



# Hydrogen Release Behavior

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Project SCS010

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000



# Overview

## Timeline

- Project start date Oct 2003
- Project end date Sep 2015
- Percent complete 60%

## Barriers

- 2007 Targets:
  - Provide expertise and technical data on hydrogen behavior, risk, and hydrogen and fuel cell technologies
- 2007 Barriers:
  - G. inadequate representation at international forums
  - N. insufficient technical data to revise standards
  - P. large footprint requirements for hydrogen fueling stations
  - Q. parking and other access restrictions

## Budget

Total project funding (to date)

- DOE share: \$13.6M (\$11.7M\*)
  - FY09 Funding: \$2.5M (\$2.1M\*)
  - FY10 Planned Funding: \$1.5M
- (\* R&D core, no IEA contracts)

## Partners

- SRI: combustion experiments
- IEA Contractors: W. Hoagland, and Longitude 122 West
- CSTT, ICC, NFPA, HIPOC, ISO, NHA, NIST, CTFCA, HYPER, IEA, NREL



# Objectives

- **Hydrogen codes and standards need a defensible and traceable basis:**
  - use quantitative risk assessment for risk-informed decision making and identification of risk mitigation strategies
  - 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
- **Provide advocacy and technical support for the codes and standards change process:**
  - consequence and risk: HIPOC, ISO TC197, NFPA (2, 52, 55, 502)
  - international engagement (addressing barrier G):
    - ISO TC197, WG11, TG1 on fueling station separation distances
    - IEA Task 19 Hydrogen Safety, recommended analysis practices
    - Global Technical Regulations, fuel system safety
    - Regulations Codes and Standards



# Approach

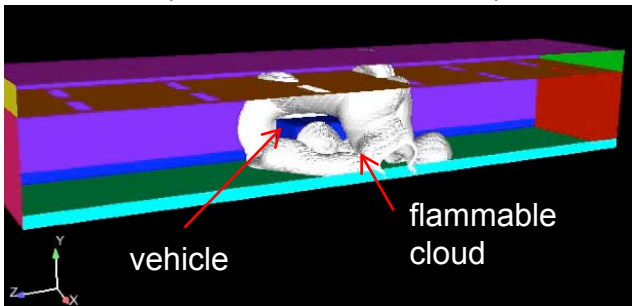
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- Develop and validate models for hydrogen behavior
  - Partial confinement and over-pressure
  - Ignition: auto-ignition
  - Ignition: lean limits
  - LH2 releases and cold vapor cloud dynamics
- Develop quantitative risk analysis methodology
  - Event frequencies
  - Risk metrics
- Support risk-informed decision-making for the codes and standards development process
  - Separation distances
  - Risk reduction and mitigation strategies

# Hydrogen vehicle releases in tunnels

- Most likely scenario: localized vehicle fire  
vehicles are designed to safely vent and tunnels are designed to handle fire loading
- Less likely scenario: delayed ignition of hydrogen  
Resulting from thermally-actuated (TPRD) tank blow-down.

Simulation of H<sub>2</sub> Vehicle TPRD Release  
in a Transversely Ventilated Tunnel  
(2 seconds into release)

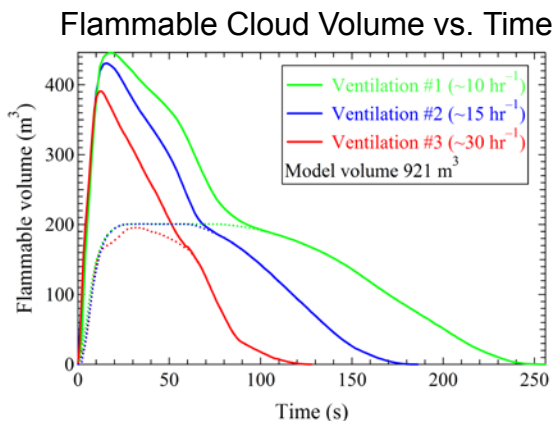


## Computational effort:

- Several tunnel geometries as in NFPA 502 examined
- Computational simulations of the release and ignition deflagration performed

## Results:

- Maximum flammable volume occurs near 30s
- Tunnel ventilation does not dilute or extract hydrogen mixture over that time scale



Results reported to NFPA 502 technical committee



# A risk perspective for hydrogen vehicle releases in tunnels

Risk assessment of a thermally-activated H<sub>2</sub> vehicle (TPRD) tank release involves:

- (1) Frequency of occurrence of specific incident
- (2) Evaluation of severity of consequence

$$\text{Risk} = \text{Freq.} \times \text{Consequence}$$

## Addressing Frequency:

- Very little statistical data for hydrogen releases from vehicles is available
- Some data is available for gasoline-powered vehicles in tunnels
- Estimated freq. of vehicles being involved in tunnel fire in U.S is  $3 \times 10^{-7}/\text{yr}$  to  $3 \times 10^{-5}/\text{yr}$

