

## Project SA5

# Hydrogen Release Behavior

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# Overview

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## Timeline

- Project start date Oct 2003
- Project end date Sep 2015
- Percent complete 33%

## Budget

- Total project funding (from FY03)
  - DOE share: \$8.3M
- FY06 Funding: \$1.5M
- FY07 Funding: \$2.9M (\$2.1M for hydrogen release and risk)

## Partners

- SRI: combustion experiments
- ISO/IPHE Contractor: R. Mauro
- IEA Contractors: W. Hoagland & Associates, and Longitude 122 West
- Interactions with CSTT, ICC, NFPA, NHA, NIST, CTFCA

## Barriers & Targets

### 2006 MYRDDP Section 3.6.4.1 Targets:

- Provide expertise and technical data on hydrogen behavior and hydrogen technologies
- Hydrogen storage tank standards for portable, stationary and vehicular use

### 2006 MYRDDP Section 3.6.4.2 Barriers:

- J. Lack of National Consensus on Codes & Standards
- K. Lack of Sustained Domestic Industry Support at International Technical Committees
- N. Insufficient Technical Data to Revise Standards
- P. Large Footprint Requirements for Hydrogen Fueling Stations



# Objectives

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- Development of new hydrogen codes and standards needs a traceable technical basis:
  - characterize small-scale gaseous leaks, determine barrier wall effectiveness
  - perform physical and numerical experiments to quantify fluid mechanics, combustion, heat transfer, cloud dispersion behavior
  - develop validated engineering models and CFD models for consequence analysis
  - use quantitative risk assessment for risk-informed decision making and identification of risk mitigation strategies
  - Develop heat transfer and flow models to optimize 70 MPa fueling
- Provide advocacy and technical support for the codes and standards change process:
  - consequence and risk: ICC and NFPA(2, 55)
  - international engagement: HYPER (EU 6<sup>th</sup> Framework Program), *Installation Permitting Guidance for Hydrogen and Fuel Cell Stationary Applications*



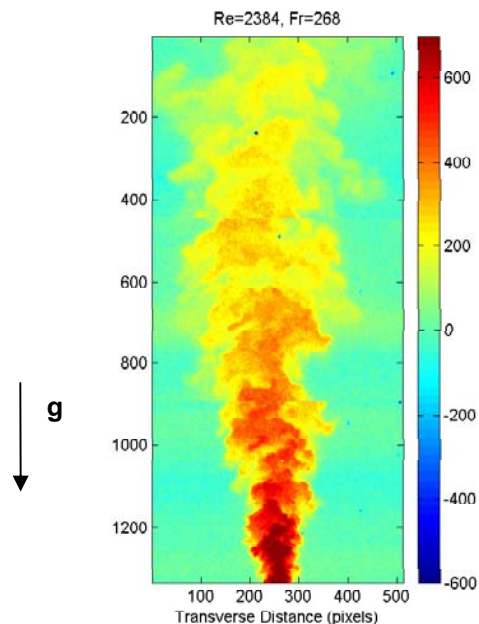
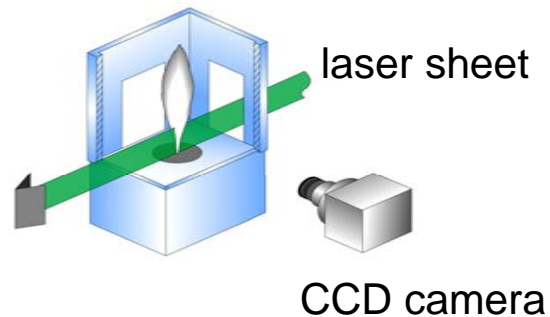
# Approach

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- Conduct characterization experiments for hydrogen releases using imaging techniques to quantify plume characteristics (visible length, heat flux, concentration contours), validate engineering models against the experimental results
- Introduce more risk-informed decision making in the codes and standards development process using quantitative risk assessment (QRA); provide a traceable technical basis for new codes
- Characterize mitigation effectiveness of barriers/deflectors for hydrogen releases using experiments and models; validate Navier-Stokes calculations (CFD) of hydrogen jet flames and simulations of jet deflection; partner with HYPER on combustion hazards
- Develop fueling model to characterize the 70 MPa fast-fill process; apply model to identify optimal fuel strategy for the SAE J2601 interface standard

# Rayleigh scattering is used to map concentration contours of small/slow leaks

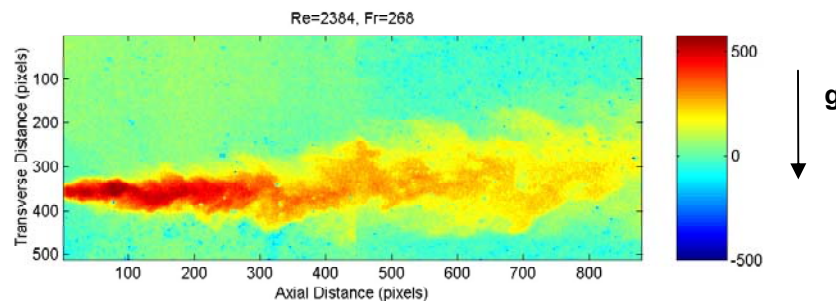
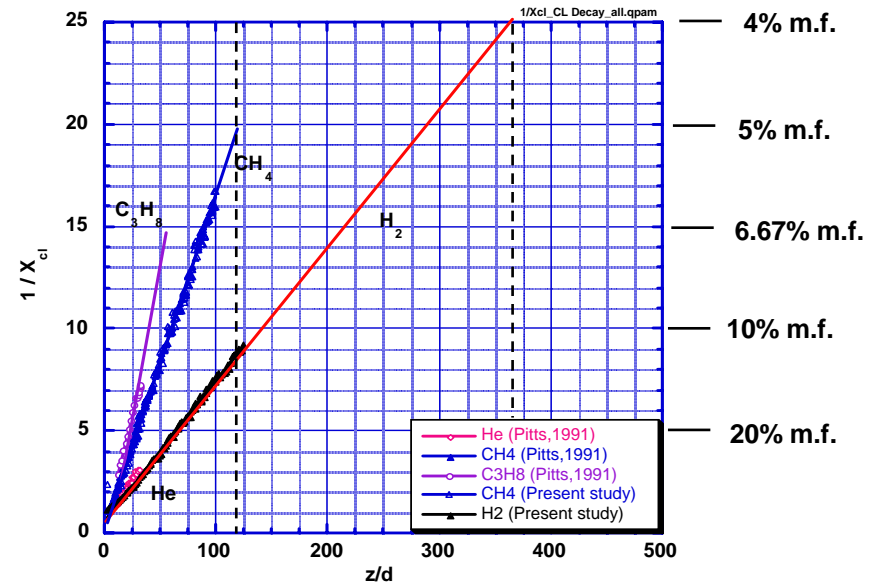
Rayleigh scattering system



