Hydrogen Release Behavior

Sandia National Laboratories, Livermore, CA

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Project SCS010

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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

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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

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Approach

- 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

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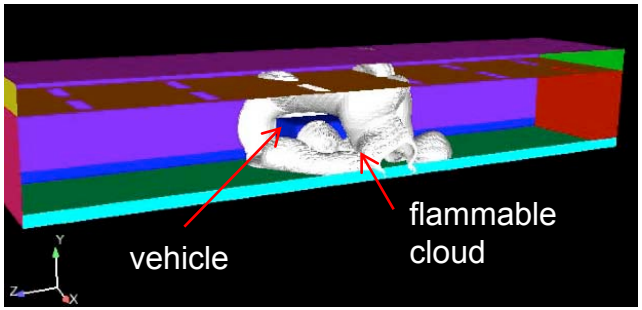
Hydrogen vehicle releases in tunnels

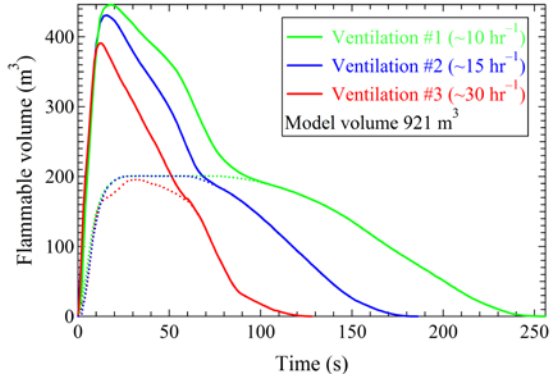
- Most likely scenario: localized vehicle fire
  vehicles are designed to safely vent and tunnels are designed to handle fire loading

- Less likely scenario: delayed ignition of hydrogen
  Resulting from thermally-actuated (TPRD) tank blow-down.

Simulation of H_2 Vehicle TPRD Release in a Transversely Ventilated Tunnel (2 seconds into release)



Flammable Cloud Volume vs. Time



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

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A risk perspective for hydrogen vehicle releases in tunnels

Risk assessment of a thermally-activated H_2 vehicle (TPRD) tank release involves:

(1) Frequency of occurrence of specific incident

(2) Evaluation of severity of consequence

Risk = Freq. x 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 **$3x10^{-7}$/yr** to **$3x10^{-5}$/yr**

Addressing Consequence:

- Risk from H_2 vehicle fires in tunnels should not increase existing risk of everyday life
  - U.S. ave. individual fatality risk from all types of accidents = **$5x10^{-4}$/yr**
- Only a fraction of hydrogen vehicle fires tunnel fires will result in TPRD release, ignition, and subsequent fatality

Estimated risk of H_2 vehicle TPRD release in tunnels does not significantly increase level of individual risk

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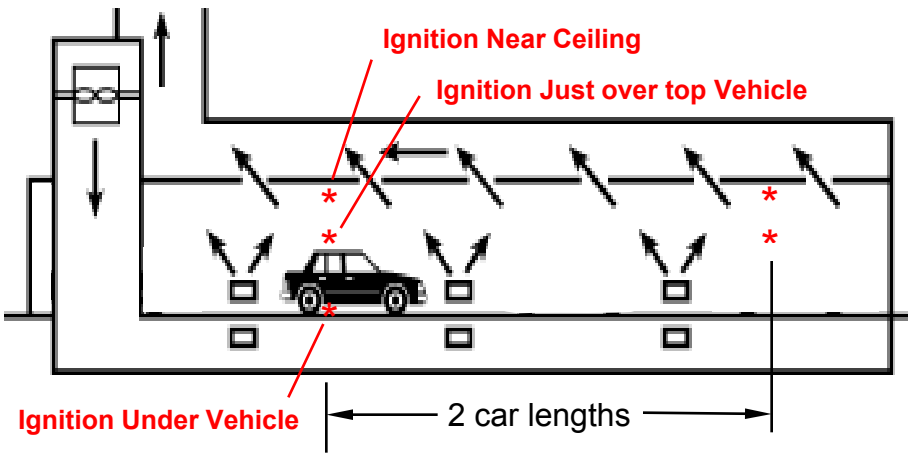
Effects of ignition location, time, and ventilation on resulting overpressure investigated

