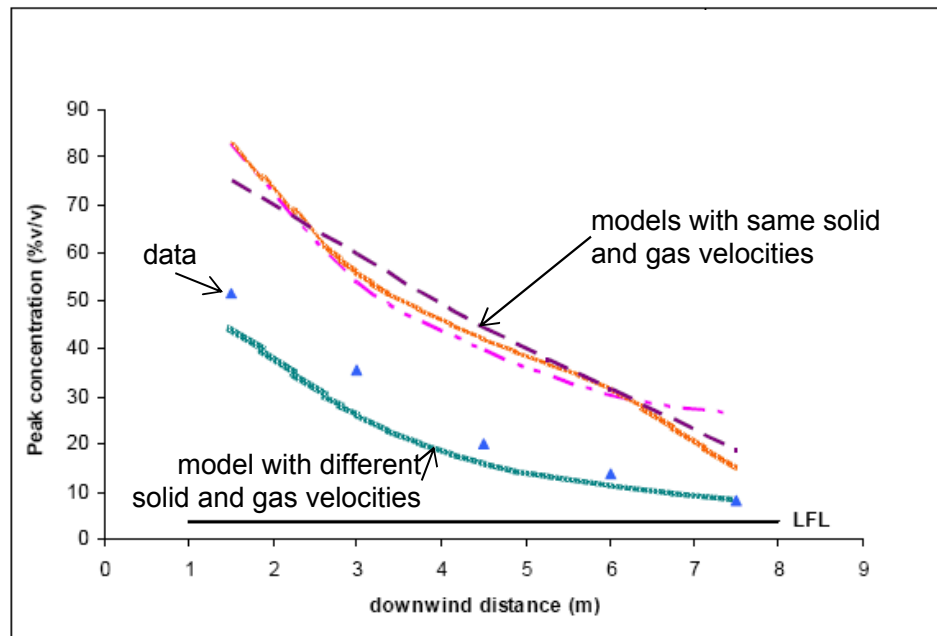
- Storage pressure = 180 psi
- Release (saturation) temperature = 20 K
- Release angle = 0°
- Release height = 25 ft