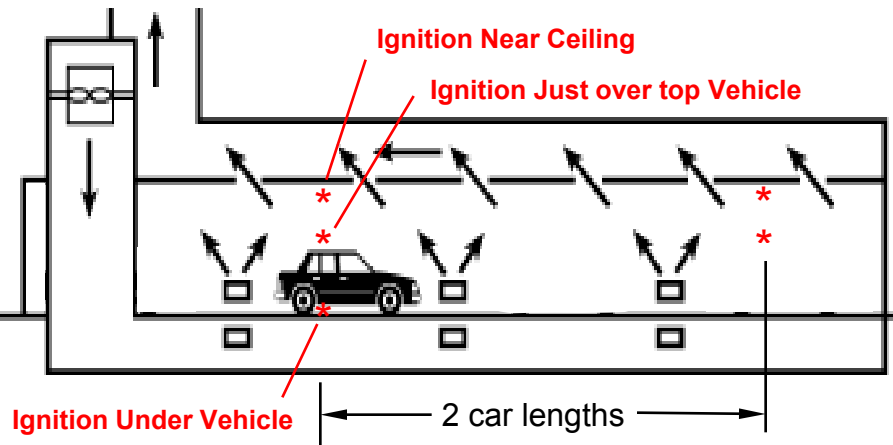
## Addressing Consequence:

- Risk from H<sub>2</sub> vehicle fires in tunnels should not increase existing risk of everyday life
  - U.S. ave. individual fatality risk from all types of accidents =  $5 \times 10^{-4}/\text{yr}$
- Only a fraction of hydrogen vehicle fires tunnel fires will result in TPRD release, ignition, and subsequent fatality

*Estimated risk of H<sub>2</sub> vehicle TPRD release in tunnels does not significantly increase level of individual risk*

# Effects of ignition location, time, and ventilation on resulting overpressure investigated

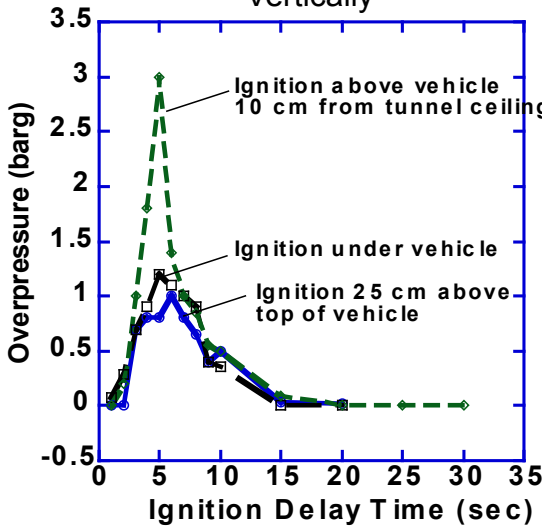
## Transversely-Ventilated Tunnel



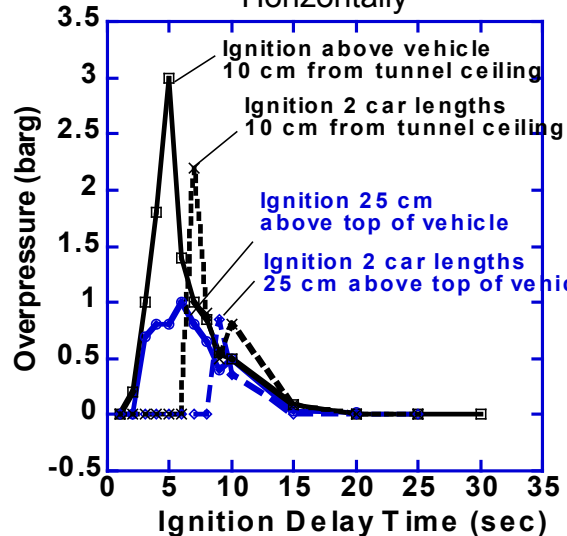
## Results:

- Peak overpressure occurs about 5 sec after PRD release (near car ignition)
- Overpressure greater for ignition near ceiling
- Ignition 2 car lengths away from release generates lower overpressure (peak at 8 sec)
- Overpressure highest for ignition at ceiling
- Overpressure lower with no tunnel ventilation

