VIII.5 Hydrogen Safety, Codes and Standards R&D – Release Behavior

Chris Moen (Primary Contact), Jay Keller, Bill Houf, Robert Schefer, Jeffrey LaChance
Sandia National Laboratories (SNL)
P.O. Box 969
Livermore, CA 94551-0969
Phone: (925) 294-3709
E-mail: cmoen@sandia.gov

DOE Technology Development Manager: Antonio Ruiz
Phone: (202) 586-0729; Fax: (202) 586-2373
E-mail: Antonio.Ruiz@ee.doe.gov

Start Date: FY 2002
End Date: Project continuation and direction determined annually by DOE

Efforts during this year were directed toward the following program components: (1) Scenario Analysis, Risk Assessments for Safety, and (2) Codes and Standards Advocacy.

Objectives

(1) Scenario Analysis, Risk Assessments for Safety
- Develop a scientific basis for evaluating credible safety scenarios, providing technical data for codes and standards decisions.
- Identify critical safety scenarios and gather technical data to support codes and standards decisions.
- Analyze hydrogen-related engineered systems and components for safety issues and identify probable hazards.
- Develop benchmark experiments and a defensible analysis strategy for risk assessment of hydrogen systems.
- Develop engineering models for rapid scenario assessment and risk analysis.

(2) Codes and Standards Advocacy
- Provide technical program management and support for the Safety, Codes and Standards Program element within the Hydrogen, Fuel Cells and Infrastructure Technologies program.
- Participate in the hydrogen codes and standards development/change process.

Technical Barriers

This project addresses the following technical barriers from the Codes and Standards section of the Hydrogen, Fuel Cells and Infrastructure Technologies 2007 Multi-year Research, Development and Demonstration Plan:

(N) Insufficient Technical Data to Revise Standards
(P) Large Footprint Requirements for Hydrogen Fueling Stations
(Q) Parking and Other Access Restrictions

Contribution to Achievement of DOE Safety, Codes & Standards Milestones

This project will contribute to achievement of the following milestones from the Codes and Standards section of the Hydrogen, Fuel Cells and Infrastructure Technologies 2007 Multi-year Research Development and Demonstration Plan:

- **Milestone 3:** Complete detailed scenario analysis risk assessments. (4Q, 2007)
- **Milestone 4:** Complete analytical experiments and data collection for hydrogen release scenarios as needed to support code development. (2Q, 2008)

Accomplishments

- The effectiveness of barriers in deflecting hydrogen jet flames and reducing the extent of hazardous radiation heat flux levels was determined through a combined experimental and numerical program. Our numerical model of reacting hydrogen jets was validated against measured jet flame parameters.
- Overpressure arising as a result of ignition in the partially confining geometry of barriers was measured and modeled using the FLACS code.
- A quantitative study of the ignitable gas composition envelope in turbulent hydrogen leaks determined that conventional flammability limits for static hydrogen mixtures are not consistent with ignitability limits in turbulent leaks.
- Developed 1-dimensional (D) and 2-D computational analysis to identify parameters (release size, pressure and downstream geometry) that control auto-ignition phenomena in high-pressure hydrogen releases.
- Participated in the European Union HYPER project and contributed to Work Packages 4 and 5. The United Kingdom Health and Safety Executive made experimental measurements of the jet flame barrier deflection and the associated overpressure arising

from ignition. The University of Ulster as well as other HYPER and HYSAFE partners are using our experimental data for model validation.

- As part of our participation in the International Energy Agency Task 19 on hydrogen safety, we established recommendations for risk criteria and harm criteria for use internationally in evaluating the acceptance of hydrogen facilities.
- A method for generating hydrogen-specific data for use in quantitative risk assessments was established and used to generate hydrogen leakage frequencies for a number of components.
- We evaluated the risk associated with different types of hydrogen refueling stations looking at the importance of different hydrogen generation methods.
- Sandia personnel participated in the National Fire Protection Association (NFPA) 2 working group to modify separation distance guidance. The separation distances are captured in a table that has also been recommended for incorporation into NFPA 55.
- A heat transfer correlation for modeling 70 MPa fast-fill fueling was calibrated against Sandia experiments. Additional calibration will be performed against data collected from ongoing tests of original equipment manufacturer (OEM) fuel systems at Powertech.