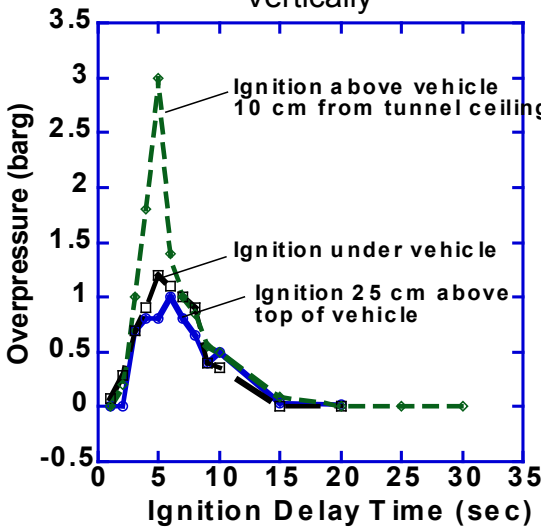
Transversely-Ventilated Tunnel



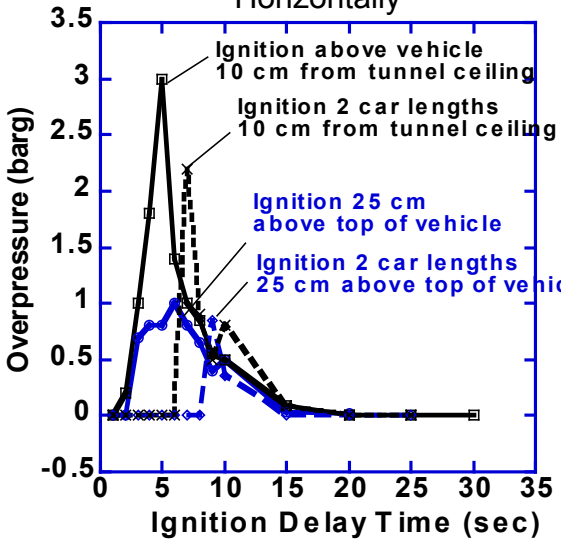
Results:

- 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

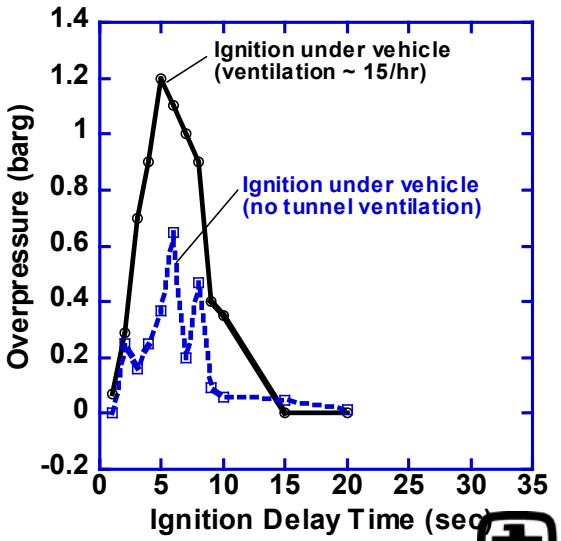
Effect of Moving Ignition Point Vertically