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

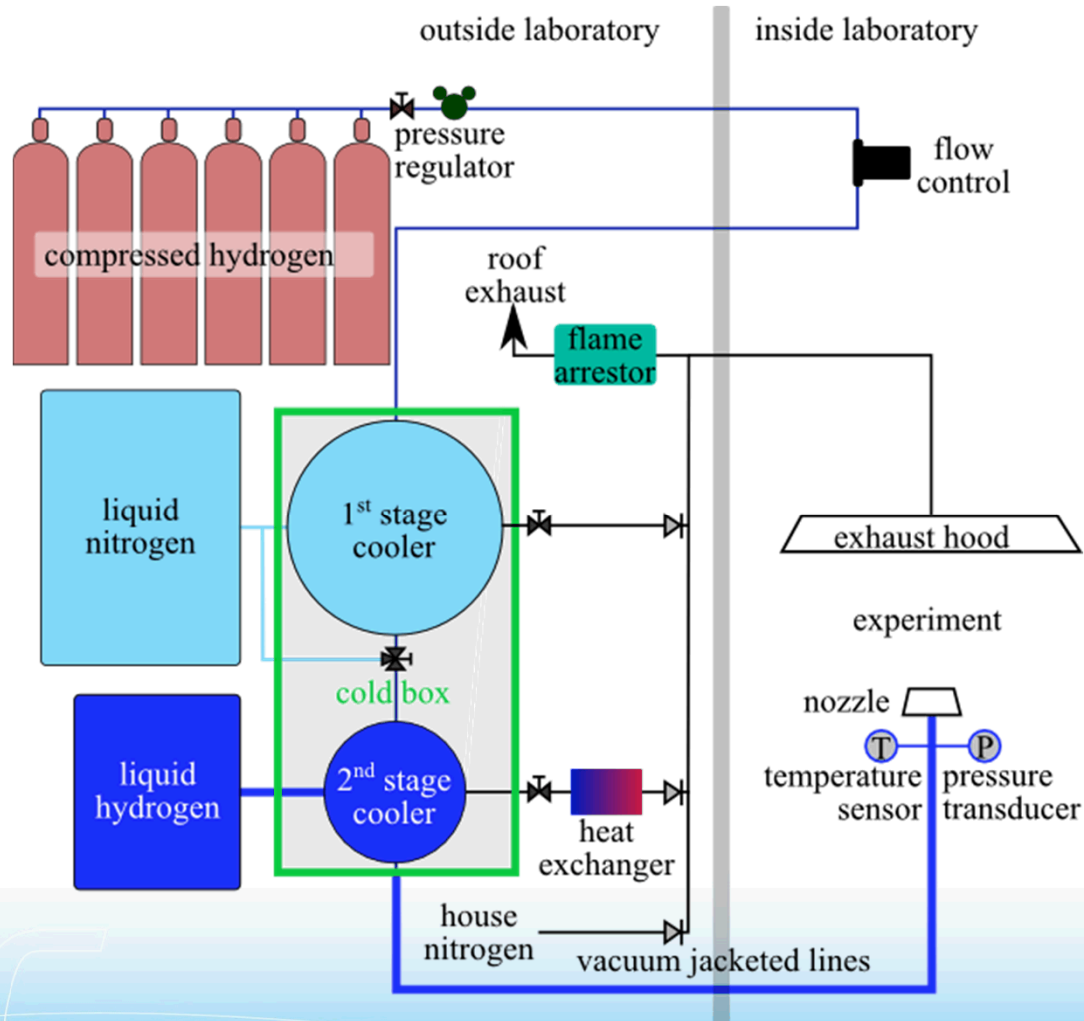
Description of Work

The approach will follow the template used previously to characterize high--pressure gaseous hydrogen releases. The concept is to integrate a novel two-stage cooler into the existing Turbulent Combustion Laboratory infrastructure to reduce the temperature of gaseous hydrogen to the desired value, potentially creating mixed--phase flows, with the hydrogen exiting through a custom nozzle. High-fidelity Rayleigh scatter imaging and Raman diagnostics will be used to measure relevant statistics of