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Introduction

A continued barrier to the deployment of commercial hydrogen technologies and infrastructure is the lack of established codes and standards. The purpose of this project is to provide the technical basis for assessing hydrogen-based systems with the accumulation of knowledge feeding into the modification of relevant codes and standards. The scenario analysis and risk assessment effort focuses 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 have developed models to quantify the hydrogen release behavior in engineered systems and combine them with QRA to support risk-informed decision-making in the code development process.

Approach

Efforts were directed toward the following program components: (1) Scenario Analysis, Risk Assessments for Safety, and (2) Codes and Standards Advocacy. Sandia is developing benchmark experiments and a defensible analysis strategy for risk and consequence assessment of unintended releases from hydrogen systems. This work includes experimentation and modeling to understand the dispersion, ignition, and combustion of hydrogen for different release scenarios. A QRA approach is used to identify and grade risk drivers to help focus decision-making and communicate research findings. As part of Codes and Standards Advocacy, Sandia participates in the codes and standards development process through organizations such as the Hydrogen Industry Panel on Codes (HIPOC) and the NFPA. This participation ensures that standards and codes organizations have the most current technical information on hydrogen behavior.

Results

Risk Assessment: QRA was used to help establish risk-informed separation distances for gaseous hydrogen storage facilities (see discussion under Code Changes). To support this effort and cooperative efforts being performed under the International Energy Agency Task 19 (hydrogen safety), risk criteria and harm criteria were surveyed and recommended values were adopted. In addition, a methodology for obtaining hydrogen-specific failure data required in a QRA was developed and utilized to obtain component leakage frequencies. The results of this data analysis was a key input into the selection of leak sizes used to determine the separation distances adopted by the NFPA technical committees. Additional QRA analyses were initiated this year focusing on the risk associated with different forms of hydrogen generation at hydrogen refueling stations and risk associated with the rest of the hydrogen infrastructure. Efforts are currently underway to evaluate the risk tradeoffs associated with the use of barriers to protect the public and facilities from hydrogen jet fires. A joint effort was initiated with NREL to establish Web-based risk assessment tools. The efforts currently underway involve developing a Failure Modes and Effects Analysis tool for identifying important accident scenarios and required prevention and mitigation features.

Barrier Wall Design: We conducted physical and numerical experiments to assess the effectiveness of barriers in deflecting hydrogen jet flames and reducing the extent of hazardous radiation heat flux levels from ignited hydrogen jet flames emanating from leaks in high pressure gaseous storage tanks. Barrier walls have been proposed as one strategy for reducing setbacks at hydrogen fueling stations. The barrier wall work requires a 3-D computational fluid dynamics (CFD) approach because of the complex geometry in the model. The CFD approach is different from our past work with engineering models and required additional validation studies. The computational model was validated against measured flame lengths, radiation heat fluxes, and concentration decay profiles in free jet flames. Vertical and inclined flat walls and a vertical three-wall configuration with panels angled at 135 degrees were studied experimentally and numerically. Both measured and predicted results demonstrate the effectiveness of barriers to deflect jet flames and reduce the extent of hazardous radiation heat flux levels. Gas confinement by the walls introduces an overpressure concern if the hydrogen ignites. Overpressures were measured and modeled and peak pressures are in the range of approximately 0.4 barg (5 psig). Comparisons between measured and predicted barrier wall results are shown in Figures 1a-c for radiation heat flux and overpressure.

Ignition of Hydrogen: Previous studies have indicated that the ignitable gas composition envelope in turbulent hydrogen leaks may not correspond well to the known flammability limits for static hydrogen mixtures. We built an experimental system to study and quantify ignition limits in turbulent hydrogen leaks. An investigation was completed to determine the probability of ignition within the jet. A laser spark system was implemented as the ignition source. Shown in Figure 2 are the measured jet light-up contours for both a methane and hydrogen jet. The hydrogen ignition contour is always at a greater radial distance than methane due to its leaner flammability limit. The hydrogen concentration field is currently being measured to determine the relationship between jet ignitability, mean concentration, and static hydrogen flammability limits.

