# IX.9 Hydrogen Release Behavior

Daniel Dedrick (Primary Contact), William Houf, Robert Schefer, Jeffrey LaChance, Greg Evans, William Winters, Isaac Ekoto, and Jay Keller Sandia National Laboratories P.O. Box 969 Livermore, CA 94551-0969 Phone: (925) 294-1552 E-mail: dededri@sandia.gov

DOE Technology Development Manager: Antonio Ruiz Phone: (202) 586-0729 E-mail: Antonio.Ruiz@ee.doe.gov

Start Date: Fiscal Year (FY) 2002 End Date: Project continuation and direction determined annually by DOE

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.

# **Objectives**

- (1) Scenario Analysis, Risk Assessments for Safety:
  - Develop a scientific basis and the associated technical data for modifying or developing new codes and standards for the commercial use of hydrogen.
  - Develop benchmark experiments and a defensible analysis strategy for risk assessment of hydrogen systems.
  - Develop and apply risk-informed decisionmaking tools in the codes and standards development process.
- (2) Hazards Mitigation Technologies for Hydrogen Applications:
  - Determine the effectiveness of ventilation, active sensing, and similar engineered safety features.
- (3) Codes and Standards Advocacy:
  - Provide technical program management and support for the Safety, Codes and Standards program element.
  - Participate in the hydrogen codes and standards development/change process.

## **Technical Barriers**

This project addresses technical barriers from the Codes and Standards section of the Fuel Cell Technologies 2007 Multi-Year Research Plan:

- (F) Limited DOE Role in the Development of International Standards
- (I) Conflicts between Domestic and International Standards
- (N) Insufficient Technical Data to Revise Standards
- (P) Large Footprint Requirements for Hydrogen Refueling Stations
- (Q) Parking and Other Access Restrictions

# Contribution to Achievement of DOE Codes and Standards Milestones

This project will contribute to achievement of the following DOE milestones from the Codes and Standards section of the Fuel Cell Technologies Program Multi-Year Research, Development and Demonstration Plan:

- Milestone 21: Completion of necessary codes and standards needed for the early commercialization and market entry of hydrogen energy technologies (4Q, 2012).
- Milestone 8: Complete investigation of safe refueling protocols for high pressure systems. (1Q, 2012)
- Milestone 9: Complete risk mitigation analysis for advanced transportation infrastructure systems. (1Q, 2015)
- Milestone 12: Complete research needed to fill data gaps on hydrogen properties and behaviors. (2Q, 2010)

#### Accomplishments

- We determined that implementation of barriers can be effective in reducing risk and separation distances to the facility lot line.
- Analysis of H<sub>2</sub> releases and delayed ignition deflagration have been performed for partially confined spaces (tunnels).
- 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 highmomentum jet data (from Forschungszentrum Karlsruhe tests).



# Introduction

The purpose of this project is to enable riskinformed development of codes and standards for hydrogen fuel cell technology that is based on a traceable, scientific foundation. Our scenario analysis and risk assessment efforts focus on defining scenarios for the unintended release of hydrogen and quantifying the consequences through scientific experimentation and modeling. Quantitative risk assessment (QRA) is used to identify risk drivers and risk mitigation strategies for the commercial use of hydrogen. We combine our validated models with QRA to support risk-informed decisionmaking in the code development process.

# Approach

We develop an understanding of combustion behavior and thermal effects from the unintended releases of hydrogen in the built environment. We consider ignition characteristics, barrier wall interactions, partially confined spaces (tunnels, garages, warehouses), and liquid hydrogen handling. Technical information is disseminated through a variety of public channels and is used by codes and standards developers writing for the International Code Council and National Fire Protection Agency (NFPA). International partnerships for vetting technical data and analysis methods occur through activities such as International Energy Agency Task 19 on Hydrogen Safety and the European HYPER project. Efforts in FY 2010 have focused on developing the basis for regulations and codes and standards development in the area of hydrogen releases in enclosures, ignition mechanisms, and liquefied hydrogen release behavior.

#### Results

#### **Risk Analysis**

Using risk information in the code development process enables rapid and effective hydrogen and fuel cell technology deployment. In FY 2010 we evaluated the use of barrier walls to reduce the risk (and thus separation distances) for hydrogen facilities. The use of properly designed barriers will remove the potential for direct contact with jet flames, reduce the distance of unignited jets, reduce the isosurfaces for various thermal radiation heat fluxes, and not result in any substantial increase in pressure that would harm people or structures. Thus, barriers provide a means to reduce the risk to the public from unintended releases of hydrogen. This reduction in risk also allows for the opportunity to reduce the separation distances at a hydrogen facility. Estimates of the risk reduction potential were generated by using the risk model developed for evaluation of the separation distances selected for incorporation into the NFPA-2 and NFPA-55 hydrogen standards [1] and the consequence results reported in [2,3]. The system configurations and associated leakage frequencies utilized in [1] were utilized in the barrier risk assessment, thus allowing for direct comparison of the risk with and without a barrier. The barrier wall was assumed to be 2.4 m high and separated from the hydrogen equipment by 1.22 m. Table 1 provides a comparison of the risk to an individual located at the facility lot line from a leak equivalent to a 3% of the maximum flow area in the hydrogen system.