release phenomena. These data will then be used to develop reduced-order engineering models that can predict unintended release characteristics from liquid hydrogen storage systems due to equipment failures.

Schedule

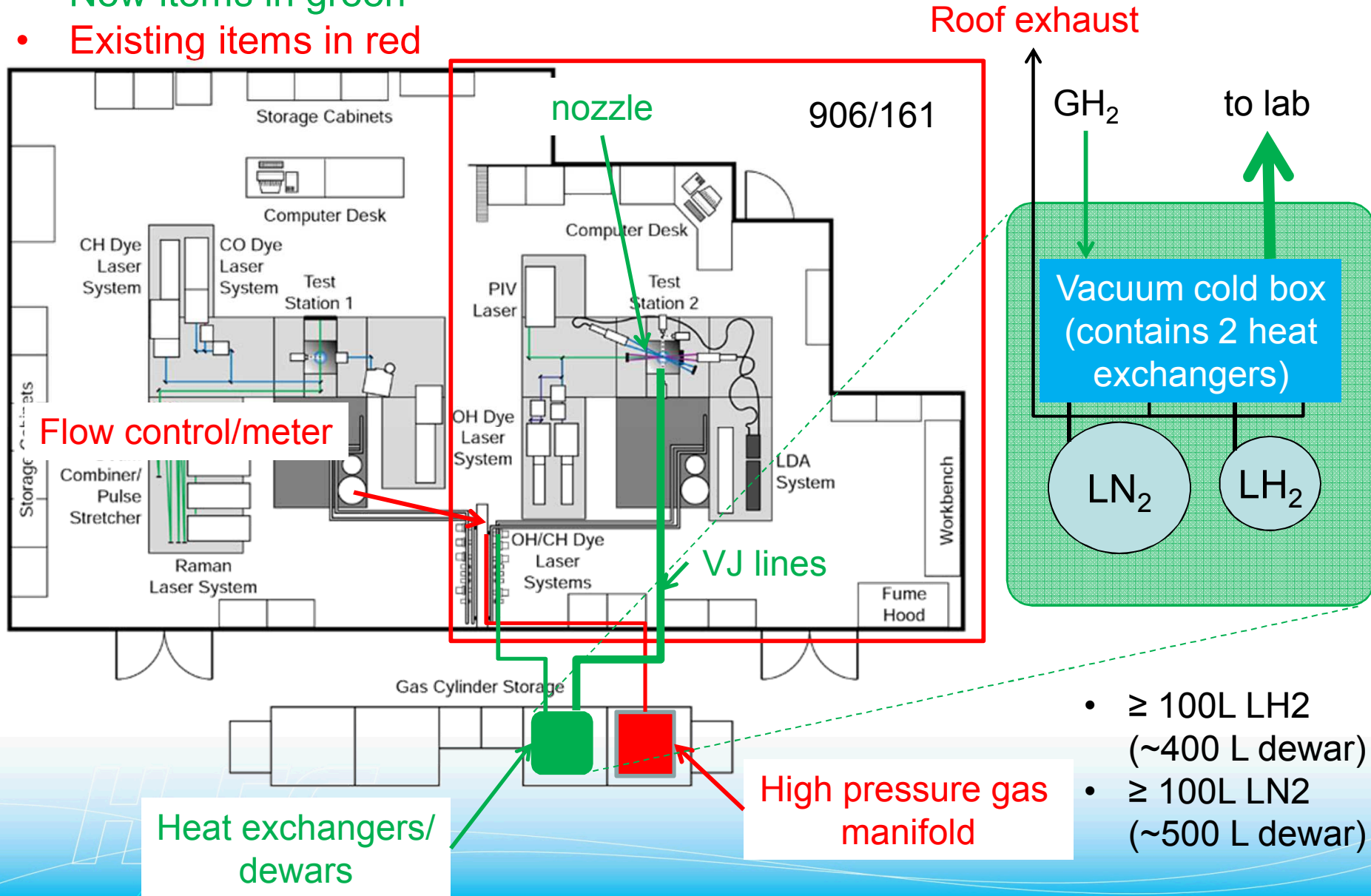
- 2015: Construct and test cold hydrogen vapor releases platform; vertical orientation (target temperature: 30 K)
- 2016:
 - Cold plume release data (2 nozzles, 6 pressures, 6 temperatures)
 - Develop/validate reduced-order cold-plume model for integration into QRA framework
- Future Work:
 - Test model 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

