

# **Vision for validating the liquid hydrogen plume model at temperatures less than 80K**

Ethan Hecht, Isaac Ekoto

Combustion Research Facility, Sandia National Laboratories, Livermore, CA

Presented at the HySAFE Research Priorities Workshop

Washington D.C., Nov. 11, 2014

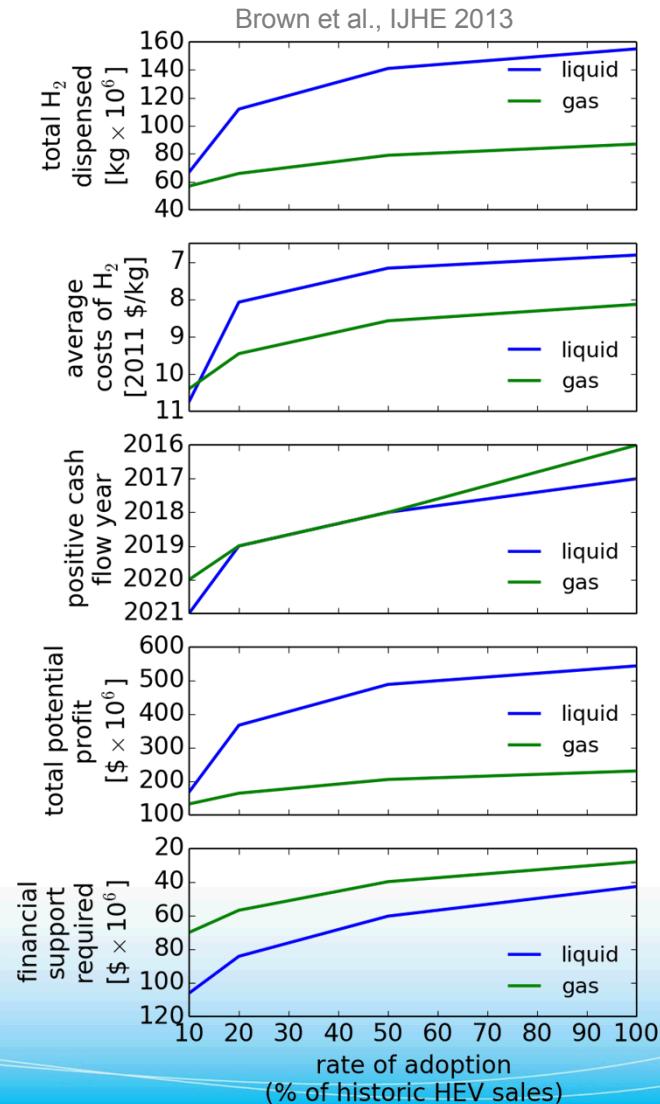


Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

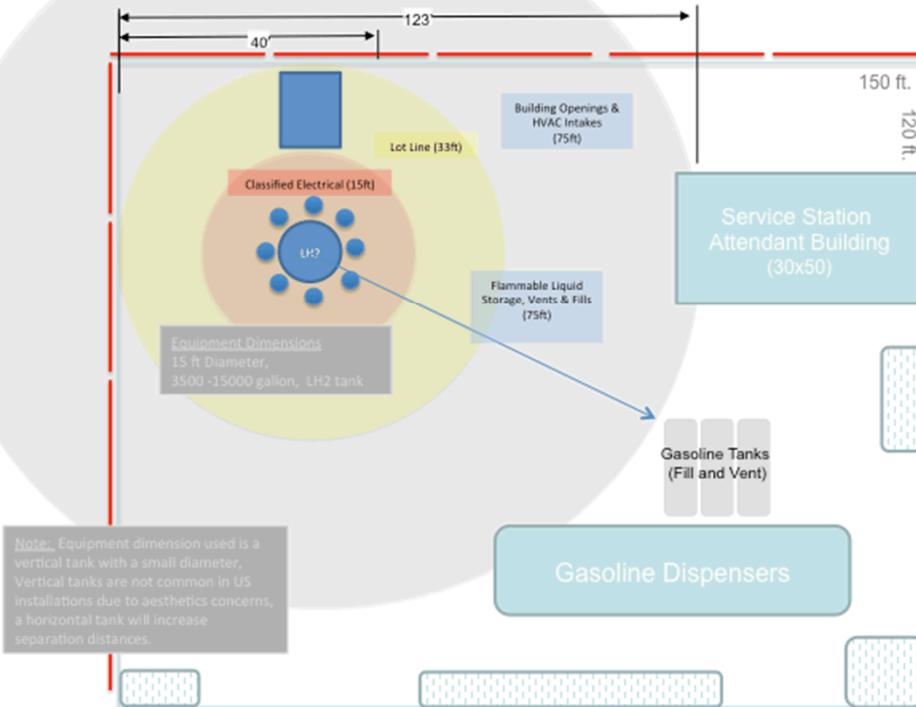
# Liquid hydrogen stations have been found to be more economically favorable than gaseous stations

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)