Princeton University has completed construction of a laboratory-scale auto-ignition experiment that will be used to make measurements at their laboratory and at Sandia where advanced laser-based diagnostics can be utilized. The experiment design is based on 1-D and 2-D computations that have shown spontaneous ignition depends on two critical issues: 1) the pressure difference and transient shock process resulting from sudden releases provides sufficient temperatures in the expanding hydrogen and air to induce chemical ignition; 2) sufficient mixing regions are produced contiguous to the site where chemical initiation occurs. A high frame-rate schlieren visualization system has been implemented to parametrically explore conditions leading to spontaneous ignition.

70 MPa Fast-Fill Refueling: A consortium was formed to study 70 MPa fast-fill fueling requirements for the Society of Automotive Engineers (SAE) J2601 standard, led by Powertech Labs. Powertech is performing the fast-fill tests while OEM partners including Chrysler, Nissan, General Motors, Ford and Toyota are contributing fueling systems. Sandia is using consortium data and data from other sources to calibrate tank heat transfer correlations to build a predictive model of the fast-fill process. Powertech has completed testing of three OEM fuel systems: Chrysler, General

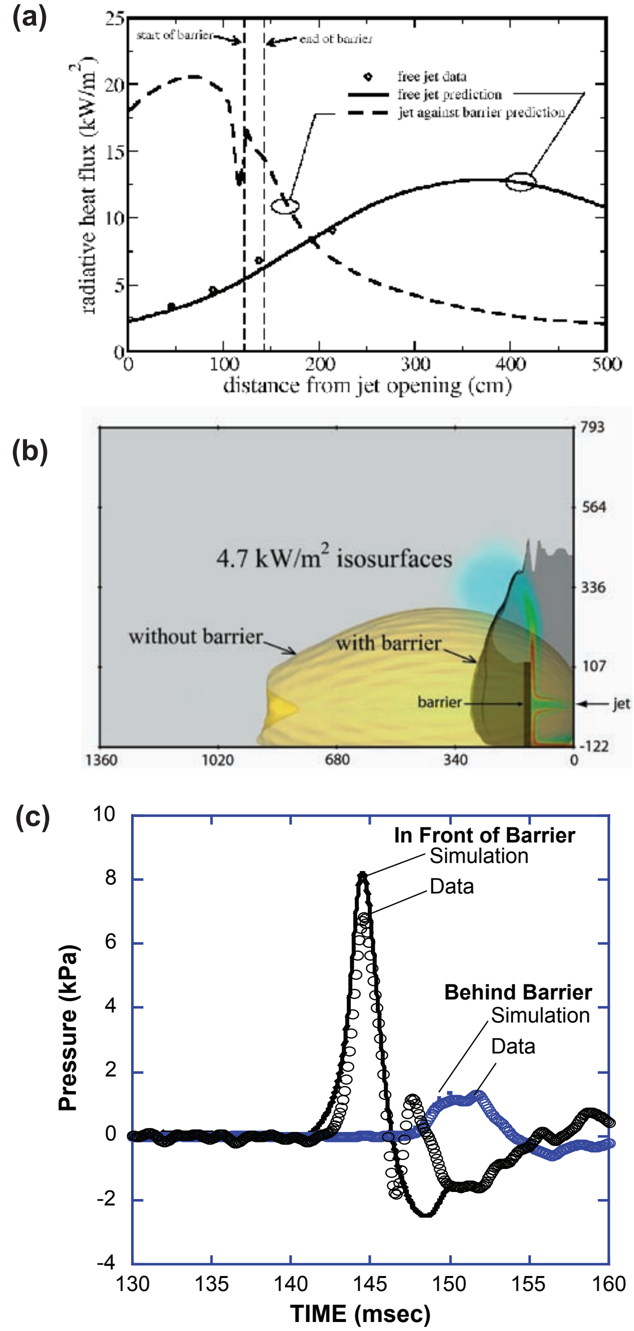

FIGURE 1. (a) comparison of measured and predicted (solid line) radiative heat flux from a horizontal free hydrogen jet flame along a line parallel to the jet (at a lateral distance of 137.6 cm from the jet centerline); also shown is the predicted heat flux (dashed line) when the jet flame is directed toward the center of a 2.4 m x 2.4 m vertical barrier; (b) side view of calculated isosurfaces for radiative heat flux of 4.7 kW/m^2 comparing horizontal and vertical extent of radiation field without and with a barrier; jet flow is from right to left with distances in centimeters; (c) comparison of simulated and experimental overpressures in single vertical wall test.