Instantaneous  $H_2$  mole fraction images  
in unignited vertical jet



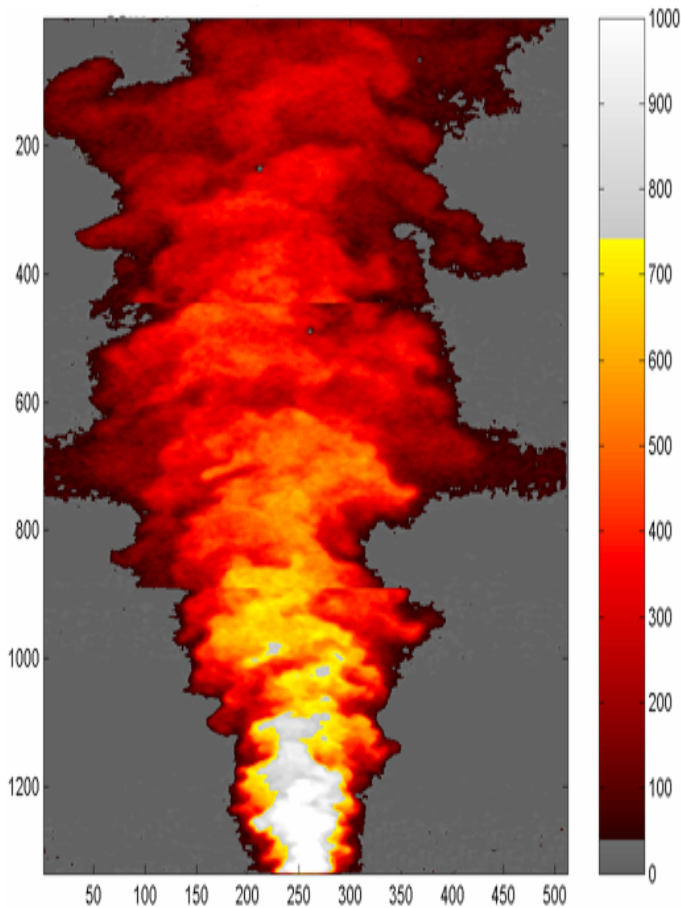
Experimentally measured centerline concentration  
decay rates in vertical buoyant jets



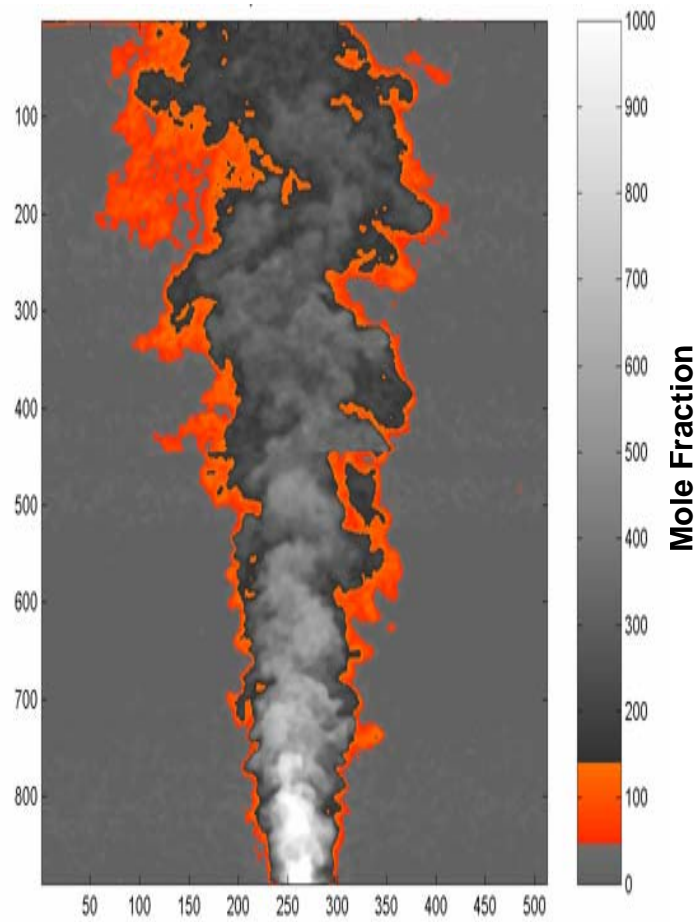
Instantaneous  $H_2$  mole fraction images  
in unignited horizontal jet