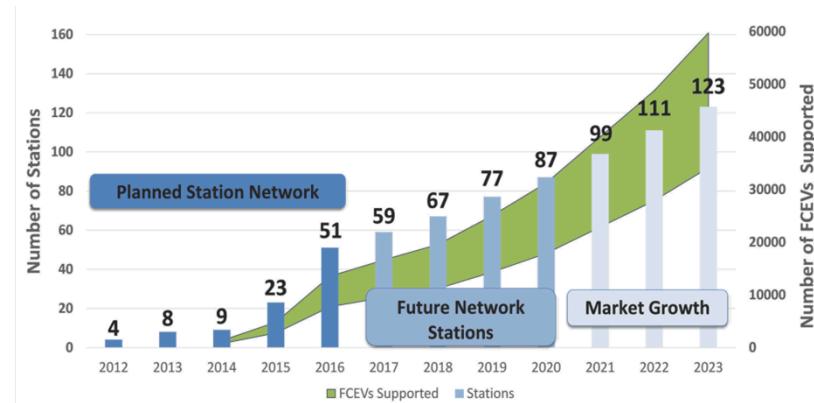


# Standoff distances in NFPA 2 for liquid hydrogen stations are often prohibitively large

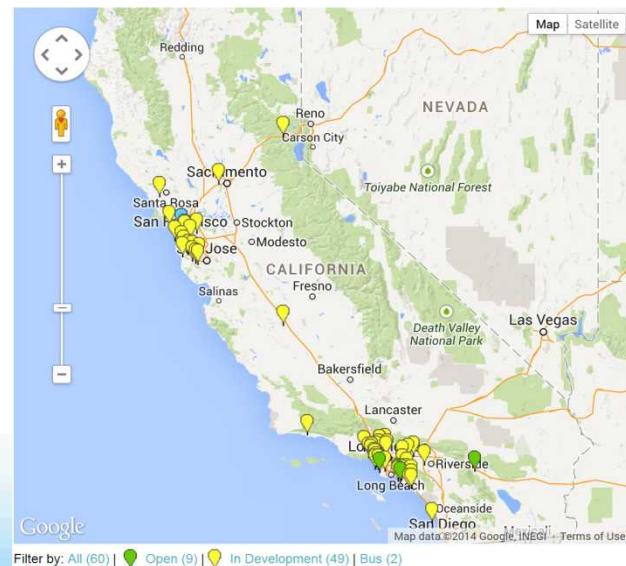


70 stations surveyed (of 343 sites), none met the NFPA 2 Ch. 6 separation distance requirements.