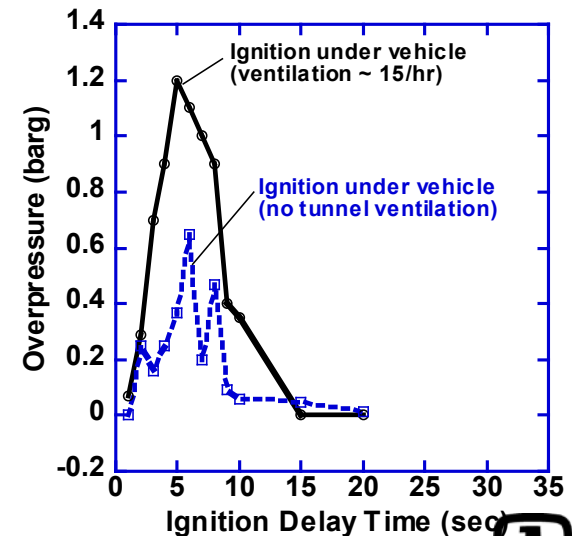
Effect of Moving Ignition Point Vertically



Effect of Moving Ignition Point Horizontally



Effect of Ventilation

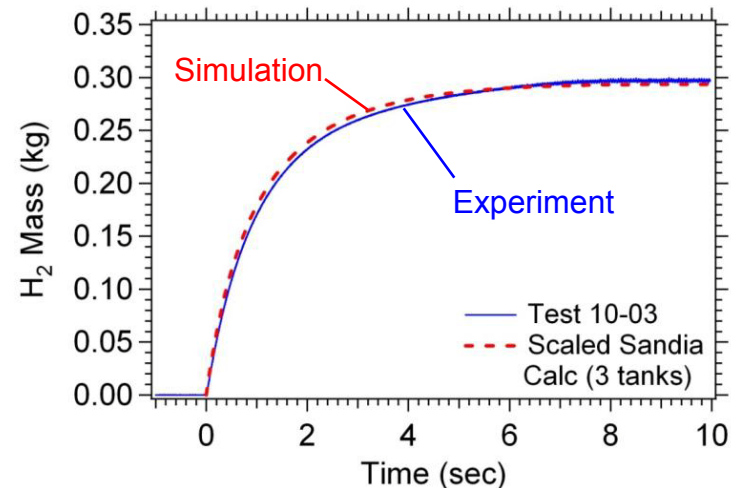


# Model validation data produced from sub-scaled tunnels tests

- Froude scaling\* used to resemble the full-scale tunnel simulations
- Scale factor (1/2.53) based on the ratio of the cross-sectional areas (0.3 Kg total GH2)
- CFD dispersion and deflagration simulations used to determine sensor placement



Comparison of Simulations and Measurements for Vehicle H<sub>2</sub> Mass Release versus Time for Scaled Tunnel Tests



Time:

$$t_S = \bar{K} t_H (S_S)^{0.5} \bar{F}$$

Mass release rate:

$$Q_S = \bar{K} Q_H (S_S)^{2.5} \bar{F}$$

Total mass released:

$$M_S = \bar{K} M_H (S_S)^3 \bar{F}$$



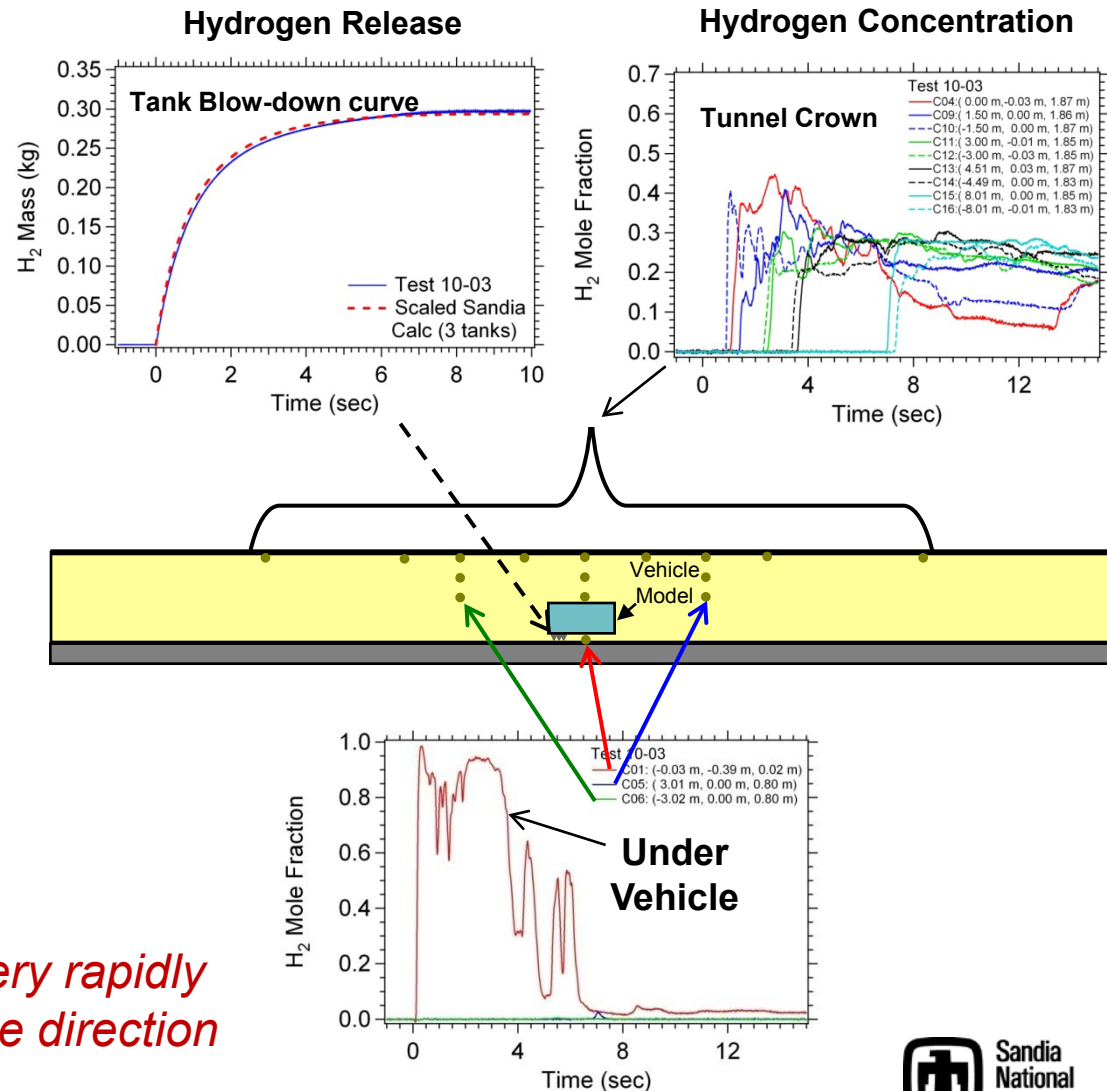
\*D.J. Hall, S. Walker, "Scaling Rules for Reduced-Scale Field Releases of Hydrogen Fluoride," Jour. of Hazardous Materials, Vol. 54, pp. 89-111, 1997."



# Experiments without ignition provide insight about the behavior of hydrogen

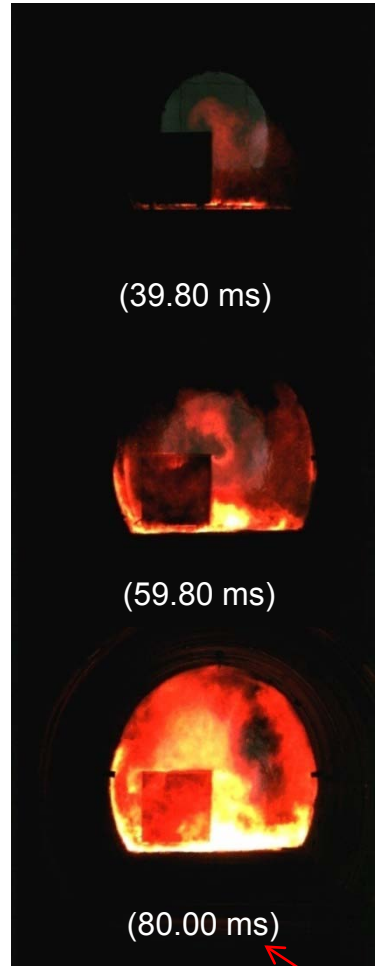
- Fast oxygen sensors were used to monitor hydrogen
  - Response time between 70 and 130 ms
- Underneath the vehicle the hydrogen concentration, rapidly approached 100%
- Hydrogen detected at the tunnel crown one second after the release

*Dispersion in the tunnel occurs very rapidly and is highly influenced by release direction*