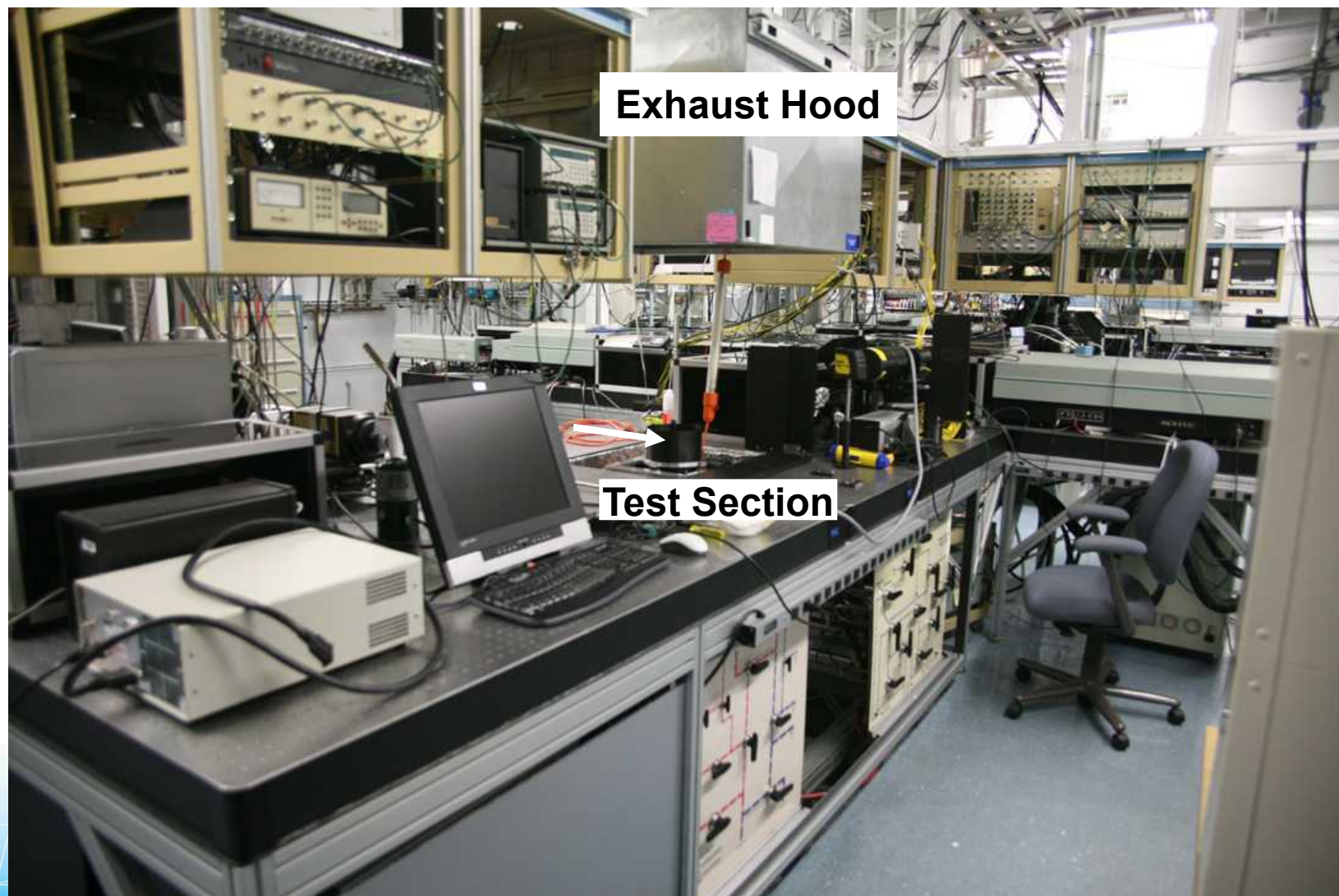


Turbulent Combustion Laboratory

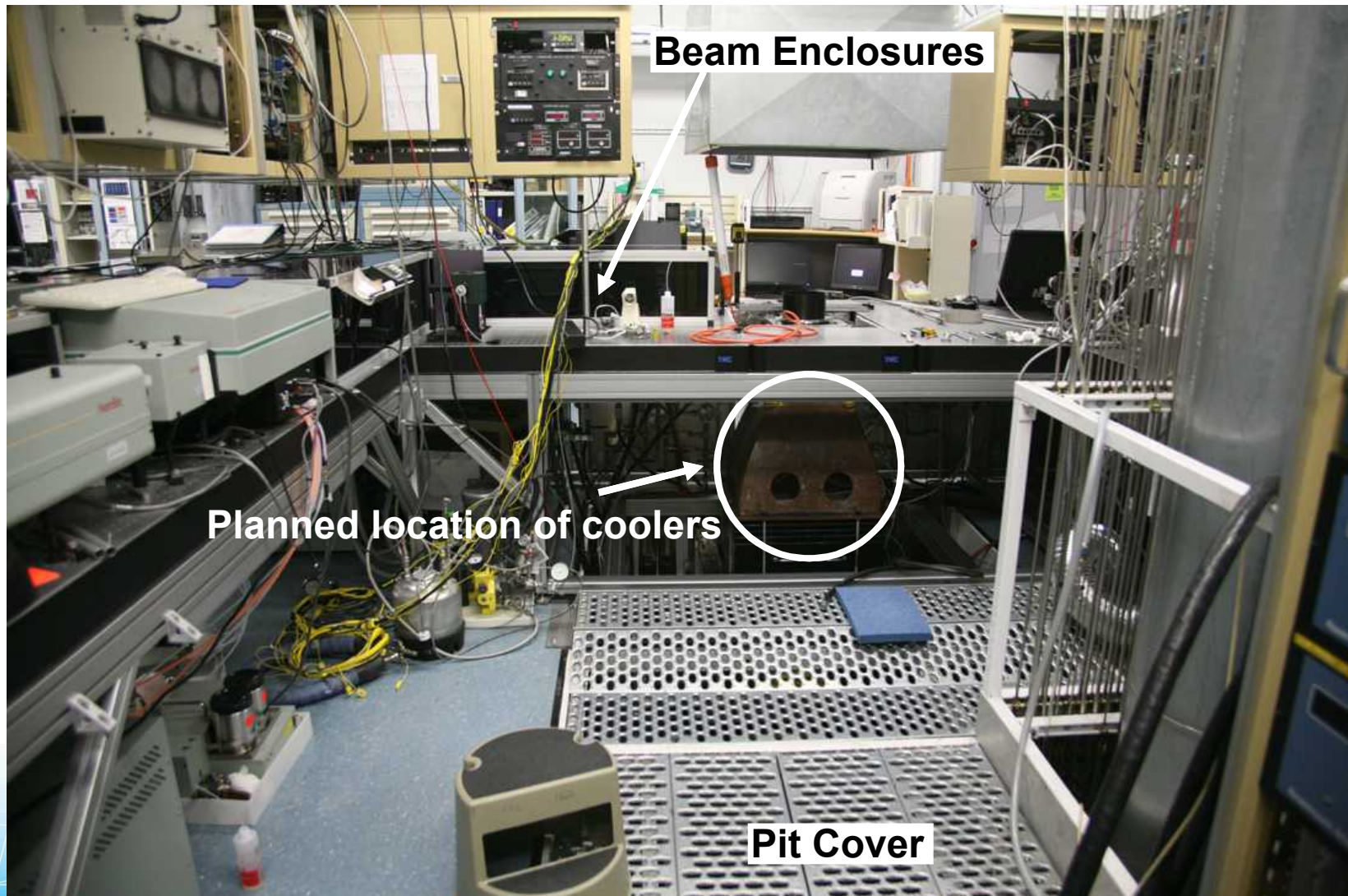
- New items in green
- Existing items in red