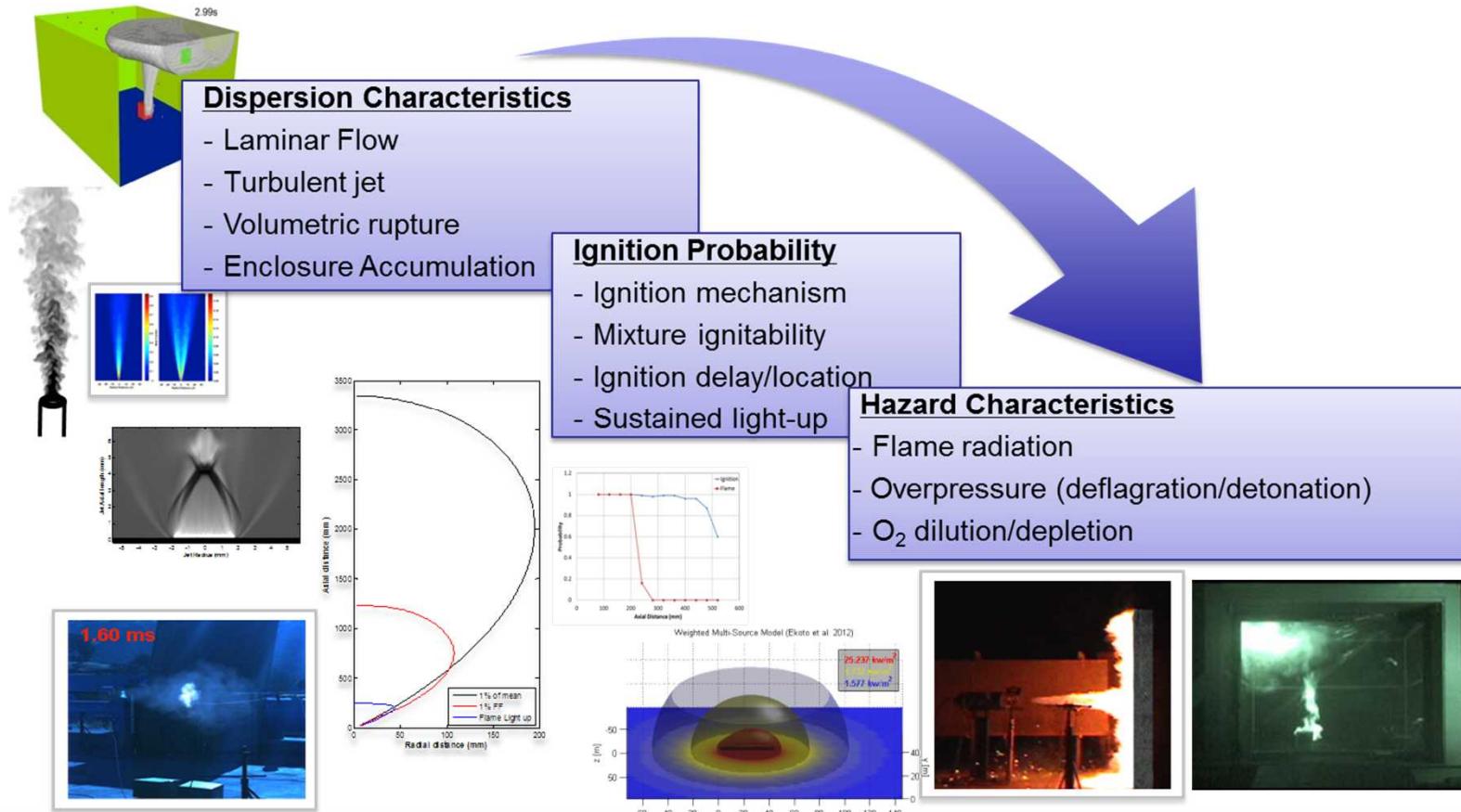
Harris, SAND-2014-3416



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



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

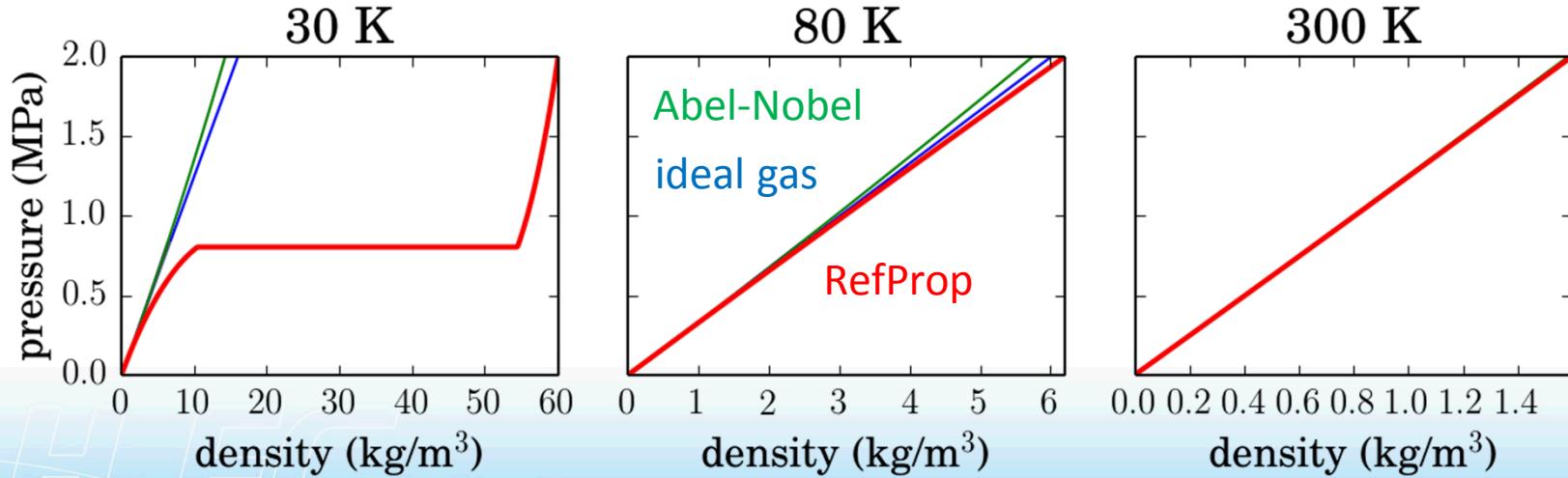


Risk requires a **Release**, then **Ignition**, forming a **Hazard**, causing **Harm**

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

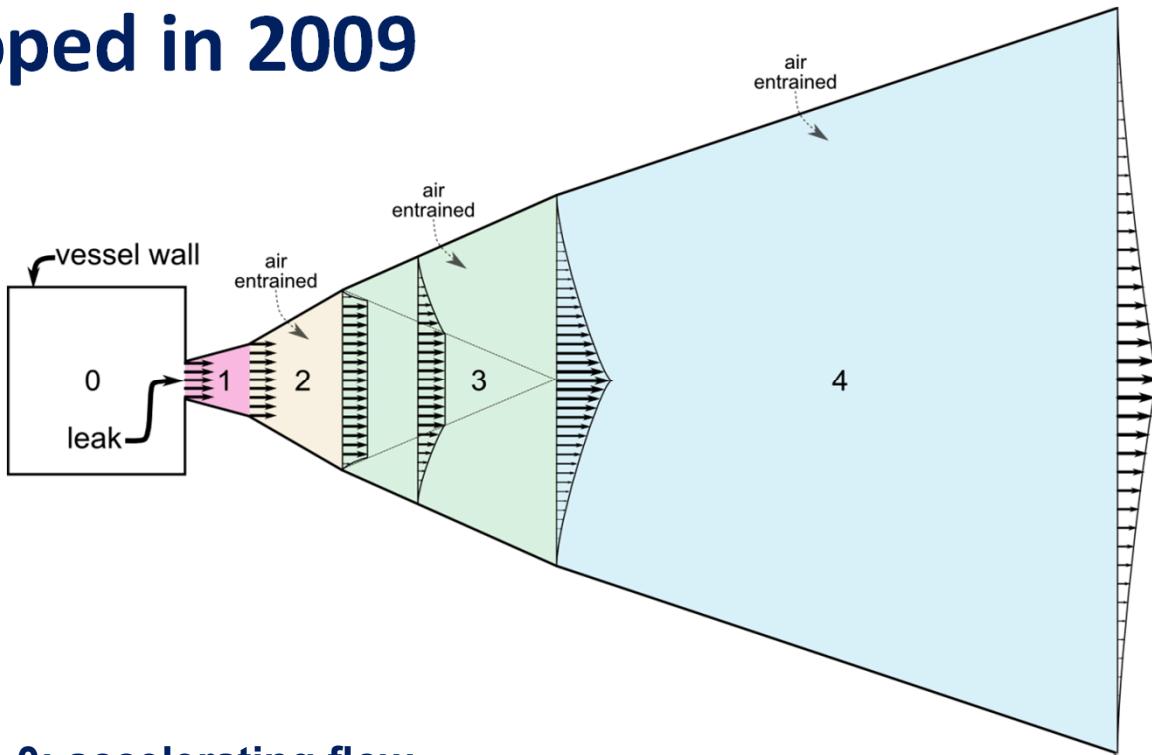
# Current network flow model (NETFLOW) must be updated for use near saturation conditions

- 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



# A conceptual model for liquid H<sub>2</sub> releases was originally developed in 2009

- Steady-state
- 1-dimensional (along streamline coordinate)