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

Time:

$$t_S = t_H (S_S)^{0.5}$$

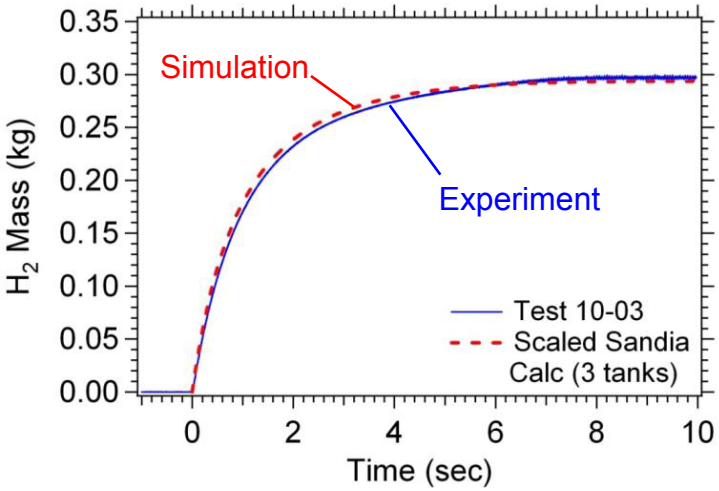
Mass release rate:

$$Q_S = Q_H (S_S)^{2.5}$$

Total mass released:

$$M_S = M_F (S_S)^3$$

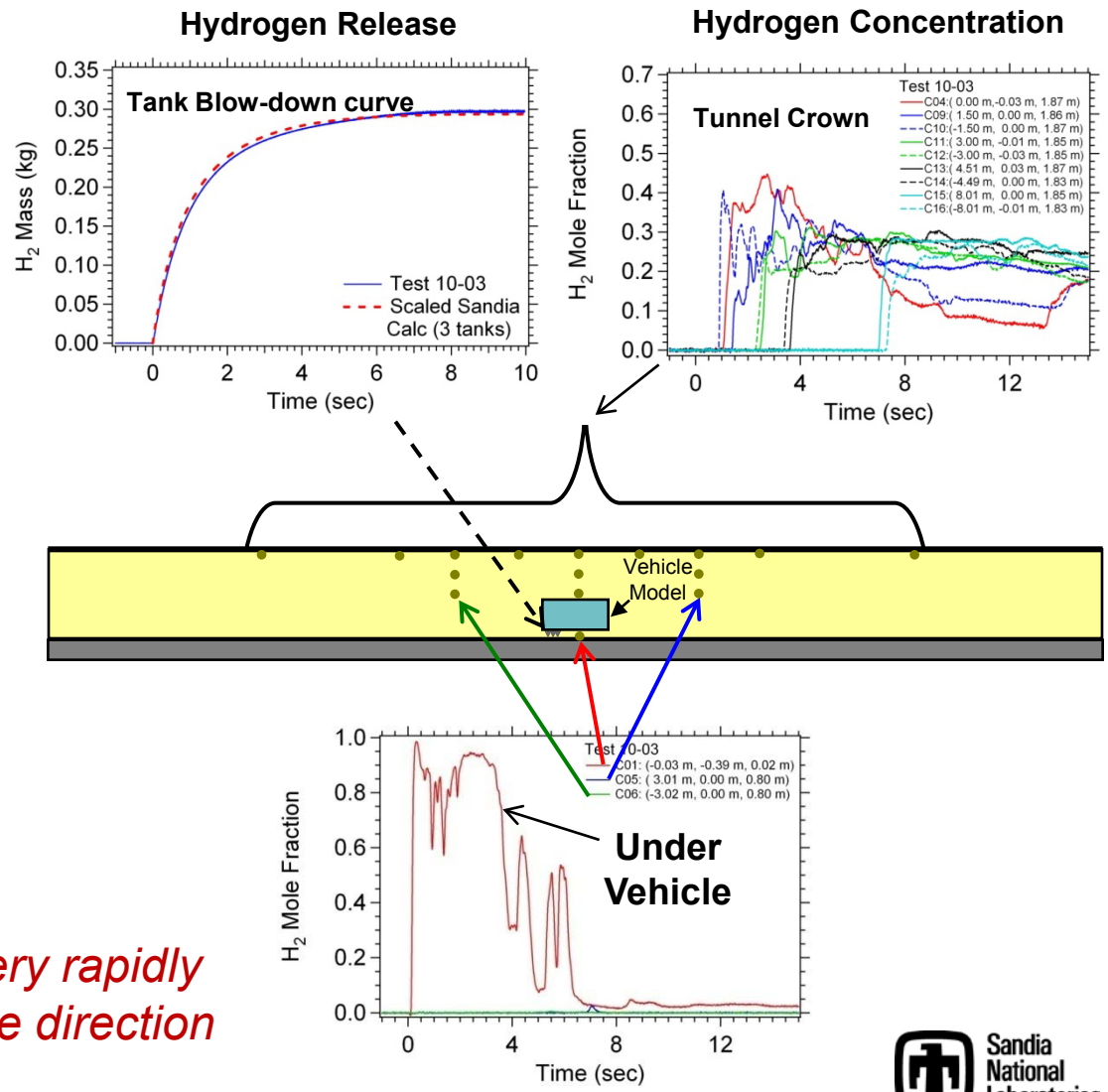
Comparison of Simulations and Measurements for Vehicle H_2 Mass Release versus Time for Scaled Tunnel Tests