System Pressure (MPa)	Leak Diameter <sup>1</sup> (mm)	Separation Distance to Facility Lot	Individual Risk at Facility Lot Line (fatalities/yr)	
		Line <sup>2</sup> w/o Barrier (m)	w/o Barrier	Barrier
1.83	9.09	14.0	2.0E-5	5.4E-6
20.78	3.28	14.0	2.1E-5	5.5E-6
51.81	1.37	8.8	3.6E-5	1.1E-5
103.52	1.24	10.4	3.5E-5	1.0E-5

TABLE 1. Estimated Risk Reduction from the use of Barriers

<sup>1</sup> Leak diameter corresponds to 3% of the largest flow area in the system. <sup>2</sup> Separation distance specified in NFPA-55, based on selected leak diameter.

As indicated in Table 1, the presence of a barrier can be used to reduce the risk to a person standing at the facility lot line. The use of a barrier can also be used to reduce the separation distances. For a risk level equivalent to the risk without a barrier, the separation distance to the facility lot line can be shortened to approximately 3.5 m for the leak diameters shown in Table 1.

#### Unintended Releases of Hydrogen in Partially Enclosed Spaces

Code language is being developed for the use of hydrogen in partially enclosed spaces. In FY 2010, we evaluated the release of hydrogen in enclosures to inform the code development processes in NFPA 2, 52, and 502. Experiments were performed in a scaled tunnel test facility (Figure 1) to provide model validation data for release simulations resulting from the venting of the thermally-activated pressure relief device (PRD) on a hydrogen vehicle in a full-scale tunnel. The tunnel test facility had a cross-sectional area that was approximately 1/2.53 that of the full-scale transversely ventilated tunnel. The release diameter was designed to match the scaled mass flow rate versus scaled time tank blow-down curve from the full-scale release. Measurements were made of the hydrogen concentration, flame speed, and ignition delay overpressure in the scaled tunnel resulting from the release produced by activation of three simulated



**FIGURE 1.** Comparison of Measured Peak Ignition Overpressure in the SRI International Test Tunnel Facility with Results from FUEGO/FLACS Model Simulations

PRD vents on the bottom of the scale-model vehicle. As part of the work a dispersion model and deflagration model of the test tunnel and vehicle geometry were developed. These models were used prior to the tests to estimate the placement of concentration and pressure sensors in the tunnel test geometry and to determine the amount of expected overpressure from ignition of the hydrogen releases. Pretest ignition deflagration simulations of the test tunnel geometry using threedimensional concentration maps from the dispersion simulations indicated that the maximum overpressure would be approximately 0.5 barg and that a peak in the overpressure would occur with increasing ignition delay time as observed in the full-scale tunnel simulations. Figure 1 shows a comparison of the peak overpressures measured in the experiments for different ignition delay times as compared to the model simulations. The ignition overpressure simulations are found to be in good agreement with the experimental data.

The same modeling approach was used in the fullscale tunnel simulations and the pretest simulations of the scaled-tunnel experiments. The good agreement between the scaled-tunnel test experimental data and pretest simulations provide validation of the simulation approach and full-scale tunnel modeling results. Results were reported to NFPA 502 – the standard for road tunnels.

#### Auto-Ignition of Unintended Hydrogen Releases

Understanding ignition mechanisms and the probability of ignition is a vital aspect of the QRA. Ignition source in a large percentage of reported hydrogen release incidents is not easily identified. Due to this uncertainty, these events are often referred to as auto-ignition events. One of the most likely ignition sources for these events is ignition of the hydrogen/ air mixture by electrostatic discharge resulting from the presence of charged particles in the flow. It is known from industrial experience that significant particle charge can develop during the high-speed flow of particle-laden gases through piping. During FY 2010, experiments were carried out to investigate the generation of static charge on iron-oxide particles in hydrogen gas flowing through pipes and the potential for these charged particles to induce an ignition event in the release. The objective of these experiments was to determine whether a static charge accumulation on iron oxide particles entrained in a hydrogen jet release could lead to a spark discharge ignition or a corona discharge ignition. Experiments were performed by adding particles to a high-pressure release of hydrogen gas flowing through a 10 foot steel pipe prior to exiting to ambient air through a nozzle.