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

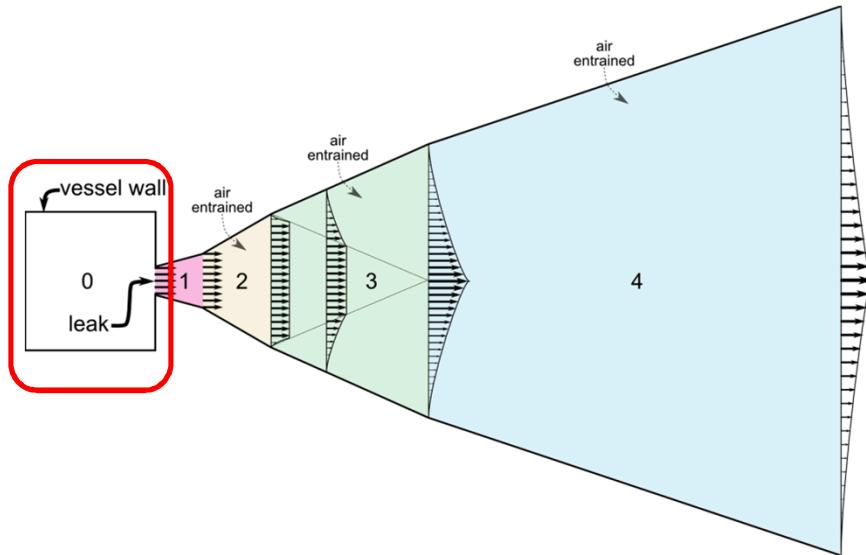
Winters, SAND Report 2009-0035

Winters & Houf, IJHE, 2011

Houf & Winters, IJHE, 2013

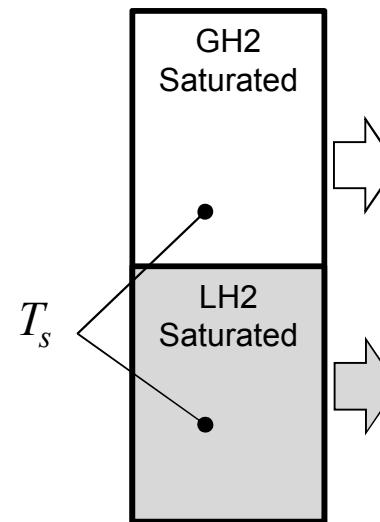
Ekoto et al., SAND2014-18776

# Accelerating flow (leak) develops from saturated storage conditions



- conserved energy with isentropic expansion

Ekoto et al., SAND2014-18776

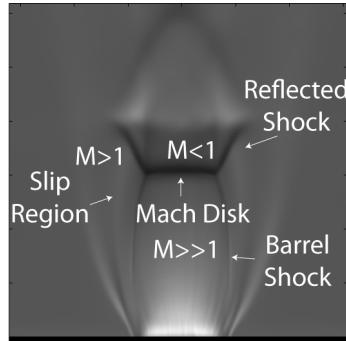
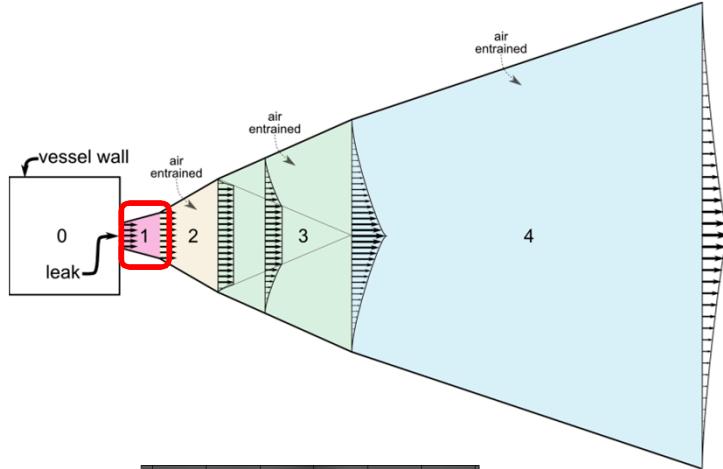


$$w_1^2 = 2(h_0 - h_1)$$

$$s_1 = s_0$$

- 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)



Ruggles & Ekoto, *IJHE*, 2012

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
Yuceil & Otugen (2002)	0.790
Harstad & Bellan (2006)	1.440
Molkov (2008)	0.993
<b>SNL Data (2011)</b>	<b>0.867</b>

\*All models updated w/ Able-Noble EOS

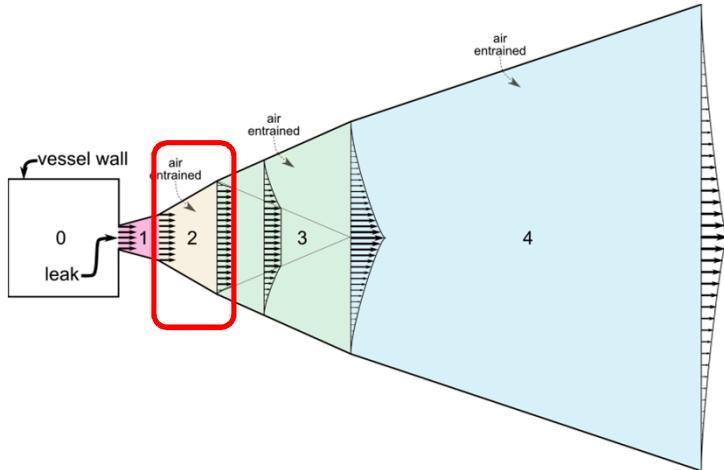
Neglects Mach Disk  
(i.e., fully supersonic)