# Comparison of jet ignitable gas envelope for hydrogen and methane

H<sub>2</sub> jet at Re=2,384; Fr = 268



CH<sub>4</sub> jet at Re=6,813; Fr = 478



H<sub>2</sub> flammability limits:  
LFL 4.0%; RFR 75%

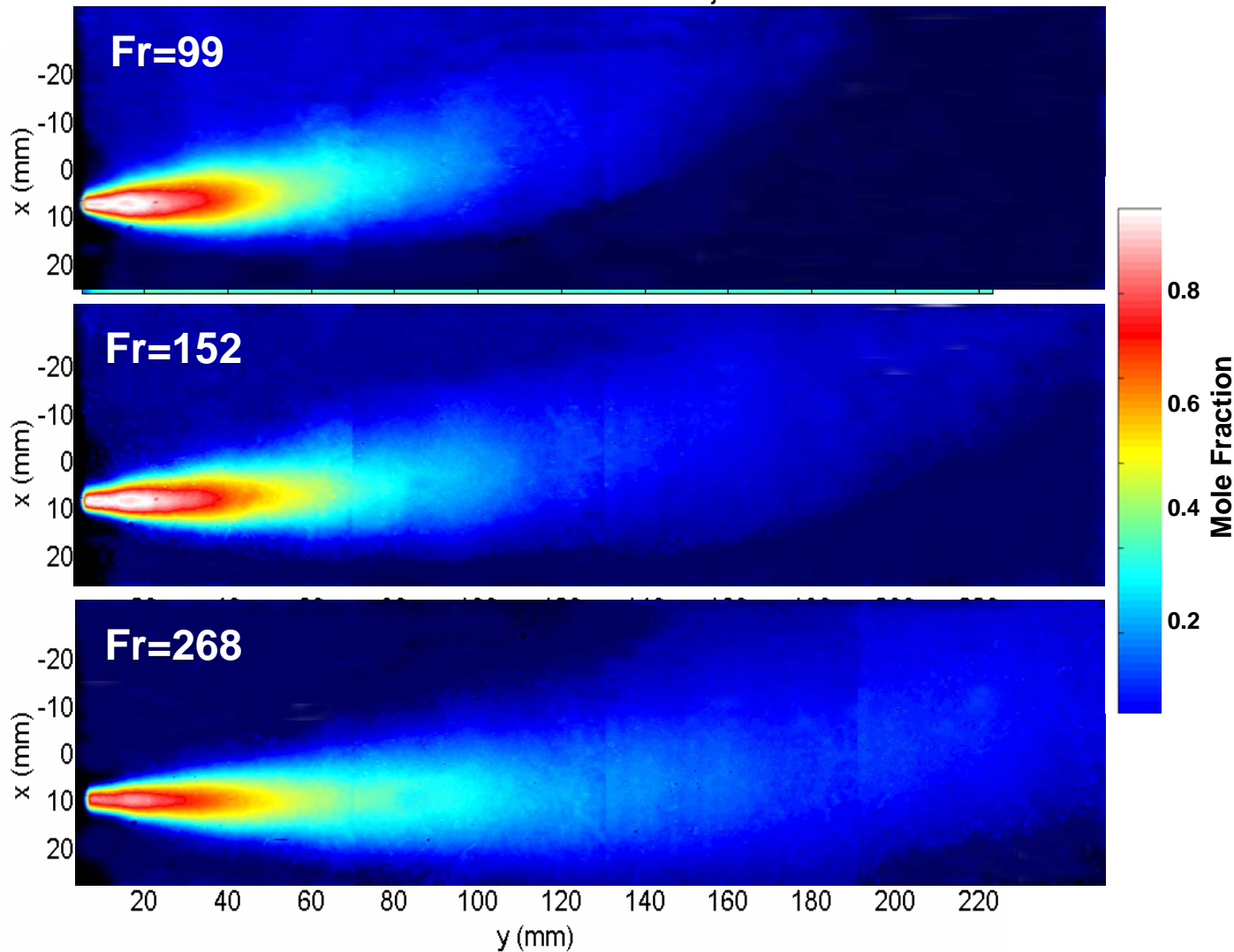
CH<sub>4</sub> flammability limits:  
LFL 5.2%; RFR 15%

*Ignitable gas envelope is significantly larger in H<sub>2</sub> jets than CH<sub>4</sub> jets.*



# Buoyancy effects are characterized by Froude number

Horizontal H<sub>2</sub> Jet ( $d_j=1.9$  mm)

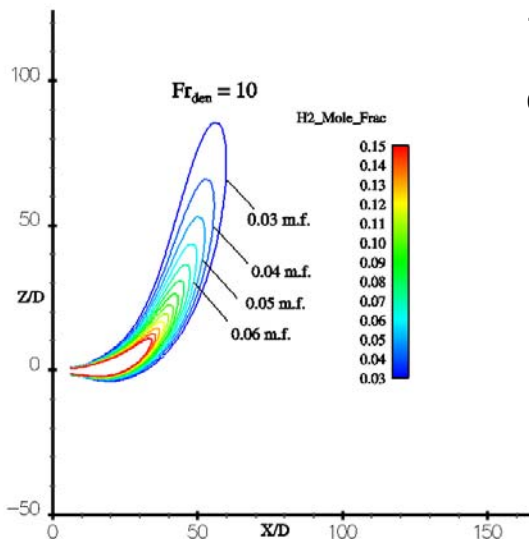


- Time-averaged H<sub>2</sub> mole fraction distributions.
- Froude number is a measure of strength of momentum force relative to the buoyant force
- Increased upward jet curvature is due to increased buoyancy at lower Froude numbers.

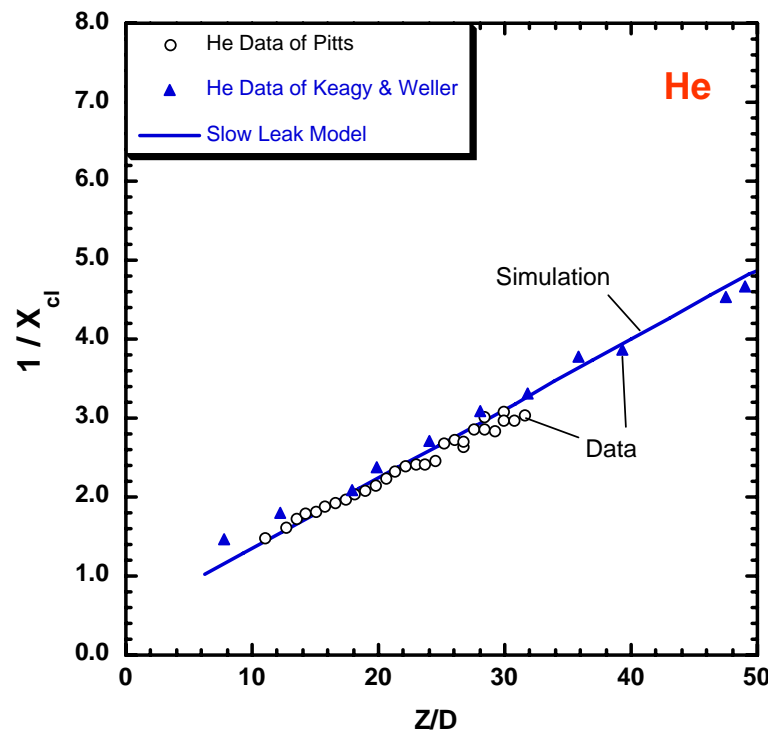
# The engineering model has been validated against data for buoyant slow leaks

The buoyantly-driven flow model :