A series of tests were performed where a circular ungrounded plate was placed in close proximity to a grounded probe in the particle-laden jet release (see Figure 2). In this configuration the ungrounded plate is charged by induction or particulate impact until the charge is high enough to arc to the nearby grounded probe. In this configuration, six ignitions occurred and in case when only 0.1 gram of iron (III) oxide particles were introduced into the flow ignition occurred in three out of four tests. In the case when no particles were introduced into the flow ignition did not occur. In addition, ignition did not occur when both probes were maintained at comparable floating electrostatic potentials. No corona-discharge events were observed during the test matrix. The results of these tests show that entrained particulates can be a source leading to spontaneous ignition in hydrogen gas releases.

#### Liquid Hydrogen Releases

Separation distances for liquid hydrogen systems are being specified in codes such as NFPA 2. We have developed an engineering model that can be utilized



**FIGURE 2.** (Top) Photograph Showing Ungrounded Circular Plate with Grounded Probe in Close Proximity (Bottom) Ignition Event as a Result of the Particle-Laden Hydrogen Release

to provide the basis for these separation distances. In FY 2010, this model was validated against highmomentum jet data from Forschungszentrum Karlsruhe of Germany. Forschungszentrum Karlsruhe conducted several experiments in which room temperature and 80 K under-expanded jets of hydrogen were vented into still air at ambient conditions. Hydrogen concentration was measured at several locations along the centerline. These jet releases were simulated using the Sandia turbulent entrainment model for cold hydrogen jets. Since the releases were choked, a source model was used to extrapolate choked conditions at the actual leak diameter to a source diameter where the pressure was atmospheric. Predicted centerline concentrations for hydrogen were compared with the Forschungszentrum Karlsruhe measurements as shown in Figure 3. Centerline concentrations for both room temperature and 80 K jets were well-reproduced by the model. The comparison shown in Figure 3 represents a validation for the cold- and ambient-temperature single phase hydrogen jet model and the high momentum source model. Further validation of the model for colder jets in which the release is two-phased will be made as validation data becomes available.

# **Conclusions and Future Directions**

This project provides key understanding to enable the deployment of early-market hydrogen systems. In FY 2010:

IX. Safety, Codes & Standards

Measured & Calculated H2 Centerline Concentration



FIGURE 3. Sandia Model Simulations of Forschungszentrum Karlsruhe Experiments

- We analyzed the use of barriers to reducing risk and separation distances to the facility lot line.
- We performed analysis of H<sub>2</sub> releases and delayed ignition deflagration 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.
- We completed experiments that identified entrained particulates as a likely a source of spontaneous ignition.
- We validated the Sandia turbulent entrainment model for cold hydrogen jets against highmomentum jet data (from Forschungszentrum Karlsruhe tests).

This project will continue to enable hydrogen and fuel cell technology deployment through developing the defensible technical basis for codes and standards. We will perform work to:

- Complete risk and consequence analysis of indoor refueling and operation of hydrogen powered industrial trucks.
- Analyze risk of unintended releases involving other confined spaces (e.g. sheds).
- Incorporate data from existing demonstration and projects into the QRA of hydrogen technologies.

- Improve the existing predictive model of ignition in turbulent flames to include sustained flame light-up probability.
- Understand ignition behavior due to environmental particulate entrainment and other mechanisms.
- Develop an understanding of high-momentum lowtemperature hydrogen plume behavior in support of NFPA 2 separation distance activities.
- Perform risk analysis of advanced storage materials in support of NFPA 2 activities.

# FY 2010 Publications/Presentations

**1.** LaChance, J. L., Tchouvelev, A.V., Engebo, A., "Development of Uniform Harm Criteria for Use in the Quantitative Risk Analysis of the Hydrogen Infrastructure," *3<sup>rd</sup> ICHS*, Ajaccio, France, September 16–18, 2009.

**2.** LaChance, J. "Risk-Informed Separation Distances for Hydrogen Refueling Stations," *IJHE*, Volume 34, Issue 14, pg. 5838, July 2009.

**3.** LaChance, J., Tchouvelev, A., Ohi, J., "Risk-Informed Process and Tools for Permitting Hydrogen Refueling Stations," *IJHE*, Volume 34, Issue 14, pg. 5855, July 2009.

**4.** Houf, W.G., Evans, G.H., James, S.C., "Simulation of Hydrogen Releases from Fuel-Cell Vehicles in Tunnels," *18<sup>th</sup> WHEC*, Essen, Germany, May 16–21, 2010.