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

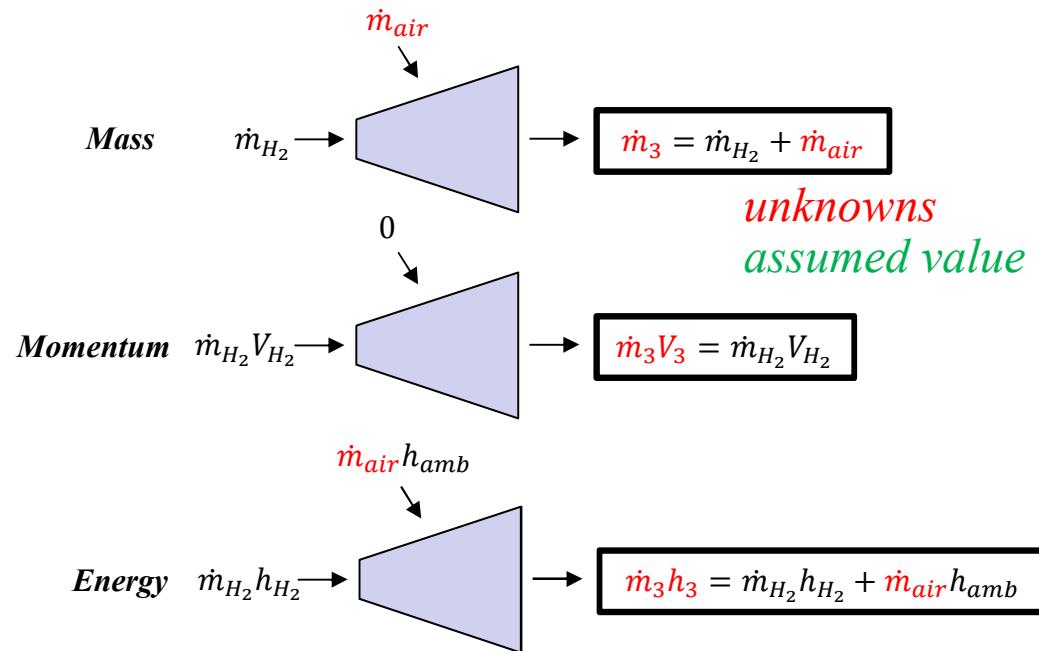
Reality is that fluid is split  
between the slip and  
Mach disk regions

*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



State modeling by NIST H<sub>2</sub> EOS:

$$h_3 = f(Y_{H_2,3}, p_{amb}, T_3)$$

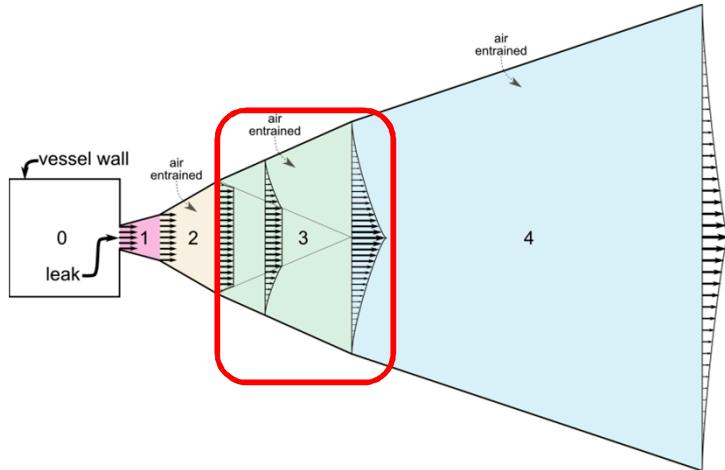
Species conservation used to close system of equations:

$$\dot{m}_{air} = \dot{m}_{H_2} \frac{1 - Y_{H_2,3}}{Y_{H_2,3}}$$

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



unknowns  
assumed value

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

*Mass*

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

*Momentum*

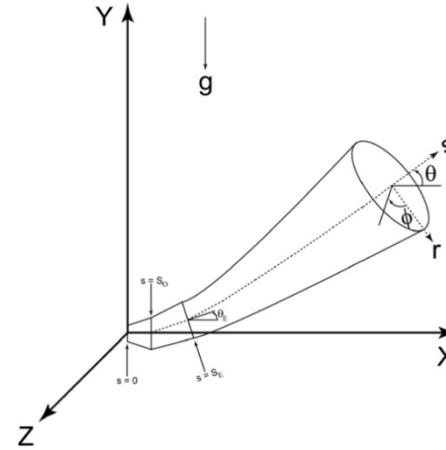
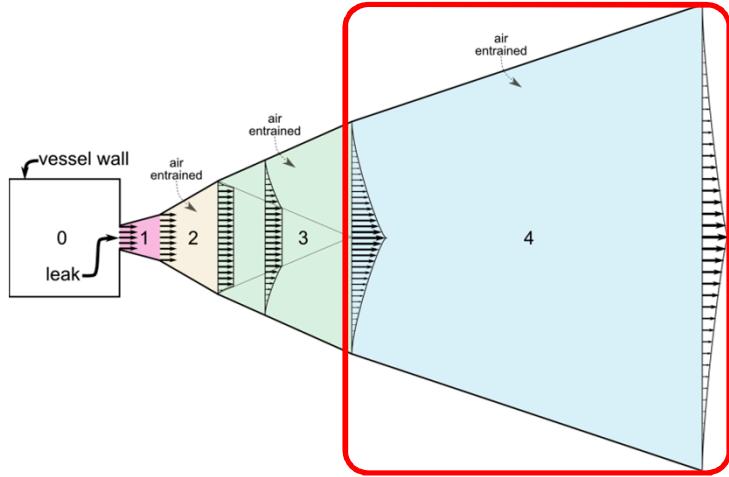
$$(\rho_{amb} - \rho_3) \frac{D_3^2}{4} = B_4^2 \left[ \frac{\rho_{amb}}{2} - \frac{\lambda^2}{2\lambda^2 + 1} (\rho_{amb} - \rho_{CL,4}) \right]$$