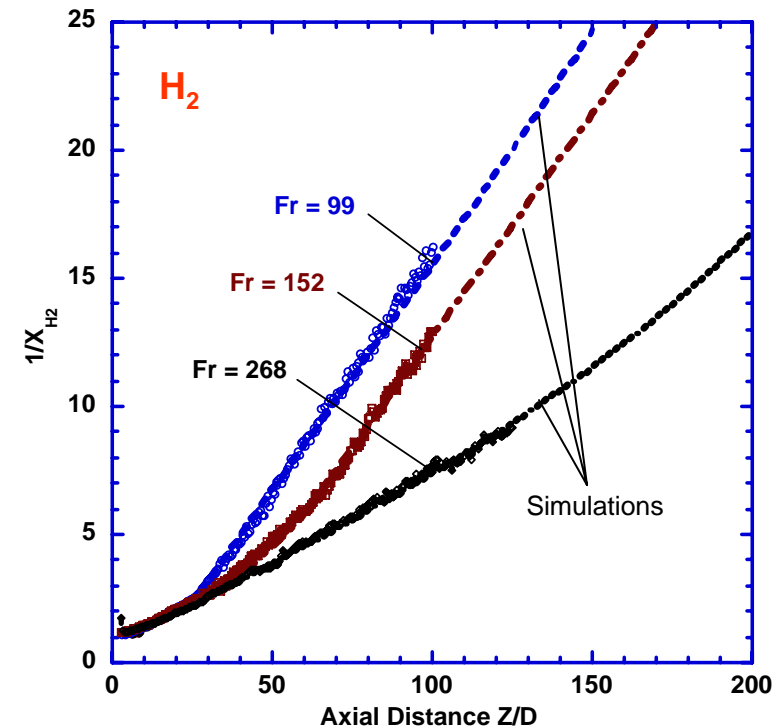
- uses a different entrainment law than our momentum jet model
- integrates along the stream line to capture plume trajectory



Comparison of model and data for concentration decay of vertical buoyant He plume



Comparison of model with data from the Sandia slow-leak experiments for buoyant H<sub>2</sub> plumes

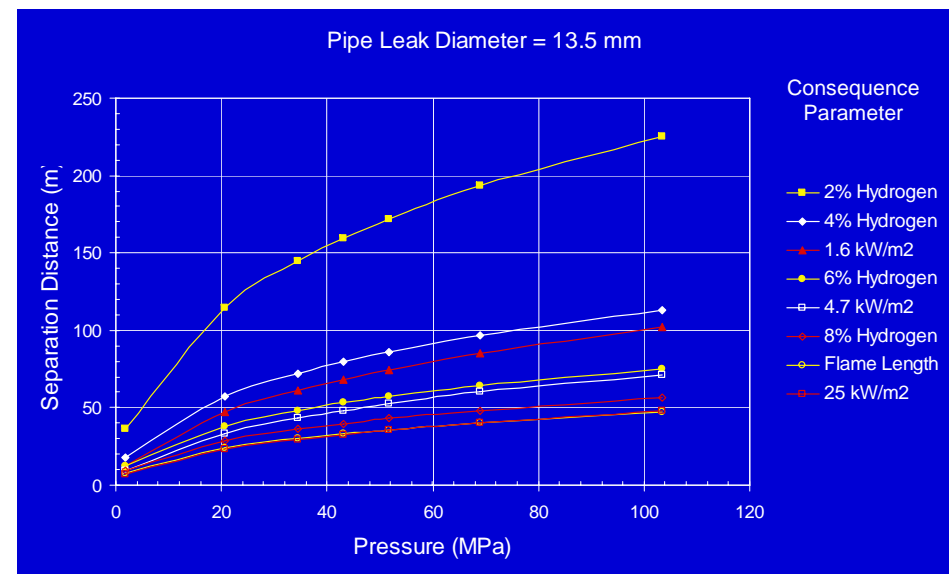
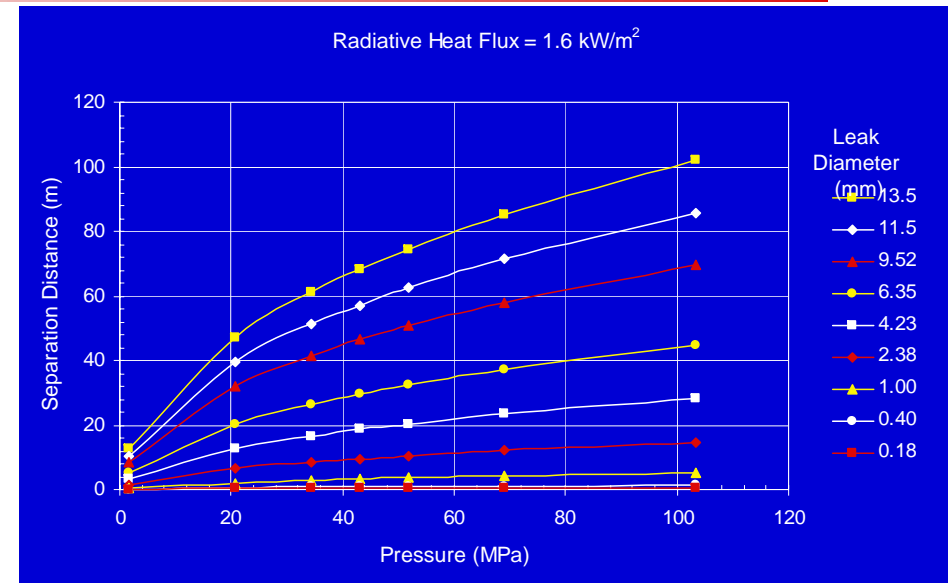


- Lower Froude number leaks are more buoyant
- Buoyancy increases entrainment rate causing faster concentration decay
- New entrainment law adds buoyancy-induced entrainment to momentum induced entrainment