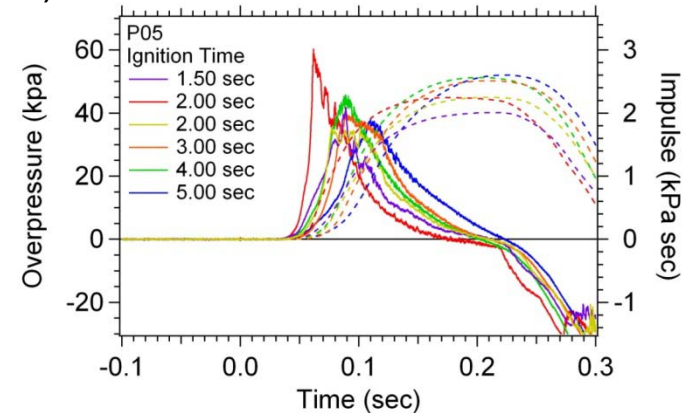


# The ignition experiments provide overpressure data as a function of ignition time

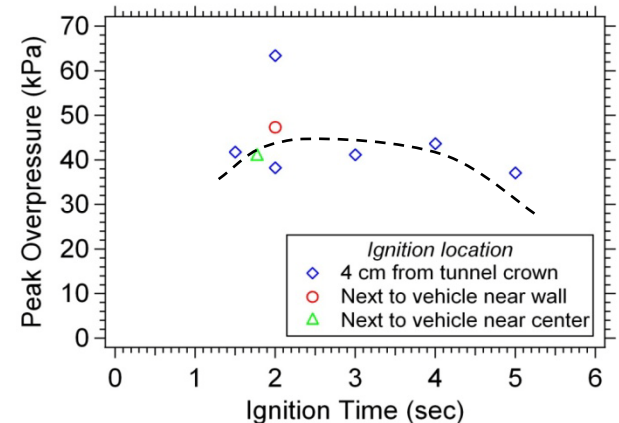
High-speed video frames  
(Ignition 1.77 sec after beginning of release)



Transient Variation of Ignition Overpressure  
(P05 - located 10.60m from tunnel center)



Peak Ignition Overpressure  
Versus Ignition Delay Time



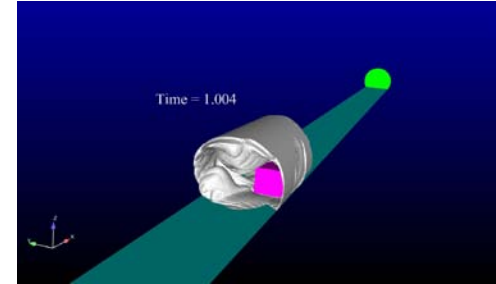
- Average maximum overpressure was: 42 kPa (0.42 barg)
- The maximum overpressure measured: 63.4 kPa at 2.00 sec ignition
- As ignition delay time increased, the impulse also increased.

*Quantification of overpressure allows for application of harm criteria*

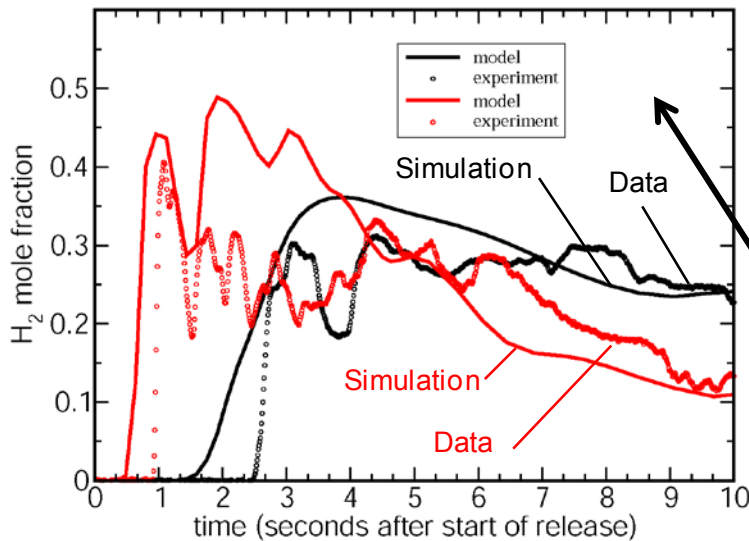
Time referenced to ignition

# Accomplishment: Experimental results show good agreement with model

- Overpressures are in good agreement with the experimental data from the tests
- 3-D calculations
  - Transient hydrogen concentration using Sandia Fuego CFD code
  - Deflagration overpressure computed in FLACS

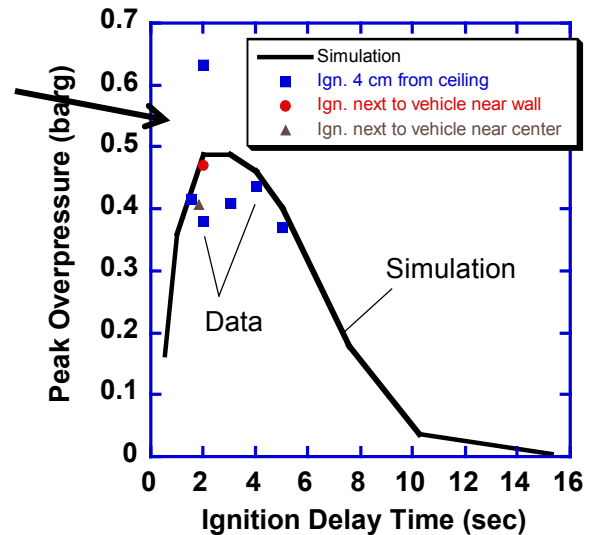


Simulation Showing Flammable H<sub>2</sub> Cloud (4-75% m.f.) around vehicle in Test Tunnel (1 sec into the release)