$s_3$

$s_4$

Winters, SAND Report 2009-0035

# 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

$\alpha_b$ : Buoyancy entrainment coefficient

$\alpha_m$ : Momentum entrainment coefficient

$g$ : Gravity constant

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

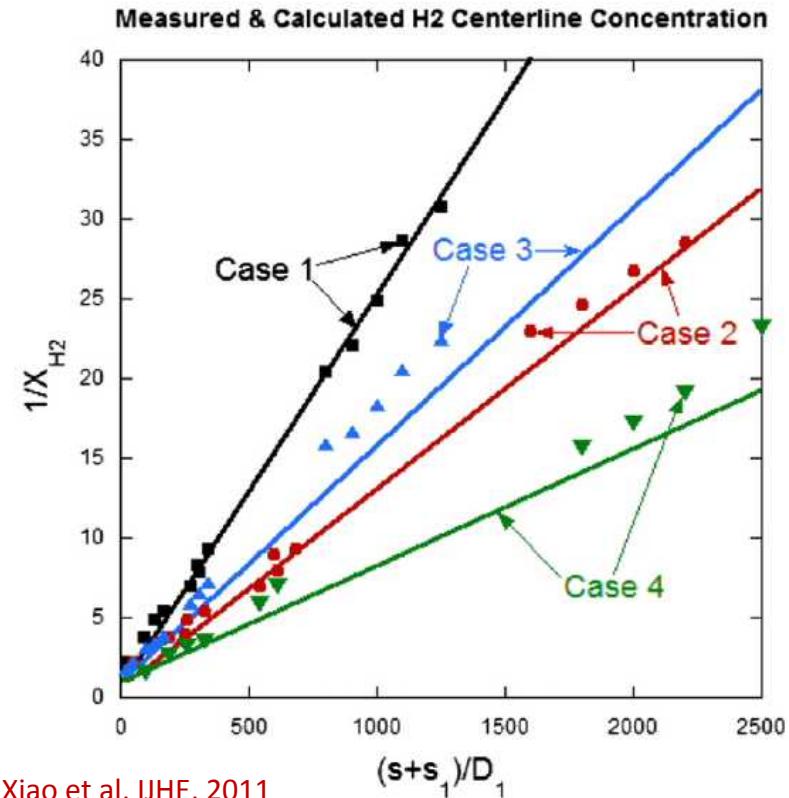
$$E_{mom} = \alpha_m \left( \frac{\pi D^2}{4} \frac{\rho V^2}{\rho_{amb}} \right)^{\frac{1}{2}}$$

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

$$\begin{aligned}
 & \text{Mass} \quad \frac{\partial}{\partial S} \int_0^{2\pi} \int_0^{\infty} \rho V r dr d\phi = \rho_{amb} E \\
 & \text{x-Mom} \quad \frac{\partial}{\partial S} \int_0^{2\pi} \int_0^{\infty} \rho V^2 \cos \theta r dr d\phi = 0 \\
 & \text{y-Mom} \quad \frac{\partial}{\partial S} \int_0^{2\pi} \int_0^{\infty} \rho V^2 \sin \theta r dr d\phi = \int_0^{2\pi} \int_0^{\infty} (\rho_{amb} - \rho) g r dr d\phi \\
 & \text{Species} \quad \frac{\partial}{\partial S} \int_0^{2\pi} \int_0^{\infty} \rho V Y r dr d\phi = 0 \\
 & \text{Energy} \quad \frac{\partial}{\partial S} \int_0^{2\pi} \int_0^{\infty} \rho V (h - h_{amb}) r dr d\phi = 0
 \end{aligned}$$

# Model results compare favorably to experiments from Karlsruhe Institute of Technology

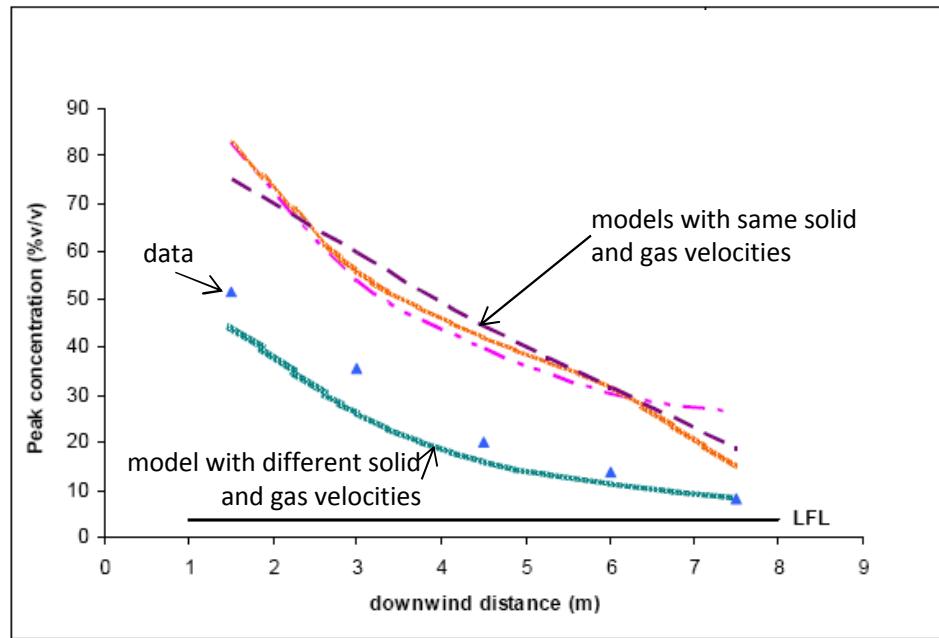
Case	Reservoir pressure [MPa]	Reservoir temperature [K]	Leak diameter [mm]
1	1.7	298	2
2	6.85	298	1
3	0.825	80	2
4	3.2	80	1