**5.** Schefer, R.W., Groethe, M., Houf, W.G. and Evans, G., "Experimental Evaluation of Barrier Walls for Risk Reduction of Unintended Hydrogen Releases," *IJHE*, Vol. 34, 1590-1606, February 2009.

**6.** Schefer, R.W., Merilo, E.G., Groethe, M.A., Houf, W.G., "Experimental Investigation of Hydrogen Jet Fire Mitigation by Barrier Walls," *3<sup>rd</sup> ICHS*, Ajaccio, Corsica, September 16–19, 2009.

**7.** Schefer, R.W., Evans, G.H., Zhang, J., Ruggles, A.J., Greif, R., "Ignitability Limits for Combustion of Unintended Hydrogen Releases: Experimental and Theoretical Results," *3<sup>rd</sup> ICHS*, Ajaccio, Corsica, September 16–19, 2009.

**8.** Houf, W.G. Evans, G.H., Schefer, R.W., Merilo, E. Groethe, M. "A Study of Barrier walls for mitigation of unintended releases of hydrogen," *3<sup>rd</sup> ICHS*, Ajaccio, Corsica, September 16–19, 2009.

**9.** Winters, W.S., Houf, W.G., "Simulation of Small-Scale Releases from Liquid Hydrogen Storage Systems," *3<sup>rd</sup> ICHS*, Ajaccio, Corsica, September 16–19, 2009.

**10.** Brennan, S., Bengaouer, Carcassi, M., Cerciara, Evans, G., Friedrich, Gentilhomme, O., Houf, W., et al., "Hydrogen and Fuel Cell Stationary Applications: Key Findings and Experimental Work in the HYPER Project," *3<sup>rd</sup> ICHS*, Ajaccio, Corsica, September 16–19, 2009 (Selected for Special Issue of IJHE).

**11.** Houf, W., Schefer, G., Evans, G, Merilo, E., Groethe, M., "Evaluation of Barrier Walls for Mitigation of Unintended Releases of Hydrogen, *IJHE*, March, 2010.

**12.** LaChance, J., Phillips, J., Houf, W., "Risk Associated with the Use of Barriers in Hydrogen Refueling Stations," *18th WHEC*, Essen, Germany, May 16–21, 2010.

**13.** Houf, W.G., Schefer, R.W., Keller, J., Blake, C., Hoagland, B., Pitts, W., Royle, M., Ruban, S., Jallais, S., Bengaouer, A., Shirvill, L., Gautier, T., Suzuki, J., Willoughby, D., "An Overview of IEA Annex 19, Subtask B: Experimental Data Bases Relevant to Hydrogen Safety Standards, Development, *18<sup>th</sup> WHEC*, Essen, Germany, May 16–21, 2010.

**14.** Houf, W.G., Evans, G.H., James, S.C., "Simulation of Releases from Hydrogen Fuel-Cell Vehicles in Tunnels," NHA Conf. & Expo, Long Beach, California, May 3-6, 2010.

**15.** Houf, W.G. "Summary of Recent Accomplishments from Sandia Hydrogen Releases Program," IEA Task 19 Meeting, Paese di Lava, Corsica, France, Sept 14–15, 2009.

**16.** Houf, W.G. "IEA Task 19 Subtask B WHEC Abstract and Paper, IEA Task 19 Meeting, Paese di Lava, Corsica, France, September 14–15, 2009.

**17.** Houf, W.G. "Unintended Hydrogen Releases in Tunnels," NFPA 502 Technical Committee on Road Tunnels and Highway Fire Protection Meeting, San Diego, CA, Sept. 30, 2009.

**18.** Brennan, S., Houf, W., Schefer, R., Evans, G., et al., "Towards Minimizing Hazards in Hydrogen and Fuel Cell Stationary Applications: Key Findings of Modeling and Experimental Work in the HYPER Project, Hazards XXI Symposium, Manchester, UK Nov. 9-12, 2009.

# References

1. LaChance, J., Houf, W., Middleton, B., Fluer, L., "Analysis to Support Development of Risk-Informed Separation Distances for Hydrogen Codes and Standards," Sandia National Laboratories Report, SAND2009-0874, March 2009.

**2.** Houf, W. and Schefer, R., "Predicting Radiative Heat Fluxes and Flammability Envelopes from Unintended Releases of Hydrogen," Int. J. Hydrogen Energy 32 (2007) 1435-1444.

**3.** Houf, W., Schefer, R., Evans, G., Merilo, E. and Groethe, M., "Evaluation of Barrier Walls for Mitigation of Unintended Releases of Hydrogen," Int. J. Hydrogen Energy 35 (2010) 4758-4775.