Peak Ignition  
Deflagration  
Overpressure

H<sub>2</sub> mole fraction  
(near tunnel  
ceiling)

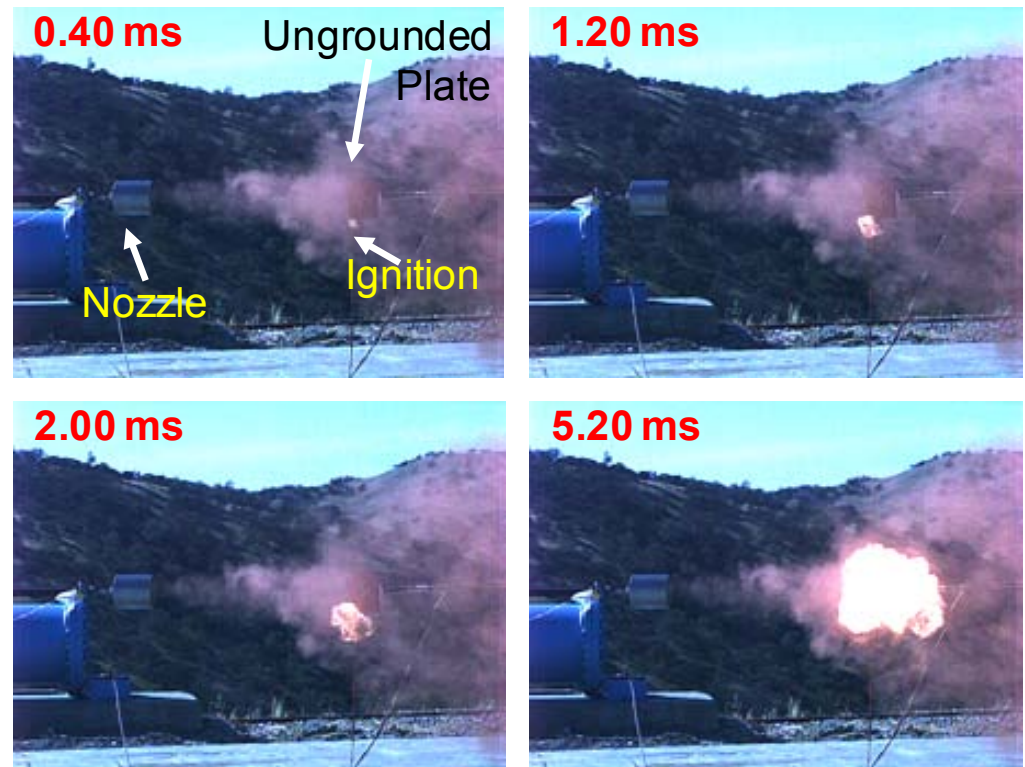


*Validated model allows for parameter investigations of mitigation strategies*

# Ignition behavior characterization: “spontaneous ignition”

- Investigate the mechanisms of static charge ignition
  - spark discharge
  - corona discharge
- Research was conducted in two stages:
  1. Quantification of level of electric charge imparted to particles
  2. Ignition of released hydrogen with spark or corona discharge from entrained particles