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

# As moisture and air condense, multi-phase flows may have droplet/particle slip

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



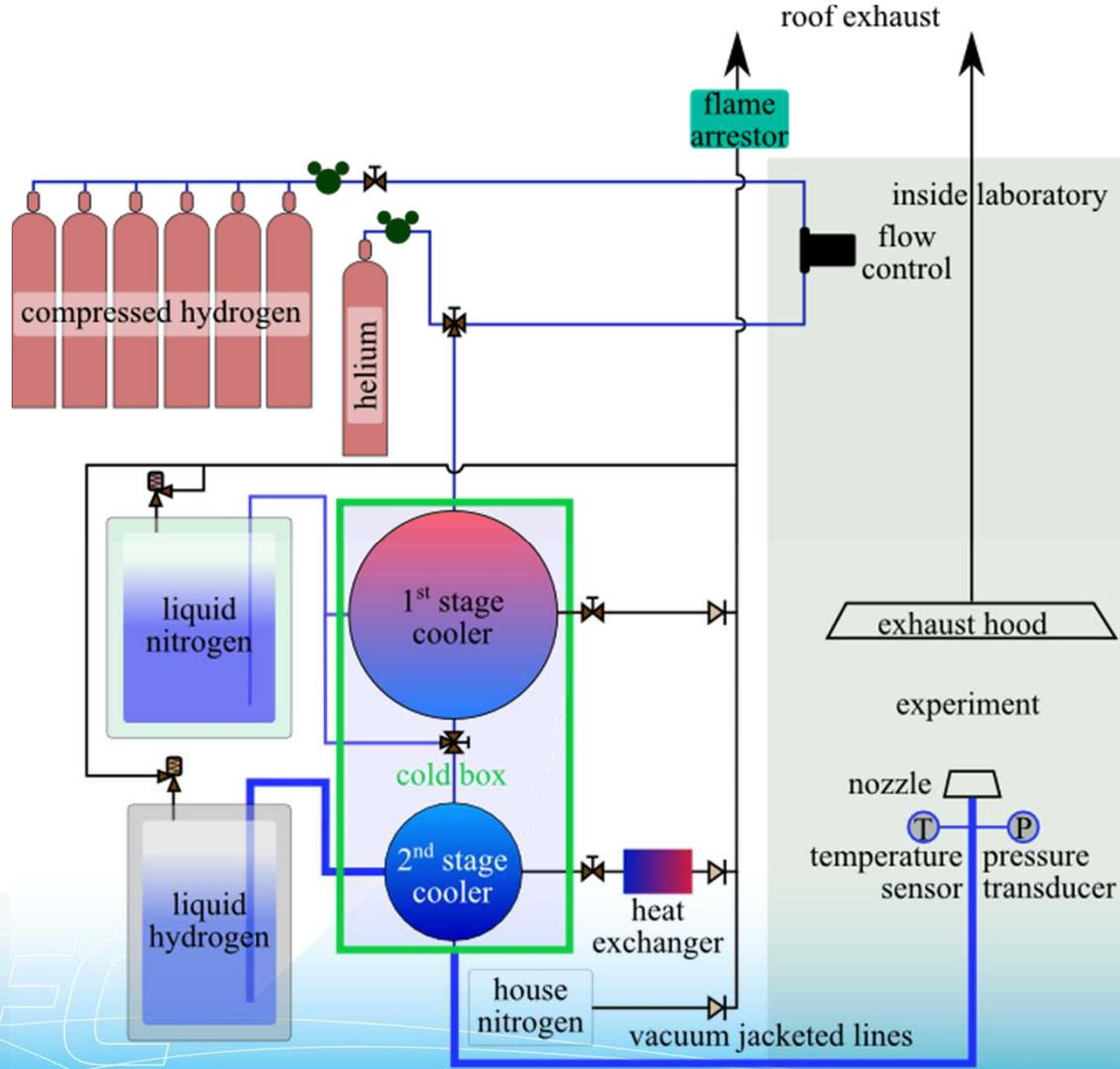
HSL Measurements: Sample probes  
Hooker et al, ICHS, 2011

ADREA-HF CFD Simulations  
Giannissi et al, ICHS, 2013

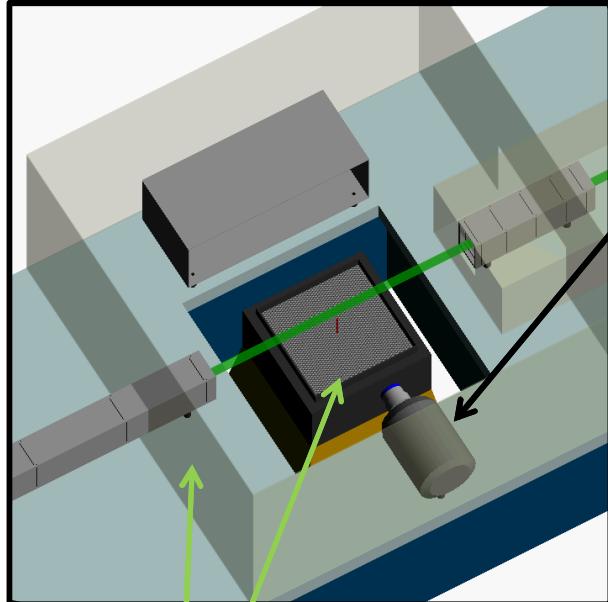
*Substantial differences in model results suggest 2-phase effects cannot be neglected for LH<sub>2</sub> releases*