TCL: 906/161 Main Work Area

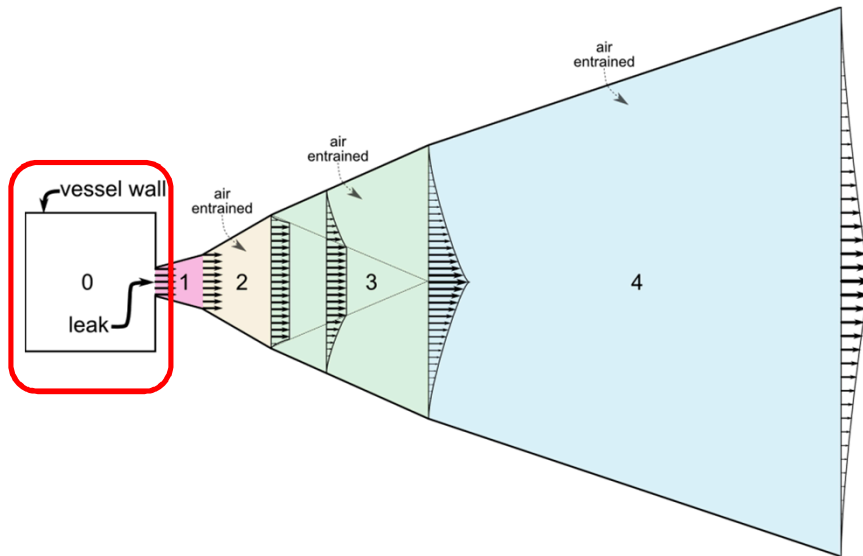


TCL: 906/161 Back Side



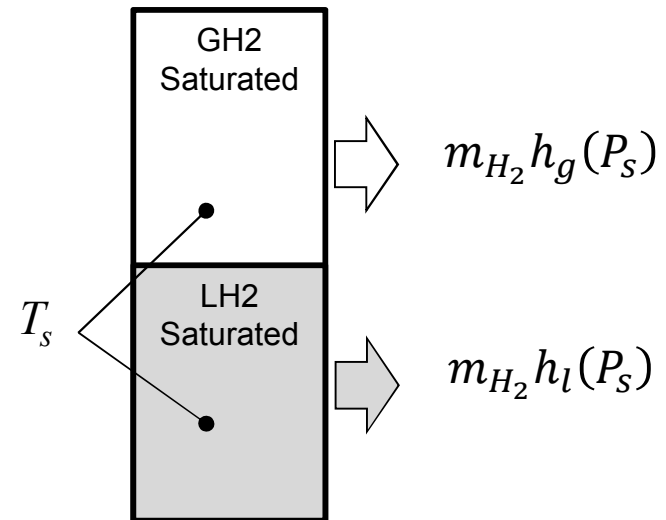
Backup

Accelerating flow (leak) develops from saturated storage conditions

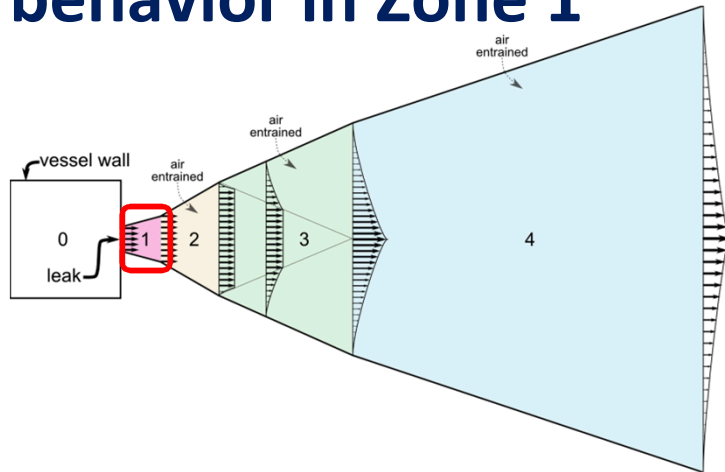


- conserved enthalpy from the gas or liquid space.