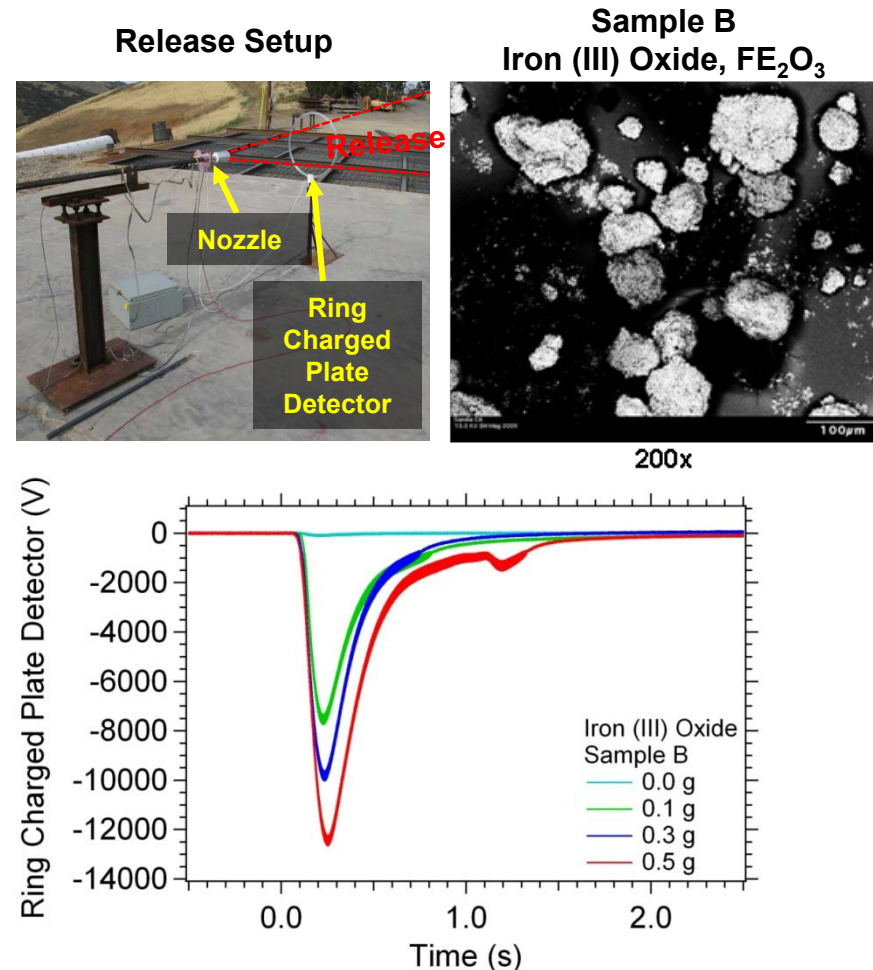
High-Speed Video Frames from Experiment



SRI Test Site

# The effect of different particle materials, sizes, and mass loadings was investigated

- Four iron oxide samples were tested
  - Three sizes of iron (III) oxide
  - One size of iron (II) oxide.
- Iron oxide particles were positively charged in all tests.
  - *Iron (III) oxide produced higher charge than iron (II)*
- Charge increased with increasing total mass of particulate.



Accumulated charge as a function of time and mass loading

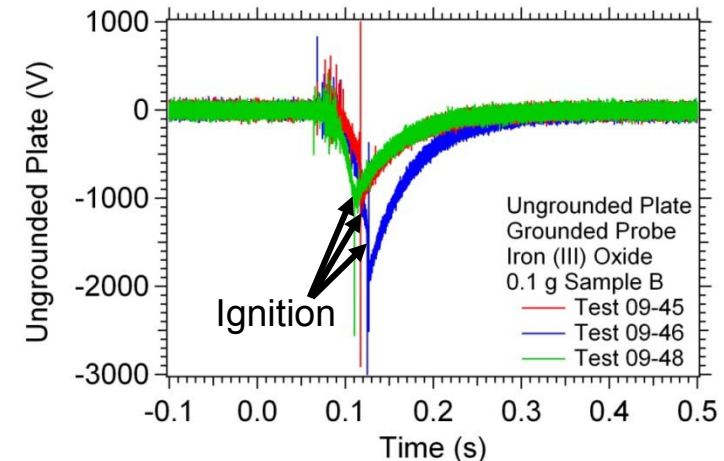
# Accomplishment: Entrained particulates are a likely source of spontaneous ignition

## Infrared Video Frames from Experiment



## Results:

- Plate in close proximity to a grounded probe caused ignition to occur in 6 of 8 tests
- Ignition occurred in 3 of 4 tests with as little 0.1 g of iron (III) oxide particles present
- All ignition events observed in this study occurred in close proximity to ungrounded metal objects.
- Tests repeated without particles to verify that particles were the source of ignition
- No evidence of corona induced ignition observed



- Disturbance in voltage indicates ignition event

*Will ignition result from externally entrained particulates?*

# Accomplishment: Validation of turbulent entrainment model for cold hydrogen

Table 1. Reservoir conditions of the under-expanded hydrogen jet experiments and computed gas states for the actual orifice and the virtual jet origin after expansion to 0.1 MPa.