*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

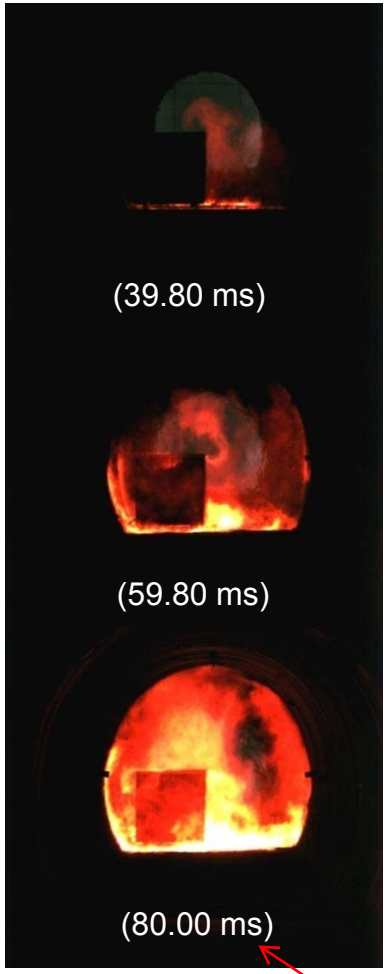
The ignition experiments provide overpressure data as a function of ignition time

- 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

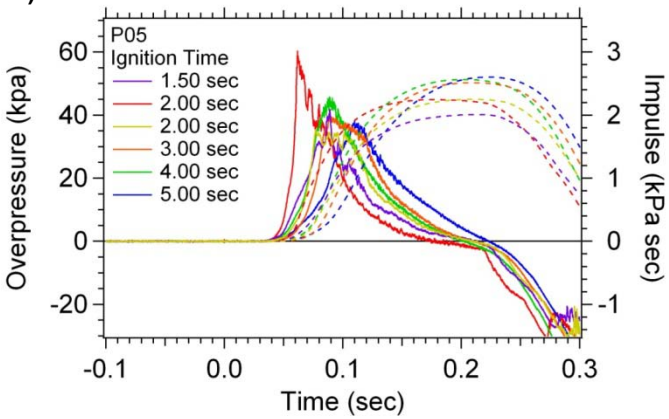
High-speed video frames

(Ignition 1.77 sec after beginning of release)