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

# We plan to retrofit our lab to generate the necessary low temperature data for model validation



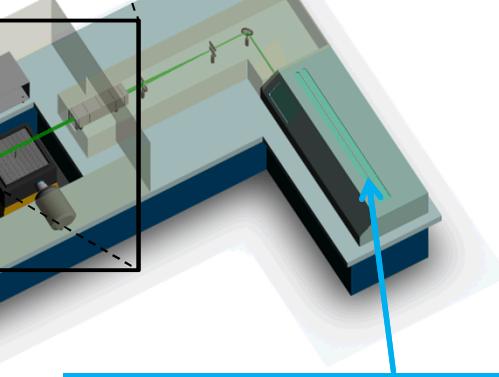
# Optical diagnostics with carefully controlled boundary conditions will provide validation data



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

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

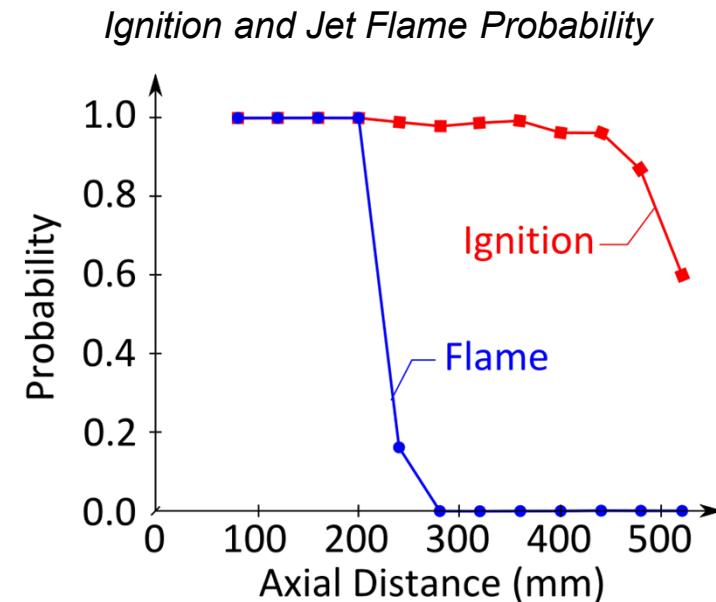
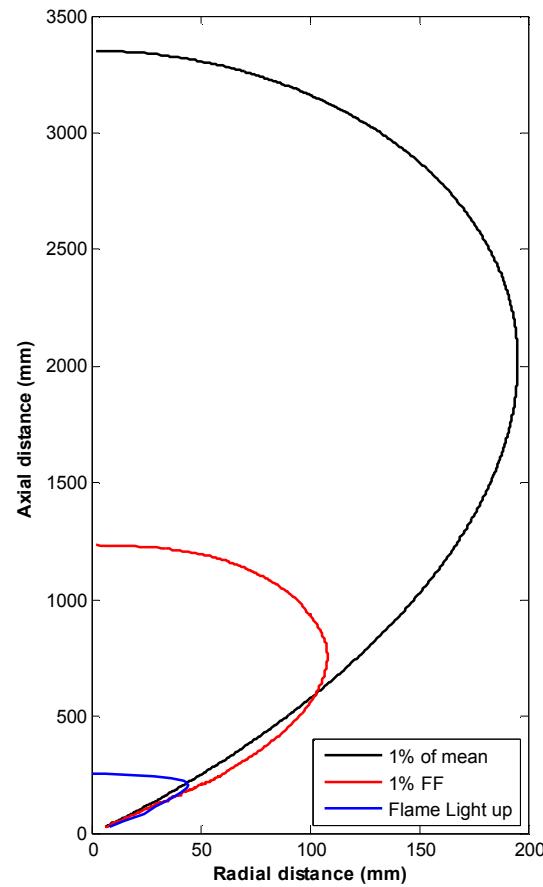
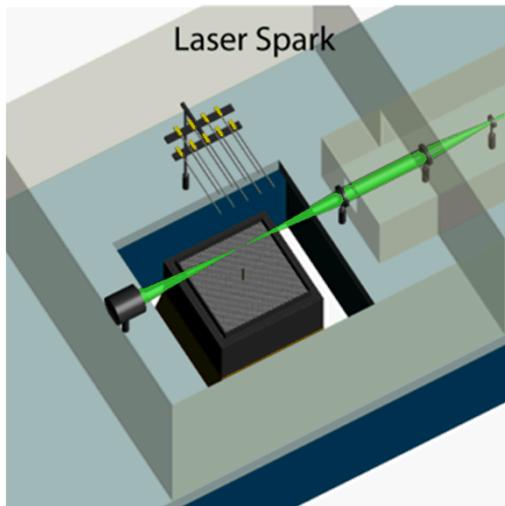


Nd:YAG injection seeded laser (1 J/pulse @ 532 nm)



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

# Future work to verify and quantify ignition boundaries



# Summary and conclusions

## Experimental plans:

- update network flow model
- build out laboratory system
- planar laser Rayleigh scattering to measure jet spreading
- particle imaging velocimetry to measure velocity
- model validation and updating
- ignition quantification

## Challenges for liquid H<sub>2</sub> reduced-order modeling:

- accurate state modeling
- pool spreading and evaporation
- humidity effects
- multiphase flow models, with velocity slip
- interactions with surfaces (e.g. barriers, ground)

# 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<sub>2</sub> Safety, Codes, and Standards team - Daniel Dedrick, Chris San Marchi, Katrina Groth, and Chris LaFleur