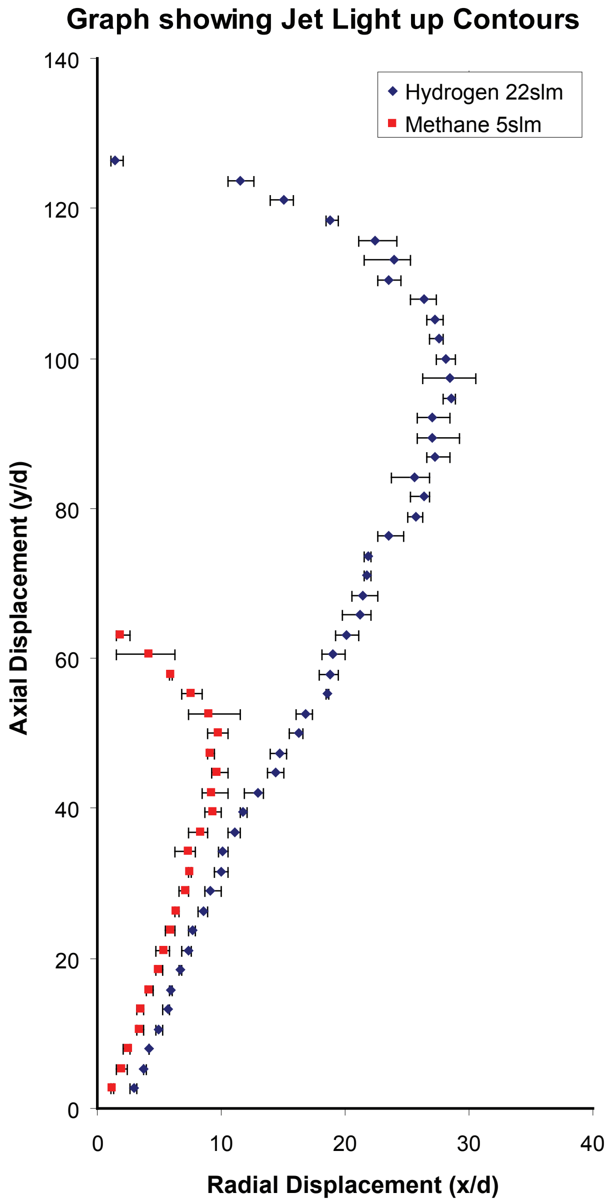

FIGURE 2. Graph Showing Jet Light-Up Contour for Turbulent Methane nd Hydrogen Jets

Motors, and Nissan. Tests on the Ford and Toyota systems are in progress. While the consortium test data has been useful for the intended purpose of providing requirements to the SAE J2601 standard, the accuracy has been insufficient for use in model calibration.

Code Change Process: Marty Gresho, Sandia fire marshal, is chairing the NFPA 2 Hydrogen Technology Committee. Sandia researchers, Bill Houf and Jeff LaChance, participate in the NFPA 2 task group on separation distances. The task group created a separation distance table based on the work published by Sandia. The table has been approved by NFPA technical committees for incorporation into NFPA 55. Bob Schefer was appointed to the HIPOC committee this year and coordinates lab research with code development data requirements.

Conclusions

- Characterized flame behavior and heat transfer in release scenarios involving flame impingement on barrier walls. Evaluated wall configuration effectiveness at deflecting flames and mitigating hazards due to radiative heat transfer and overpressure produced during flame ignition.
- Quantified ignitable gas envelopes in turbulent hydrogen leaks. Verified that traditional flammability limits for static hydrogen/air mixtures are not applicable to unintended releases.
- Applied engineering models to identify processes important to auto-ignition in high-pressure hydrogen releases. Developed experiment to verify model findings.
- Established new risk-informed separation distances that have been adopted in several NFPA codes.
- Thirty publications and presentations were delivered.