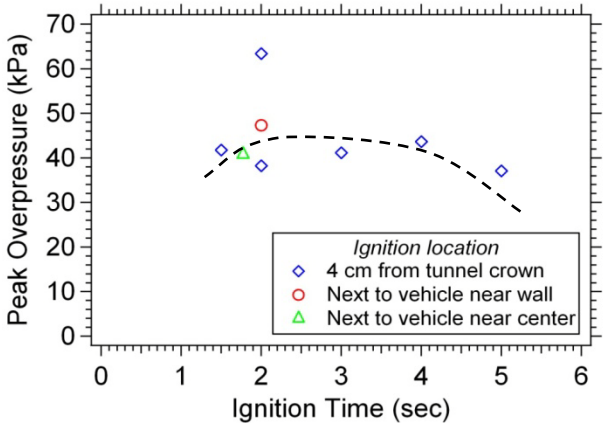


Time referenced to ignition

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



Peak Ignition Overpressure Versus Ignition Delay Time



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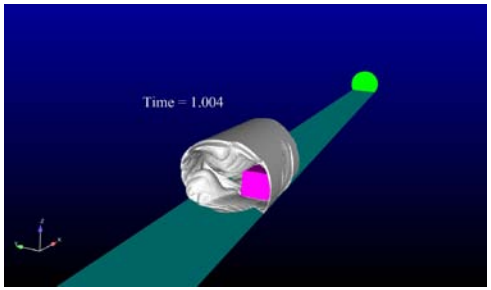
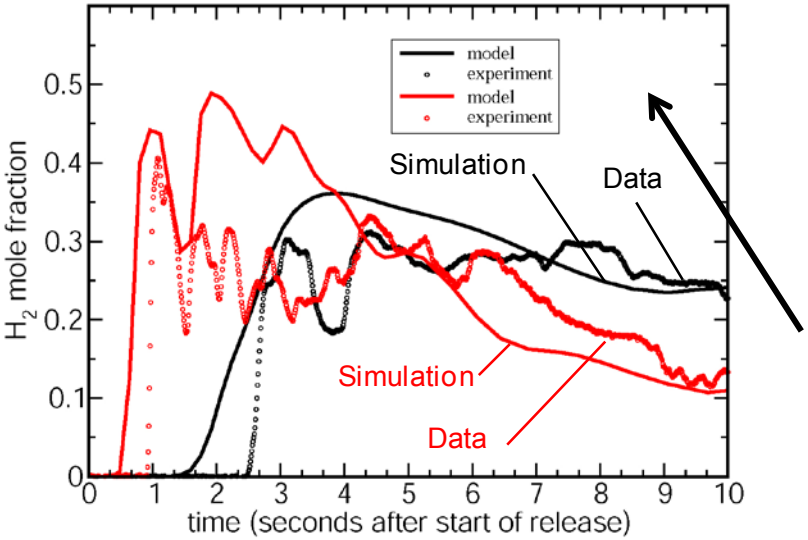
Accomplishment: Experimental results show good agreement with model

- 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

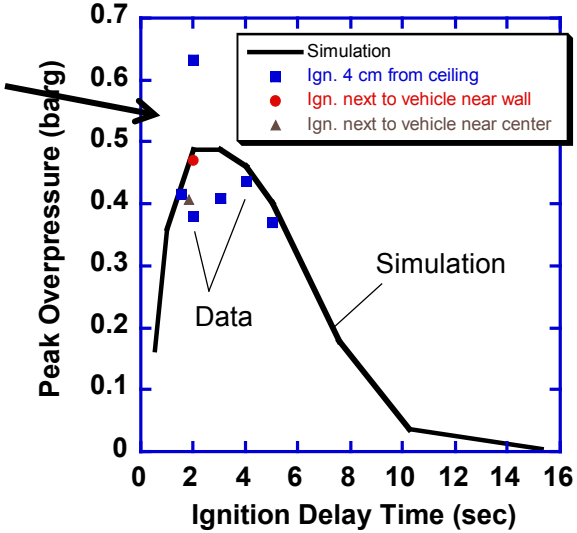


Simulation Showing Flammable H_2 Cloud (4-75% m.f.) around vehicle in Test Tunnel (1 sec into the release)



H_2 mole fraction (near tunnel ceiling)