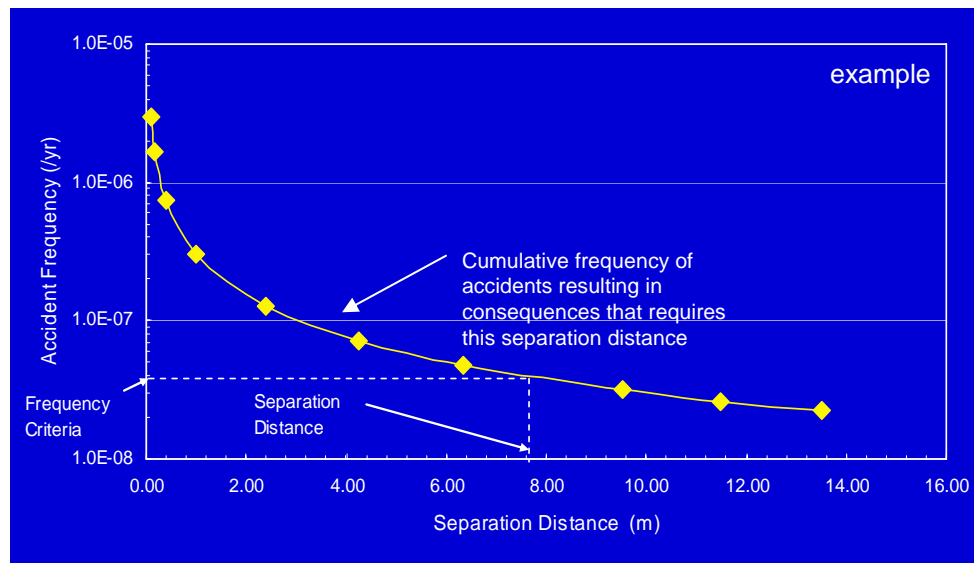
# Consequence-based separation distances for hydrogen facilities can be large

- Current code separation distances are not reflective of future fueling station operations (e.g., 70 MPa)
- Facility parameters (e.g., operating pressure and volume) should be used to delineate separation distances
- Consequence-based separation distances (i.e., single event) can be large depending on pressure, leak size, and consequence parameter
- QRA insights are being considered by NFPA-2 to help establish meaningful separation distances and other code requirements



# Risk-informed code development framework

- Quantitative risk assessment (QRA) provides code developers with risk insights to help define codes and standards requirements:
  - requires quantification of consequences from of all possible accidents
  - requires definition of event frequencies
  - requires definition of acceptable risk levels and metrics
- Accounts for parameter and modeling uncertainty present in analysis; evaluates importance of risk assumptions through sensitivity analysis

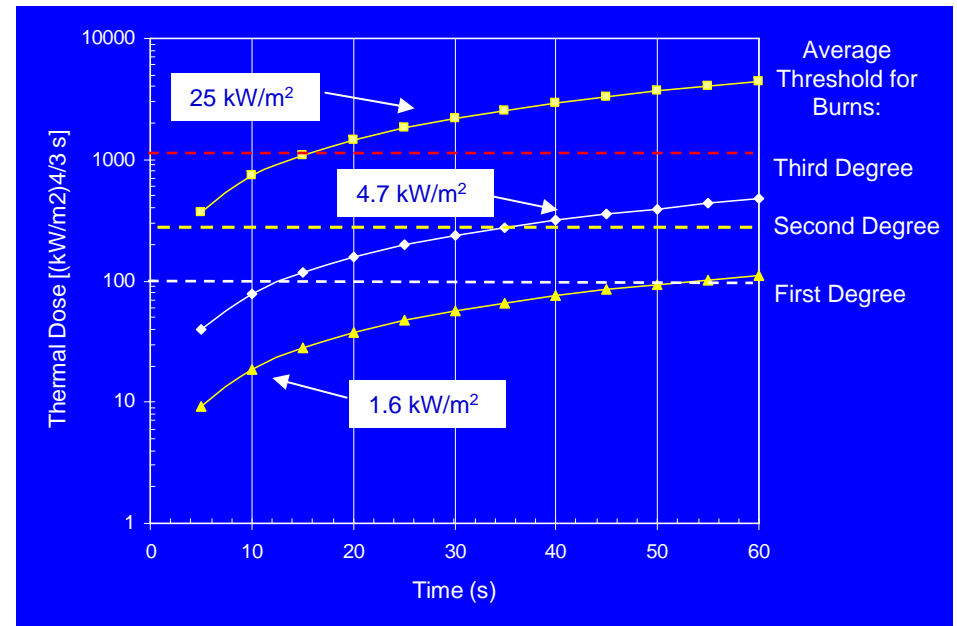


$$\text{Risk} = \text{Frequency} \times \text{Consequence}$$

# QRA requires data!

## Consequence parameters

- radiant heat flux levels for jet fires (from ICC Fire Code):
  - 1.6 kW/m<sup>2</sup> – no harm to individuals for long exposures
  - 4.7 kW/m<sup>2</sup> – injury (second degree burns) within 35 s
  - 25 kW/m<sup>2</sup> – equipment and structural damage (long exposure); third degree burns within 15 s
- Ignitable hydrogen concentration limits:
  - 4%, 6%, and 8% concentrations



## Appropriate failure rate data

- component leakage data
- component failure data
- phenomenological probabilities

## Accident frequency criteria

- suggested range of criteria
  - 10<sup>-6</sup>/yr to 2x10<sup>-4</sup>/yr

Component	Mean Component Leakage Frequency		
	Small Leak	Large Leak	Rupture
Vessel	1E-3/yr	1E-4/yr	1E-5/yr
Pipe	5E-5/m-yr	5E-6/m-yr	5E-7/m-yr
Refueling Hose	0.1/yr	1E-2/yr	1E-3/yr
Pump	3E-3/yr	3E-4/yr	3E-5/yr
Compressor	3E-2/yr	3E-3/yr	3E-4/yr
Electrolyser	1E-4/yr	1E-5/yr	1E-6/yr
Vaporizer	1E-3/yr	3E-4/yr	5E-5/yr
Valve	1E-3/yr	1E-4/yr	1E-5/yr
Pipe Joints/Unions	3E-2/yr	4E-3/yr	5E-4/yr
Flange	3E-4/yr	3E-5/yr	NA
Filter	3E-3/yr	3E-4/yr	3E-5/yr
Instrument Line	1E-3/yr	3E-4/yr	5E-5/yr