Winters, SAND 2001-8422

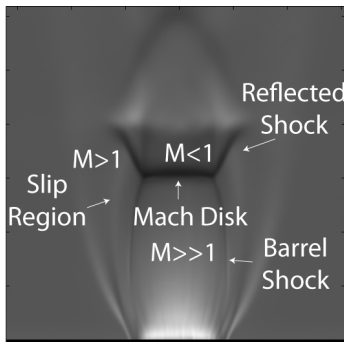


Pseudo source models are used to account for choked flow behavior in Zone 1



Several source models have been developed to predict the mass weighted effective diameter, (i.e., the critical scaling parameter): $d^* \equiv$

$$d_{eff} \sqrt{\rho_{eff} / \rho_{amb}}$$



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

Ruggles & Ekoto, *IJHE*, 2012

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

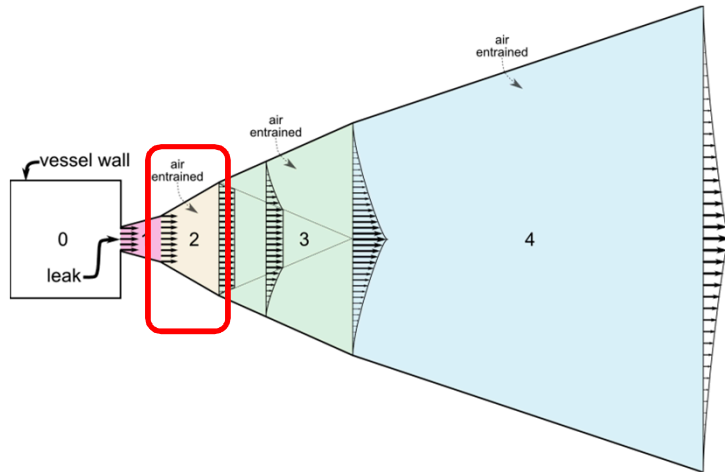
Assumes **all** flow goes through
Mach disk (i.e., fully subsonic)

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

*All models updated w/ Able-Noble EOS

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



unknowns
assumed value

Mass

$$\dot{m}_{H_2} \rightarrow \text{Zone 2} \rightarrow \boxed{\dot{m}_3 = \dot{m}_{H_2} + \dot{m}_{air}}$$

Momentum

$$\dot{m}_{H_2} V_{H_2} \rightarrow \text{Zone 2} \rightarrow \boxed{\dot{m}_3 V_3 = \dot{m}_{H_2} V_{H_2}}$$

Energy

$$\dot{m}_{H_2} h_{H_2} \rightarrow \text{Zone 2} \rightarrow \boxed{\dot{m}_3 h_3 = \dot{m}_{H_2} h_{H_2} + \dot{m}_{air} h_{amb}}$$

Winters, SAND Report 2009-0035

State modeling by NIST H₂ 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:

$$E_{mom} \equiv \frac{1}{\rho_{amb}} \frac{d\dot{m}}{dS} \approx \frac{1}{\rho_{amb}} \frac{\dot{m}_{air}}{S_3} \Rightarrow S_3 = \frac{\dot{m}_{air}}{E_{mom} \rho_{amb}}, \text{ where } E_{mom} = \alpha_m \left(\frac{\pi D_{H_2}^2 \rho_{H_2} V_{H_2}^2}{4 \rho_{amb}} \right)^{\frac{1}{2}}$$

Zone 3 treated as discrete region w/ boundary conditions specified from self-similar profiles at Zone 4

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

unknowns
assumed value

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

Winters, SAND Report 2009-0035

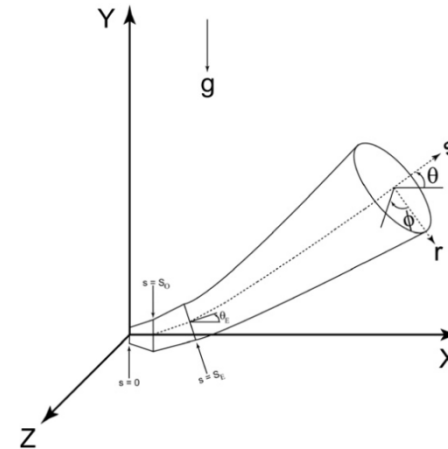
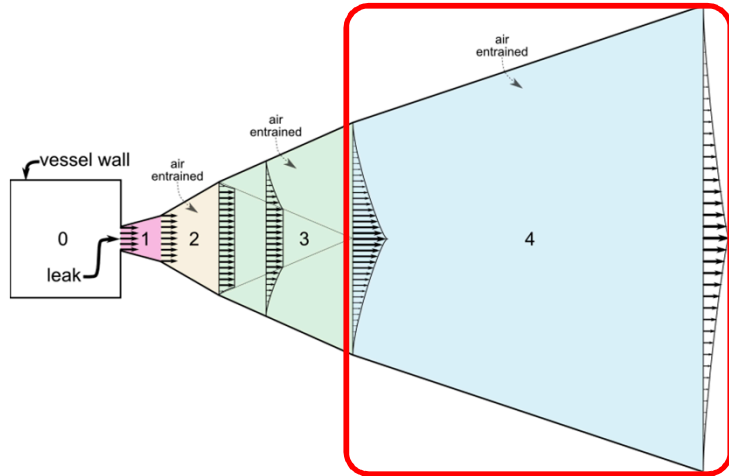
Mass