Peak Ignition Deflagration Overpressure



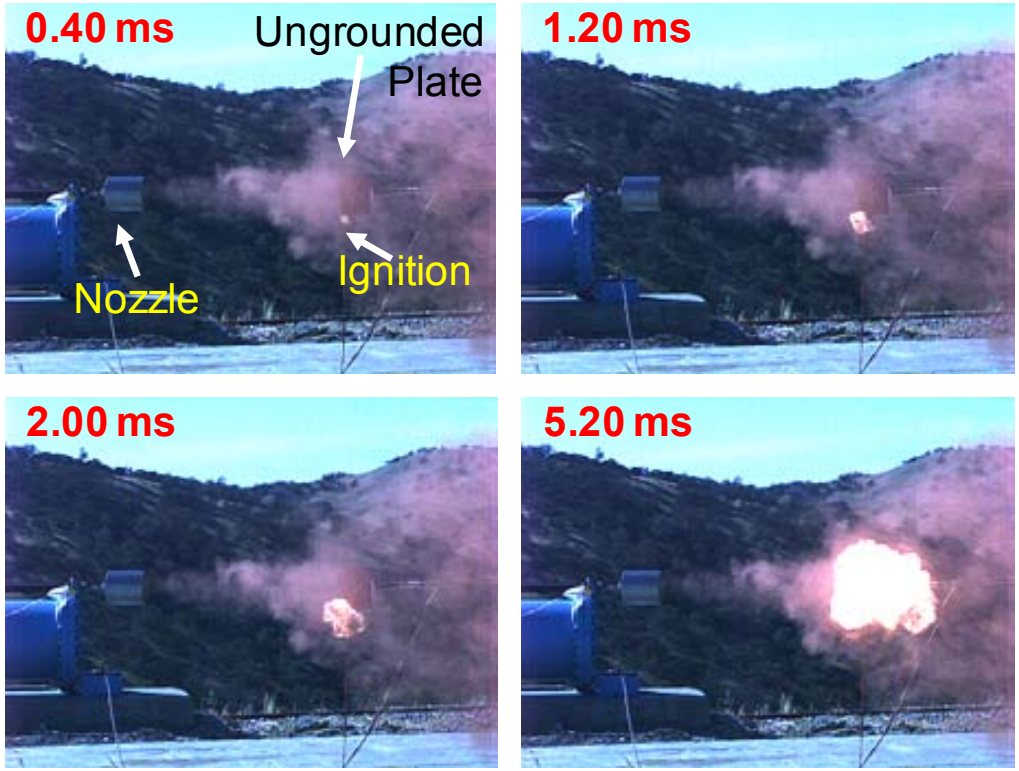
Validated model allows for parameter investigations of mitigation strategies

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

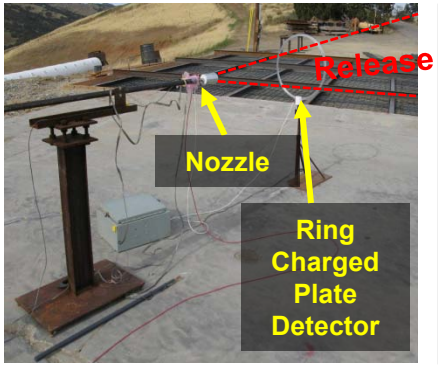


SRI Test Site

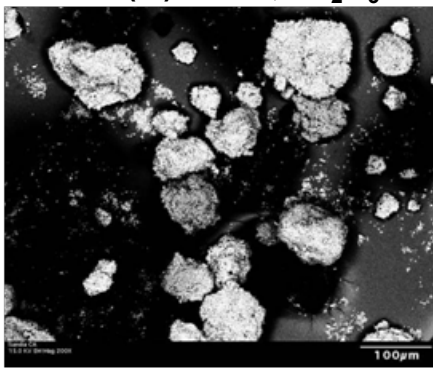
The effect of different particle materials, sizes, and mass loadings was investigated

- 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.

Release Setup



Sample B
Iron (III) Oxide, FE_2O_3



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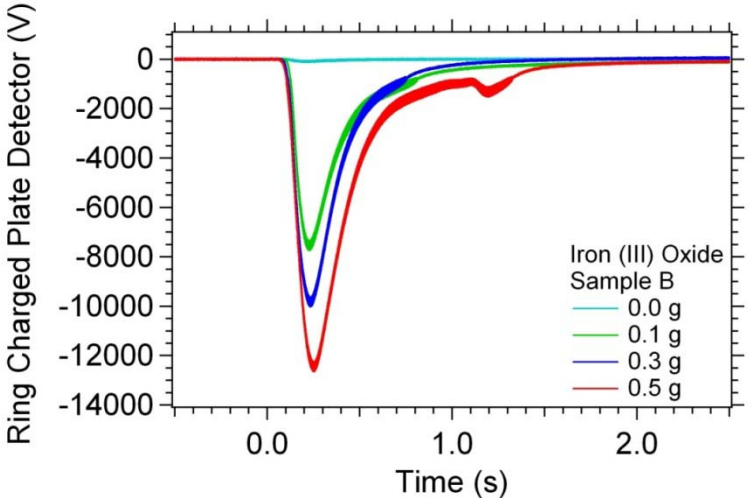