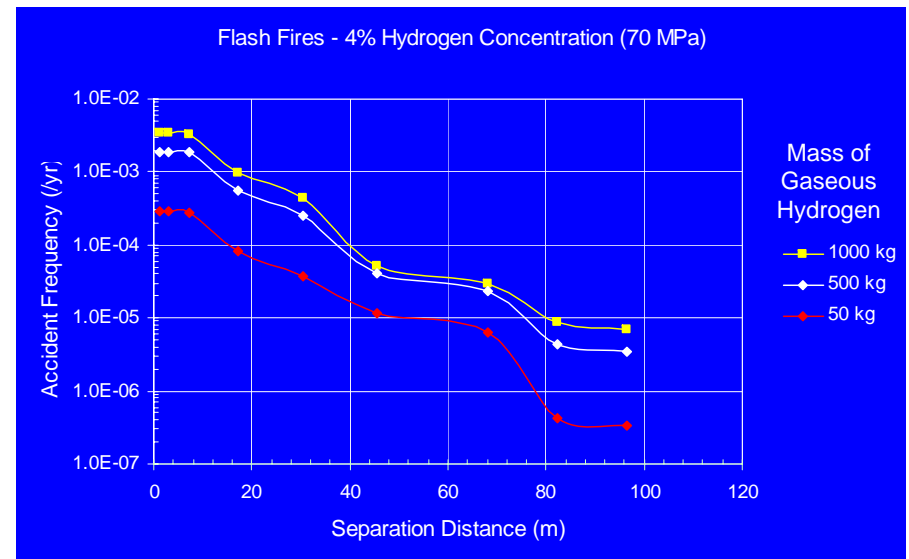
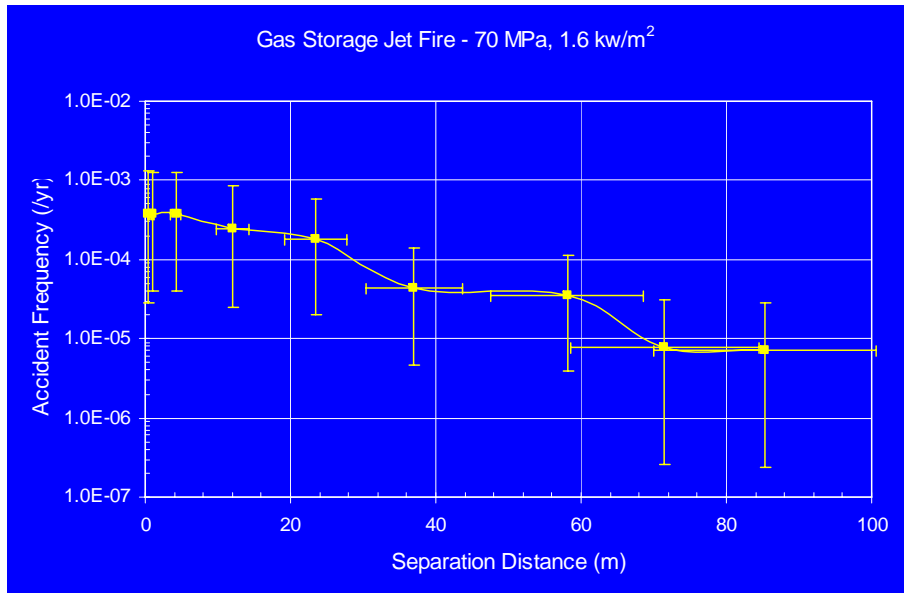
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- Gas Storage Leaks - Flash Fires (Operating Pressure = 70 Mpa)
- Accident Frequency (yr)
- Separation Distance (m)
- Hydrogen Concentration
- 4% H<sub>2</sub>
  - 6% H<sub>2</sub>
  - 8% H<sub>2</sub>
- | Separation Distance (m) | 4% H <sub>2</sub> Accident Frequency (yr) | 6% H <sub>2</sub> Accident Frequency (yr) | 8% H <sub>2</sub> Accident Frequency (yr) |
|-------------------------|---|---|---|
| 0                       | ~2.0E-03                                  | ~2.0E-03                                  | ~2.0E-03                                  |
| 5                       | ~1.8E-03                                  | ~1.5E-03                                  | ~1.0E-03                                  |
| 10                      | ~1.2E-03                                  | ~8E-04                                    | ~5E-04                                    |
| 20                      | ~6E-04                                    | ~3E-04                                    | ~4E-05                                    |
| 30                      | ~3E-04                                    | ~4E-05                                    | ~3E-05                                    |
| 45                      | ~4E-05                                    | ~2E-05                                    | ~4E-06                                    |
| 65                      | ~2E-05                                    | ~3E-06                                    | -   |
| 85                      | ~4E-06                                    | -   | -   |
| 95                      | ~3E-06                                    | -   | -   |

	Risk-Informed Separation Distances Required for Flash Fires in High Pressure Systems (distance in meters)					
	Pipe Leaks			Gas Storage Leaks <sup>1</sup>		
Risk Criteria	35 MPa	70 MPa	105 MPa	35 MPa	70 MPa	105 MPa
2E-4/yr	0	0	0	13-26	16-32	19-36
5E-5/yr	0	0	0	17-30	22-44	24-49
1E-5/yr	0	0	0	29-59	38-76	44-87
5E-6/yr	0	0	0	40-72	40-82	46-92


<sup>1</sup> Range corresponds to distances for 8% - 4% H<sub>2</sub> concentration by volume.

# Uncertainty and sensitivity analysis

- Accident frequency sensitivity:
  - distribution of component leak size versus frequency is a critical parameter
  - ignition probabilities are also critical parameters
- Consequence-related sensitivity:
  - consideration of leak orientation can reduce separation distances
  - inclusion of temporal effects is not important for jet fires
- Facility-related sensitivity:
  - reducing stored gas mass or increasing gas cylinder size can reduce leakage frequency and risk-based separation distance (i.e., less-complicated system)