Future Directions

- Investigate and quantify overpressure phenomena produced during initial ignition of hydrogen releases in the presence of barrier walls.
- Experimentally determine and develop a computational model to predict ignition limits for lean hydrogen/air mixtures for sustainable flames in turbulent jets and plumes.
- Perform laboratory-scale and full-scale experiments to identify mechanisms responsible for auto-ignition of high-pressure hydrogen releases.
- Continue to assess what issues are important for safety codes and standards involved with liquid hydrogen. Explore available literature and identify areas where data gaps exist and develop experiments and/or models that will fill those gaps.
- Evaluate the risk associated with accidental releases of hydrogen in tunnels, parking structures, and storage sheds.
- Use network flow models and improved tank heat transfer correlation to develop optimum control strategies for hydrogen tank filling. Develop Web-based risk tools for evaluating hydrogen refueling stations.

FY 2008 Publications/Presentations

1. Schefer, R. W., Groethe, M., Houf, W. G. and Evans, G. (2008), "Experimental Evaluation of Barrier Walls for Risk Reduction of Unintended Hydrogen Releases", International Journal of Hydrogen Energy (submitted).

2. Schefer, R. W. and Houf, W. G. (2008), "Investigation of Small-Scale Unintended Releases of Hydrogen: Momentum–Dominated Regime", International Journal of Hydrogen Energy (accepted).

3. Schefer, R. W., Houf, W. G. and T. C. Williams (2008), "Investigation of Small-Scale Unintended Releases of Hydrogen: Buoyancy Effects", International Journal of Hydrogen Energy (accepted).

4. Houf, W. G., Evans, G. and Schefer, R. W, (2008), "Analysis of Jet Flames and Unignited Jets from Unintended Releases of Hydrogen," Special Issue of International Journal of Hydrogen Energy (Invited).

5. Houf, W. G. and Schefer, R. W. (2007) "Predicting Radiative Heat Fluxes and Flammability Envelopes from Unintended Releases of Hydrogen", *International Journal of Hydrogen Energy* **32**, 12, pp. 2081-2093.

6. Houf, W. G. and Schefer, R. W. (2008) "Analytical and Experimental Investigation of Small-scale Releases of Hydrogen," *International Journal of Hydrogen Energy* **33**, 4, pp. 1435-1444. February 2008.

7. Schefer, R. W. Houf, W. G., Williams, T. C., Bourne, B. and Colton, J. (2007), "Characterization of High-Pressure, Under-Expanded Hydrogen-Jet Flames", International Journal of Hydrogen Energy, Vol. 32, 12, August, 2007, pp. 2081-2093.

8. LaChance, J. L., "Risk-Informed Separation Distances for Hydrogen Refueling Stations," 2nd International Conference on Hydrogen Safety, San Sebastian, Spain, September 11-13, 2007.

9. LaChance, J. L., Tchouvelev, A. V., and Ohi, J., "Risk-Informed Process and Tools for Permitting Hydrogen Fueling Stations," 2nd International Conference on Hydrogen Safety, San Sebastian, Spain, September 11-13, 2007.

10. Houf, W. G., Evans, G. and Schefer, R, W., "Research and Development on Unintended Releases for Hydrogen Safety Codes and Standards," IEA Task 19 Meeting, San Sebastian, Spain, Sept. 10, 2007.

11. Houf, W. G., Evans, G. and Schefer, R. W., "Analysis of Jet Flames and Unignited Jets from Unintended Releases of Hydrogen," 2nd International Conference on Hydrogen Safety, San Sebastian, Spain, September 11-13, 2007.

12. Houf, W. G., Evans, G. and Schefer, R. W., "Research and Development on Unintended Releases for Hydrogen Safety Codes and Standards," HYPER Work Package 4 & 5 Meeting, San Sebastian, Spain, Sept. 14, 2007.

12. Schefer, R. W. and Houf, W. G., "Unintended Hydrogen Releases: Experiments and Modeling", Japanese New Energy and Industrial Technology Development Organization (NEDO) Meeting, Sandia National Laboratory, Livermore, CA, November 13, 2007.