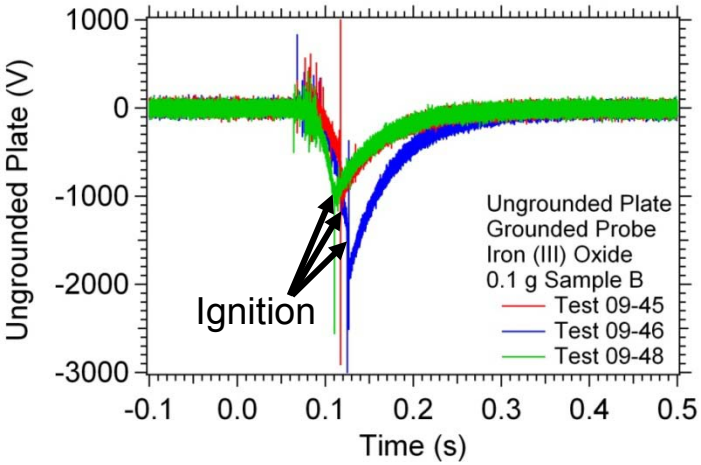
Accumulated charge as a function of time and mass loading

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

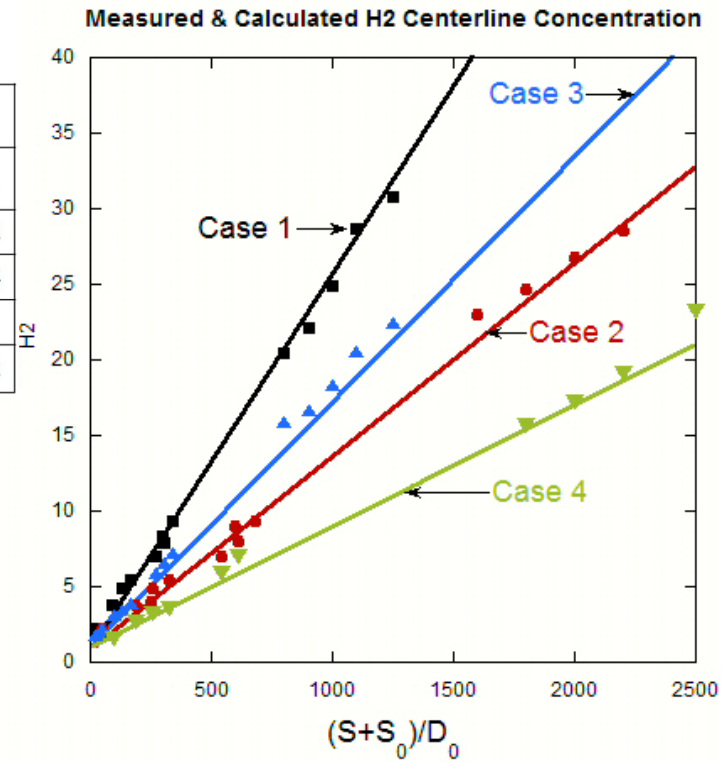
Will ignition result from externally entrained particulates?

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)	ρ_r (kg/m^3)	D_0 (mm)	P_e (MPa)	T_e (K)	ρ_e (kg/m^3)	v_e (m/s)	D_v (mm)	ρ_v (kg/m^3)	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.[1]
- Virtual jet origin calculated using Yuceil and Otugen[2] 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," 3rd 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.

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

green – completed
orange – on track
red – behind schedule

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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

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Summary

- Analysis of H_2 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_2 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_2 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

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