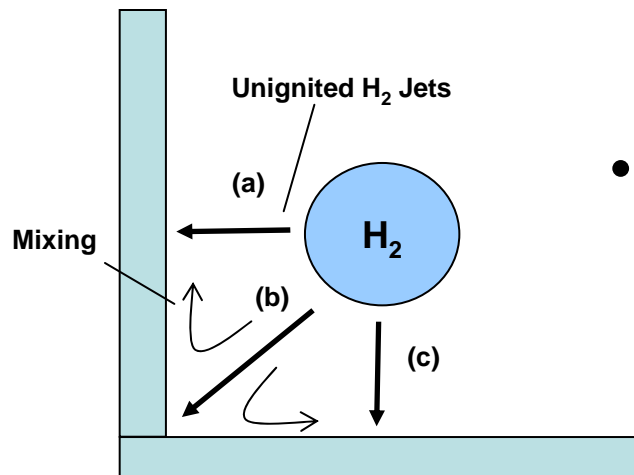






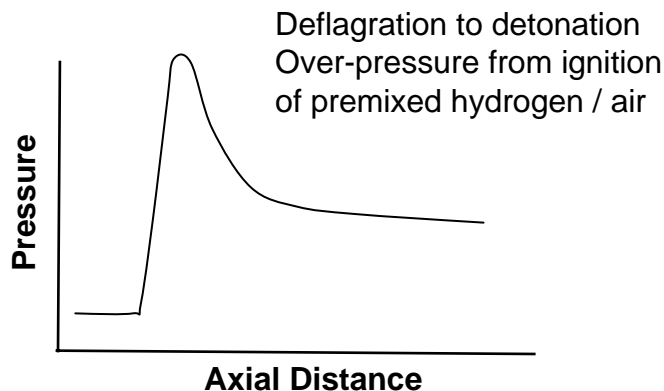
# We are studying barriers as a mitigation strategy to reduce safety distances

- Goal: determine if barriers are an effective jet mitigation technique since mixtures of  $H_2$  and air can ignite and potentially generate large overpressures.
- Collaborating with the HYPER project in Europe.

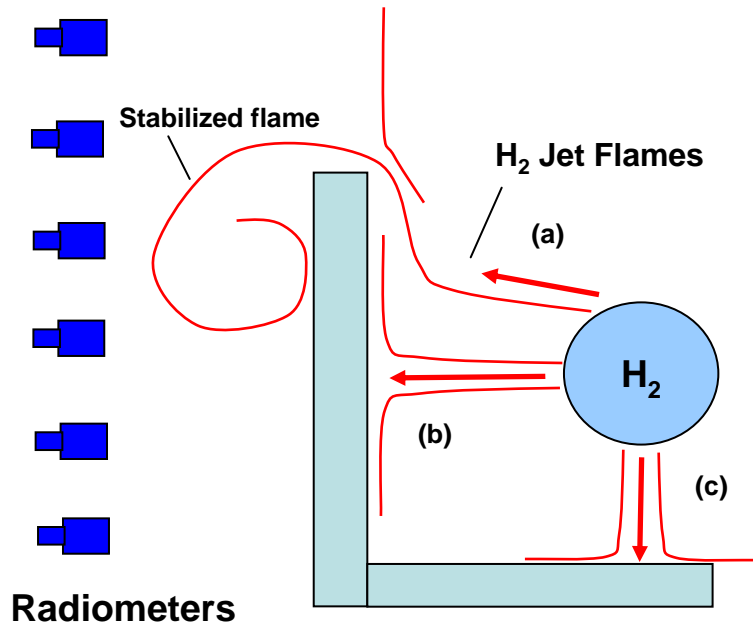


## Over-pressure characterization

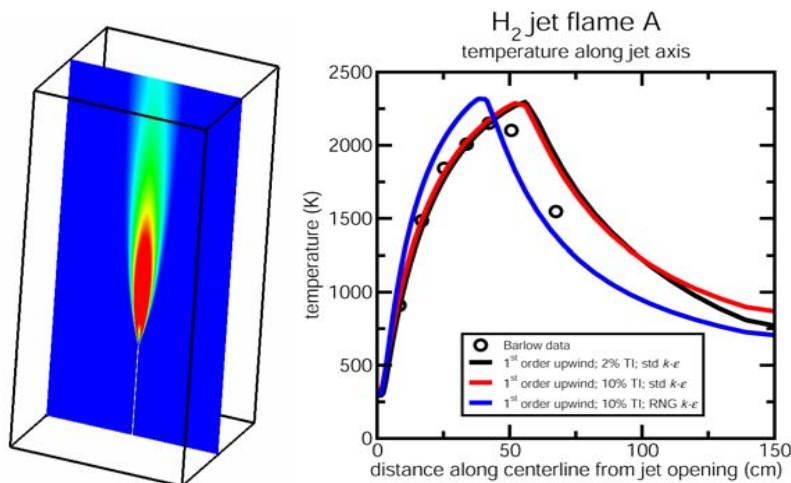
- Characterize  $H_2$  transport and mixing near barrier walls through combined experiment and modeling
- Identify conditions leading to deflagration or detonation
  - residence time and ignition timing
  - magnitude of over-pressure and duration
- Develop correlations for wall heights dependency and wall-standoff distances
- Combine data and analysis with quantitative risk assessment for barrier configuration guidance



# The behavior of $H_2$ jet flames near barrier walls is also an issue of importance



- Characterize stabilization of  $H_2$  jet flame on and behind barrier
- Characterize thermal/structural integrity of barriers
- Use CFD modeling and validation for  $H_2$  jet flames to minimize the number of tests
- Develop correlations for wall height dependencies and wall stand-off distances
- Combine data and analysis with quantitative risk assessment for barrier configuration guidance



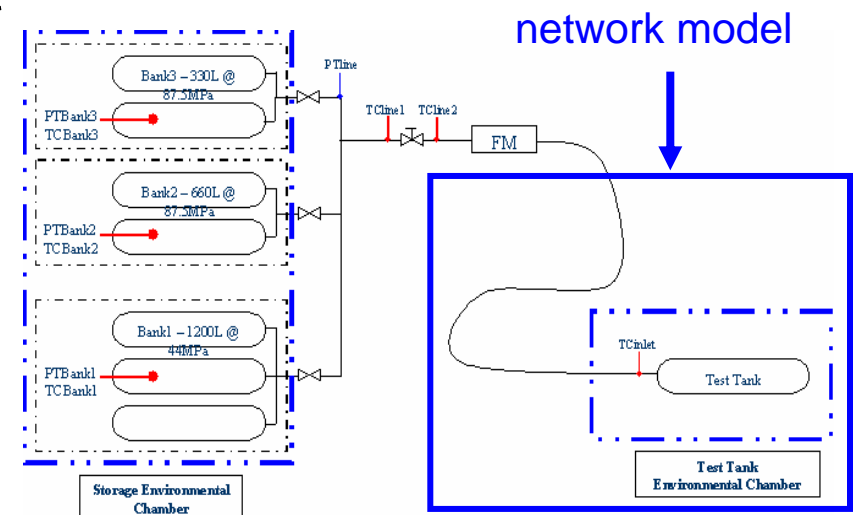
Barlow flame A (ref. Combustion and Flame, v. 117, pp. 4-31, 1999)