14. Schefer, R. W., Houf, W. G. and Evans, G. H. "Hydrogen Safety Codes and Standards: *Barrier Walls for Hazards Mitigation*," Hydrogen Codes and Standards Technical Team Meeting, Livermore, CA, January 9, 2008.

15. Schefer, R. W., Ruggles, A. and Houf, W. G., "Hydrogen Safety Codes and Standards: *Ignition of Unintended Releases*," Hydrogen Codes and Standards Technical Team Meeting, Livermore, CA, January 9, 2008.

16. Houf, W. G., "NFPA2 – Consequence-Based Separation Distances," NFPA 2 Task Group 6 Meeting, Golden, CO, Jan. 28-29, 2008.

17. Houf, W. G., Evans, G. and Schefer, R. W., "Recent Research and Development on Barrier Walls for Unintended Releases of Hydrogen, HYPER Meeting, Manchester, UK, February 21-22, 2008.

18. Houf, W. G. and Schefer, R. W. (2008), "Investigation of Small-Scale Unintended Releases of Hydrogen", SAE 2007 Transactions, Journal of Passenger Cars, March, 2008.

19. Weiner, S. Houf, W. G. and Ruiz, A., "Present and Future Directions in Hydrogen Safety Research," IEA Task 19 Meeting, St-Alexis-des-Monts, Quebec, Canada, March 2, 2008.

20. Houf, W. G., Evans, G. and Schefer, R. W., "Recent Research and Development on Barrier Walls for Unintended Releases of Hydrogen," IEA Task 19 Meeting, St-Alexis-des-Monts, Quebec, Canada, March 2, 2008.

21. LaChance, J. L., Brown, J., Middleton, B., and Robinson, D., "Data for the Use in Quantitative Risk Analysis of Hydrogen Refueling Stations," National Hydrogen Association Meeting, Sacramento, CA, March 30 - April 3, 2008.

22. Tchouvelev, A. V., LaChance, J. L., and Engebo, A., "IEA Task 19 Hydrogen Safety Effort in Developing Uniform Risk Acceptance Criteria for the Hydrogen Infrastructure," National Hydrogen Association Meeting, Sacramento, CA, March 30 - April 3, 2008.

23. Houf, W. G., Schefer, R. W. and Evans, G., "Analysis of Barriers for Mitigation of Unintended Releases of Hydrogen," 2008 Annual Hydrogen Conference and Expo USA, Sacramento, CA, March 30-April 3, 2008.

24. Diop, S., Agrawal, A. K., and Schefer, R. W., "Barrier Optimization by Optical Analysis of Compressed Hydrogen Gas Leaks", 2008 Technical Meeting of the Central States Section of the Combustion Institute, Tuscaloosa, AL, 20-23 April, 2008.

25. Schefer, R. W., "Unintended Hydrogen Releases: Technical Basis for Safety Codes and Standards Development," USCAR Directors Meeting, Livermore, CA, April 24, 2008.

26. Houf, W. G., Evans, G. and Schefer, R. W., "Recent Research and Development on Barrier Walls for Mitigation of Unintended Releases of Hydrogen, HYPER Meeting, Paris, France, April 3-4, 2008 (by teleconference).

27. LaChance, J. L. and Houf, W. G., "Risk-Informed Separation Distances for Use in NFPA Hydrogen Codes and Standards," 17th World Hydrogen Energy Conference, Brisbane, Australia, June 15-19, 2008.

28. Houf, W. G., Schefer, R. W., Evans, G. and Groethe, M., "Barriers for Mitigation of Unintended Releases of Hydrogen", 17th World Energy Conference, Brisbane, Australia, 15-19 June, 2008.

29. Schefer, R. W., Groethe, M., Houf, W. G and Keller, J. O., "Experimental Evaluation of Barrier Walls for Risk Reduction of Unintended Hydrogen Releases", 17th World Energy Conference, Brisbane, Australia, 15-19 June, 2008.

30. Houf, W. G., Evans, G. and Schefer, R, W., HYPER Work Package 4 Interim Report on Releases, Fire and Explosions, Chapter 6: "Effect of Barriers and Walls," October 31, 2008.