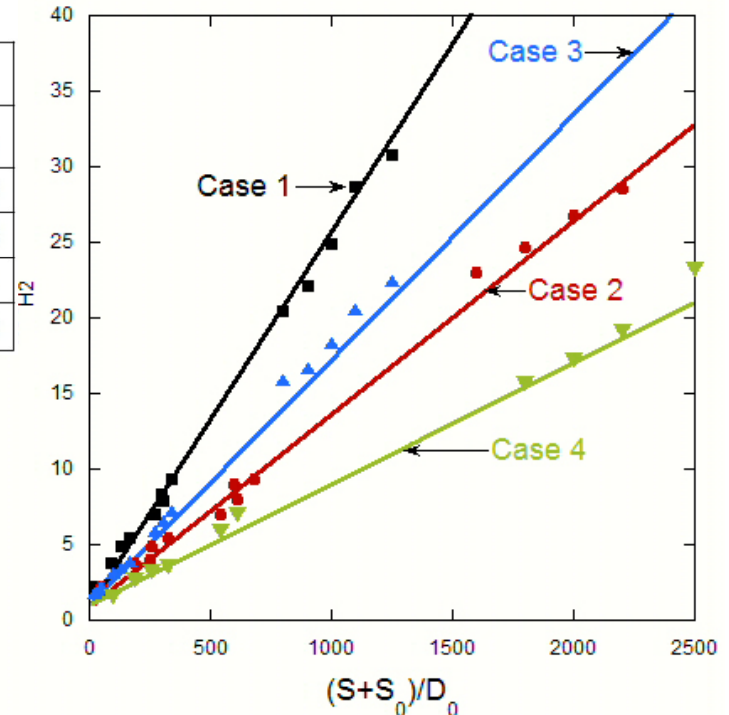
Cases	Reservoir			Actual orifice					Virtual jet origin			
	$P_r$ (MPa)	$T_r$ (K)	$\rho_r$ (kg/m <sup>3</sup> )	$D_0$ (mm)	$P_e$ (MPa)	$T_e$ (K)	$\rho_e$ (kg/m <sup>3</sup> )	$v_e$ (m/s)	$D_v$ (mm)	$\rho_v$ (kg/m <sup>3</sup> )	$T_v$ (K)	$v_v$ (m/s)
1	1.7	298	1.369	2	0.89	246.8	0.869	1208.9	3.76	0.151	163.3	1969.2
2	6.85	298	5.354	1	3.552	246.1	3.42	1231.4	3.52	0.163	152.8	2080.4
3	0.825	80	2.527	2	0.4	60.1	1.641	640.4	2.75	0.566	43.6	979.8
4	3.2	80	10.019	1	1.513	59.5	6.603	637.8	2.44	0.669	38.1	1060.2

Reproduced from reference 1.

- Data from FZK experiments of Xiao et. al.<sup>1</sup>
- Virtual jet origin calculated using Yuceil and Otugen<sup>2</sup> source model.

- [1] J. Xiao, J. R. Travis and W. Breitung, "Hydrogen Release from a High Pressure GH2 Reservoir in Case of a Small Leak," 3<sup>rd</sup> ICHS International Conference on Hydrogen Safety, Ajaccio-Corse, France, September 16-18, 2009.
- [2] K. B. Yuceil and M. V. Otugen, "Scaling Parameters for Underexpanded Supersonic Jets," Physics of Fluids, Vol. 4, No. 12, pp. 4206-4215, December, 2002.

Measured & Calculated H2 Centerline Concentration



*Additional data needed for lower temperature (<77K) behavior validation*

# Milestones

12/09	Complete modeling parameters studies on hydrogen vehicle releases in tunnels
12/09	Evaluate risk associated with hydrogen releases in tunnels
3/10	Evaluate risk associated with hydrogen indoor refueling
9/10	Complete laboratory experiments for small-scale cryogenic leaks
9/10	Complete large-scale tests at SRI for auto-ignition under conditions approaching realistic release scenarios. Identify alternate ignition mechanisms and develop mitigation strategies

<b>green</b>	- <b>completed</b>
<b>orange</b>	- <b>on track</b>
<b>red</b>	- <b>behind schedule</b>





# Future Work

## Remainder of FY10

- Risk and consequence analysis of indoor refueling and operation of hydrogen powered industrial trucks
- Finalize risk assessment of hydrogen releases in tunnels and distribute to NFPA 2 Task Group 11
- Incorporation of Risk Data from existing demonstration and ARPA-E projects
- Light-up mechanism model for turbulent flow
- Ignition behavior due to environmental particulate entrainment

## FY11

- Complete risk and consequence analysis of indoor refueling
- Unintended releases involving other confined spaces (e.g. sheds)
- High momentum low temperature hydrogen plume behavior in support of NFPA activities
- Advanced storage materials in support of NFPA 2 activities



# Summary

- Analysis of H<sub>2</sub> releases and delayed ignition deflagration have been performed for partially confined spaces (tunnels)
  - A preliminary risk analysis indicates that the level of potential risk from H<sub>2</sub> vehicles accidents does not significantly increase the level of individual risk
  - Tunnel release modeling approach validated with scaled-tunnel experiments
  - ***Validated approach can be used for H<sub>2</sub> releases in other partially enclosed spaces (warehouses, sheds, etc)***
- Experiments have shown that entrained particulates originating from tanks or piping are likely a source of spontaneous ignition
- The Sandia turbulent entrainment model for cold hydrogen jets has been validated against high-momentum jet data (from FZK tests)

***This program provides key understanding to enable the deployment of early-market hydrogen systems***