# Flow and heat transfer model for the multi-client 70 MPa fast-fill study

- Develop a network flow model and heat transfer correlation for the 70 MPa fast-fill hydrogen fueling process
- Model will be calibrated against Powertech constant pressure ramp rate experiments
- The calibrated model will be used to predict fill characteristics for untested and off-design conditions
  - ambient and tank conditions
  - pre-cooling temperatures
  - fueling ramp rates
  - station-side plumbing variations
  - fuel system variations



Powertech's 70 MPa fast fill test facility equipped with hydrogen-safe environmental chambers.





# Future Work

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## Remainder of FY07

- Finish buoyancy-driven leak work and publish
- Perform risk assessment (QRA) of refueling station hazards
- Perform experiments and calculations for safety aspects of barrier walls
- Develop a network flow model for 70 MPa fueling process

## FY08

- Continue investigation of safety aspects of barrier walls and other passive mitigation strategies
- Develop scientific theory for ignition criteria for turbulent hydrogen leaks
- Extend risk analysis to identify needs for step-out technologies; study how the public perceives risk in order to develop a risk communication strategy
- Begin scoping liquid hydrogen safety issues
- Complete studies and optimization of the 70 MPa fueling process



# Summary

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- Completed engineering model for buoyant plumes and reported at 2007 NHA meeting and SAE World Congress
- QRA is being used to make risk-informed decisions regarding set-backs as part of the NFPA-2 activity
  - Sandia staff are participating with the technical committee
  - QRA incorporates Sandia hydrogen release engineering models
  - QRA methodology is vetted through international risk experts as part of our involvement in IEA Hydrogen Safety Task 19
- Barrier walls are being characterized as a jet mitigation strategy for set back reduction
  - Partnership with SRI (testing) and HYPER (analysis)
  - CFD best-practices working group





# Responses to previous year reviewers' comments

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1. *“Attempt to engage researcher as a voting member in the various technical committees on hydrogen in the model and design code activities.”; “It was not clear if the project is working with organizations such as NFPA that are establishing setback distances.”*
  - M.Gresho chairs NFPA-2, coordinates through HIPOC
  - W. Houf is a member of NFPA-55 and NFPA-2; J. LaChance contributes to NFPA-2; both are members of the NFPA-2 set-back task force
2. *“Need to re-examine the allowable risk level and programmatic impacts of a potential accident.”*
  - Risk metrics are vetted through IEA Hydrogen Safety Task 19 experts
  - Sensitivity analysis is used to bound uncertainties and model errors
3. *“Other labs have flame plume and hazard data; need better collaboration.”*
  - Other data used in buoyant plume model validations
  - Coordinating with NIST Building & Fire Research Lab
  - Participate in CFD validation workshops with NREL, NIST, CTFCA



# Publications

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1. Houf and Schefer, “Small-Scale Unintended Releases of Hydrogen” , 2007 NHA Conference, San Antonio, TX, March 19-22, 2007.
2. Houf and Schefer, “Investigation of Small-Scale Unintended Releases of Hydrogen”, SAE World Congress, Detroit, MI, April 16-19, 2007, (invited paper).
3. LaChance, "Risk-Informed Separation Distances for Hydrogen Refueling Stations“, 2007 NHA Conference, San Antonio, TX, March 19-22, 2007.
4. Schefer and Houf, “Investigation of small-scale unintended releases of hydrogen: momentum-dominated regime”, submitted to *International Journal of Hydrogen Energy*.



# Presentations

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1. LaChance, "Risk-Informed Safety Distances for Hydrogen Refueling Stations", IEA Task 19 Hydrogen Safety Experts Meeting, Vancouver, Canada, September 6, 2006.
2. Schefer, Houf, Moen and Keller, "Hydrogen Safety Codes and Standards: Unintended Releases", IEA Task 19 Hydrogen Safety Experts Meeting, Vancouver, Canada, September 6-8, 2006.
3. LaChance, "Risk-Informed Safety Distances for Hydrogen Refueling", NFPA Hydrogen Technology Technical Committee Meeting, Golden, CO, November 2-3, 2006.
4. Houf and Schefer, "Research and Development on Unintended Releases for Hydrogen Safety, Codes and Standards", NFPA Hydrogen Technology Technical Committee Meeting, Golden, CO, November 2-3, 2006.
5. Keller, "Sandia National Laboratories Hydrogen Program", HYPER Program Kickoff Meeting, Manchester, UK, November 15, 2006.
6. Schefer, Houf, and Evans, "Hydrogen Safety Codes and Standards: Unintended Releases", CFD Best Practices Working Group Meeting, Livermore, CA, December 8, 2006.
7. Schefer, Houf, and Evans, "Hydrogen Safety Codes and Standards: Unintended Releases", Hydrogen Codes and Standards Technical Team Meeting, Sandia National Laboratory, Livermore, CA, January 31, 2007.
8. Houf, Schefer, and Evans, "Research and Development for Hydrogen Safety Codes and Standards", Hydrogen Codes and Standards Technical Team Meeting, Sandia National Laboratory, Livermore, CA, January 31, 2007.
9. Winters, "Modeling Network and Vessel Heat Transfer," Hydrogen Codes and Standards Technical Team Meeting, Sandia National Laboratory, Livermore, CA, January 31, 2007.
10. LaChance, "Risk-Informed Separation Distances for an Example Hydrogen Refueling Station", IEA Task 19 Hydrogen Safety Experts Meeting, Tsukuba, Japan, January 31, 2007.
11. Schefer, Houf, Moen and Keller, "Hydrogen Safety Codes and Standards: Unintended Releases", IEA Task 19 Hydrogen Safety Experts Meeting, Tsukuba, Japan, January 31, 2007.
12. Houf, Evans, and Schefer, "Validation of CFD for Hydrogen Release Scenarios", CFD Best Practices Working Group Meeting, San Antonio, TX, March 19, 2007.