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

Momentum

$$\underbrace{(\rho_{amb} - \rho_3)}_{S_3} \frac{D_3^2}{4} = B_4^2 \underbrace{\left[\frac{\rho_{amb}}{2} - \frac{\lambda^2}{2\lambda^2 + 1} (\rho_{amb} - \rho_{CL,4}) \right]}_{S_4}$$

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

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

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

$$F_{rL} = \frac{V_{CL}^2 \rho_{exit}}{g B (\rho_{amb} - \rho_{CL})}$$

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

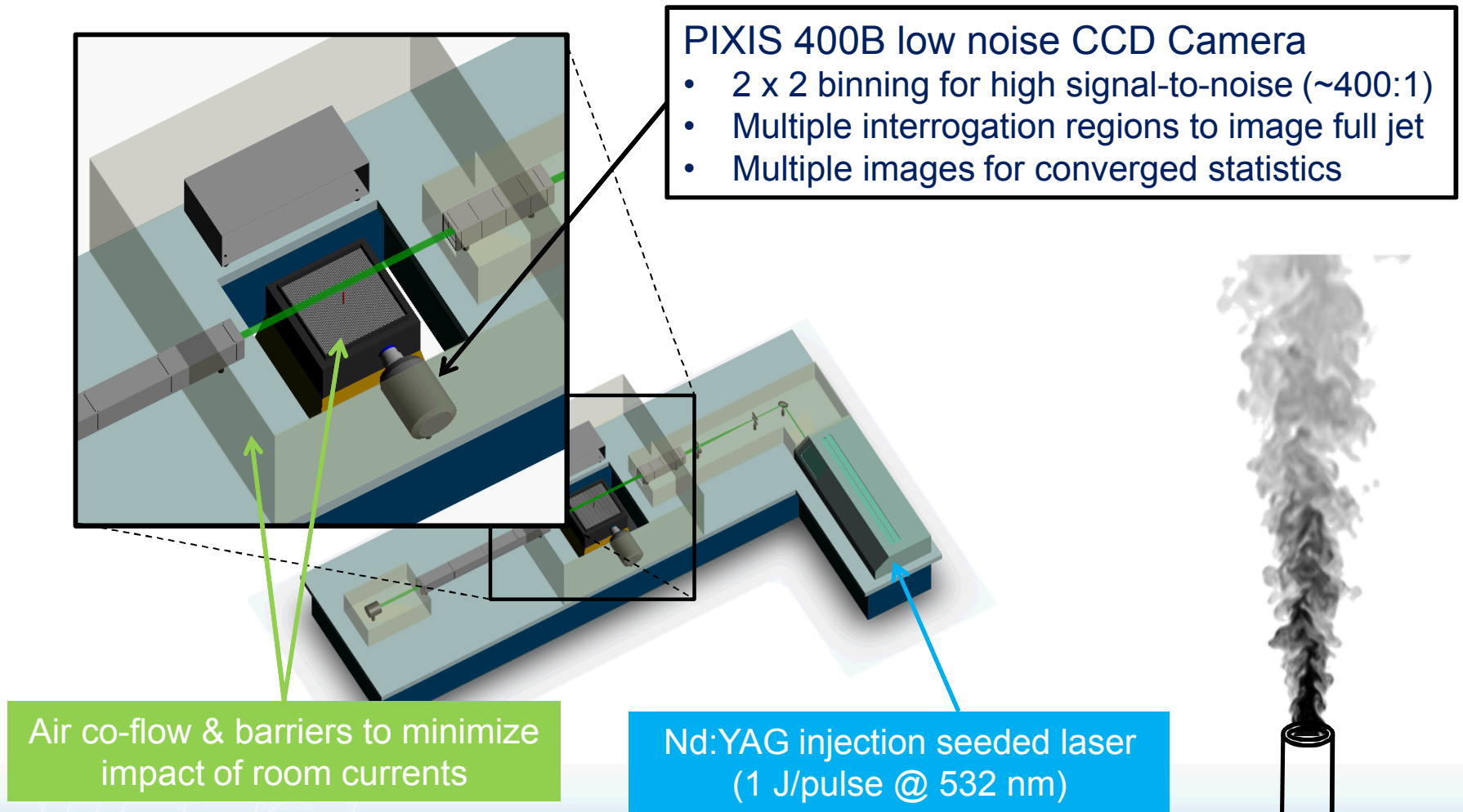
$$\text{x-Mom} \quad \frac{\partial}{\partial S} \int_0^{2\pi} \int_0^\infty \rho V^2 \cos \theta r dr d\phi = 0$$

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

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

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

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

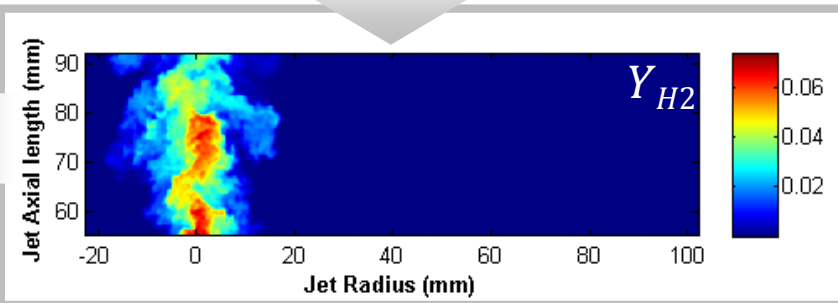
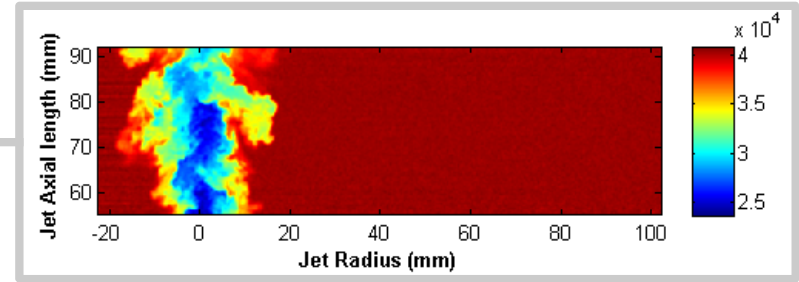
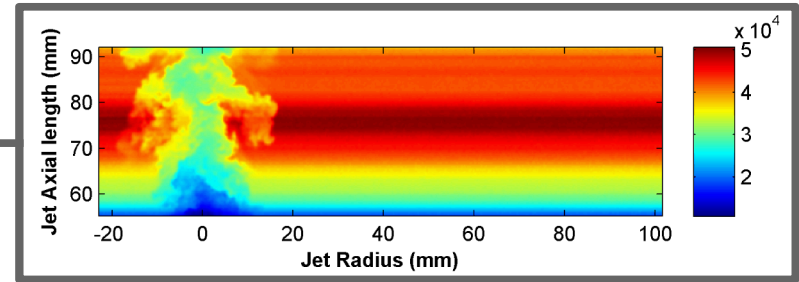
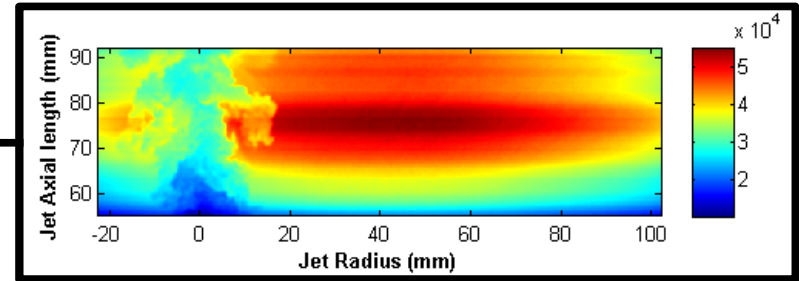


Opportunity for additional upstream measurements using complementary Raman diagnostics in an adjacent lab

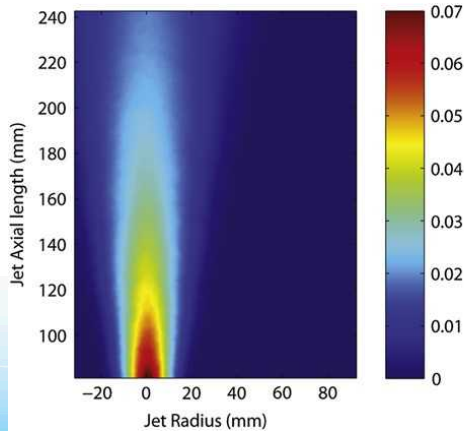
Quantitative measurement w/ good accuracy

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

