VIII.6 R&D for Safety Codes and Standards: Hydrogen Release Behavior and Risk Assessment

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Project Start Date: October 1, 2003
Project End Date: Project continuation and direction determined annually by DOE

Overall Objectives

- Build tools to enable industry-led codes and standards (C&S) revision and safety analyses to be based on a strong science and engineering basis.

- Develop and validate hydrogen behavior physics models to address targeted gaps in knowledge.

- Develop hydrogen-specific quantitative risk assessment (QRA) tools and methods to support regulations, codes and standards decisions and to enable performance-based design (PBD) code-compliance option.

- Eliminate barriers to deployment of hydrogen fuel cell technologies through scientific leadership in codes and standards development efforts.

Fiscal Year (FY) 2014 Objectives

- Develop version 1 of an integrated hydrogen-specific risk assessment toolkit (HyRAM) to enable sustained use of QRA by a broad range of users.

- Initiate research activity with industrial partners to use QRA tool to implement and validate performance-based compliance approach of National Fire Protection Association (NFPA) 2 Chapter 5.

- Develop technical plan and partnerships for building experimental test platform for hydrogen release behavior at cryogenic temperatures.

- Conduct modeling and experimental activities to develop and validate reduced order modeling of jet flame behavior and deflagration overpressures.

- Provide expert perspective on QRA and behavior models to relevant codes and standards committees to promote the adoption of science-based methods.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Safety, Codes and Standards section of the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan:

(A) Safety Data and Information: Limited Access and Availability

(F) Enabling National and International Markets Requires Consistent Regulations, Codes and Standards

(G) Insufficient Technical Data to Revise Standards

(L) Usage and Access Restrictions (parking structures, tunnels and other usage areas)

Contribution to Achievement of DOE Safety, Codes and Standards Milestones

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

- Milestone 2.8: Publish risk mitigation strategies. (2Q, 2014)

- Milestone 2.7: Provide critical understanding of hydrogen behavior relevant to unintended releases in enclosures. (4Q, 2013)

- Milestone 2.10: Understand flame acceleration leading to transition to detonation. (4Q, 2014)

- Milestone 2.11: Publish a draft protocol for identifying potential failure modes and risk mitigation. (4Q 2014)

- Milestone 2.13: Develop and validate simplified predictive engineering models of hydrogen dispersion and ignition. (4Q 2015)

- Milestone 2.19: Validate inherently safe design for hydrogen fueling infrastructure. (4Q, 2019)

- Milestone 4.7: Complete risk mitigation analysis for advanced transportation infrastructure systems. (1Q, 2015)

- Milestone 4.8: Revision of NFPA 2 to incorporate advanced fueling storage systems and specific requirements for infrastructure elements such as garages and vehicle maintenance facilities. (3Q, 2016)

FY 2014 Accomplishments

- Report: developed a metric to evaluate the development of hydrogen codes and standards and benchmarked program activity to show progress in enabling technology deployment

- Workshop: organized and led hydrogen C&S QRA user workshop to help build stakeholder awareness of risk and to identify barriers that limit industry use of QRA

- Developed an integrated reduced-order behavior model for predicting overpressures associated with transient hydrogen releases for use in risk-informed C&S development.

- Developed a detailed project plan to research and model the behavior of unintended releases of hydrogen at cold and cryogenic temperatures

- Updated existing reduced-order flame radiation models with large scale, downstream flame radiation behavior to improve prediction of downstream heat flux

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INTRODUCTION

DOE has identified safety, codes, and standards as a critical barrier to the deployment of hydrogen, with key barriers related to the availability and implementation of technical information in the development of RCS. This project provides the technical basis for assessing the safety of hydrogen fuel cell systems and infrastructure using QRA and physics-based models of hydrogen behavior. The risk and behavior tools that are developed in this project are motivated by and shared directly with the committees revising relevant codes and standards, thus forming the scientific basis to ensure that code requirements are consistent, logical, and defensible.

APPROACH

This work leverages Sandia's unique experimental and modeling capabilities and combines these efforts with stakeholder engagement and international leadership. The behavior of hydrogen releases is examined using state-of-the-art diagnostics in the Turbulent Combustion Laboratory. Results of these experiments are used to develop and validate predictive engineering tools for flame initiation, flame sustainment, radiation patterns, and overpressures. The resulting behavior models provide the foundation for QRA modeling efforts, which include scenario analysis, consequence modeling, and quantification of risk. These integrated hydrogen behavior and QRA models are then applied to relevant technologies and systems to provide insight into the risk level and risk mitigation strategies with

the aim of enabling the deployment of fuel cell technologies through revision of hydrogen safety, codes, and standards.

RESULTS

Develop Version 1 of HyRAM

Code committees and industry are both interested in using QRA to enable code development and code compliance for hydrogen systems. Gaps and limited availability of QRA tools for hydrogen form a barrier to this goal. This core research activity addresses the hydrogen QRA tool gap by integrating validated models and data into a Windows®-based engineering tool with a graphical user interface. This tool is called HyRAM, Hydrogen Risk Assessment Models.

Figure 1 is a flowchart that shows the various modules used within HyRAM. Initial elements of the flowchart were independently developed in Matlab®. The unified HyRAM tool replaces this array of independent modules to enable broader application of QRA by stakeholders. The modular architecture and open-source license set the stage for future development activities to occur collaboratively with other research organizations. HyRAM version 1 contains graphical user interfaces for "QRA mode," which enables end-to-end use of the HyRAM modules to calculate risk from jet flames for user-defined gaseous hydrogen systems. Toolkit priorities are based on published proceedings of the QRA user workshop held in June 2013. Version 1 of HyRAM, which is to be completed at the end of 2014, can be used to quantify the likelihood and thermal consequences associated with jet fires from gaseous releases from user-defined hydrogen installations. Future development activities include enabling stand-alone use of behavior models for consequence calculations and the addition of new consequence calculations (such as overpressure) to expand the type of infrastructure that can be modeled in HyRAM.

Cold and Cryogenic Hydrogen Behavior Research

Bulk liquid hydrogen storage has the benefit of a higher storage potential that enables greater station throughput over similarly sized gaseous systems. However, validated models of liquid hydrogen releases—critical information needed for risk-based strategies—do not exist, due to a lack of adequate data from science-based test platforms with full control over release boundary conditions. Sandia developed a detailed project plan to research and model the behavior of unintended releases of hydrogen at cold and cryogenic temperatures. Additionally, under a Cooperative Research and Development Agreement with industry, we have begun designing an experimental platform for generating the missing data. The preliminary design is shown in Figure 2. After installation and performance-testing of the cryogenic hydrogen release laboratory are complete (targeted for late 2015), the laboratory will be used to develop comprehensive data sets

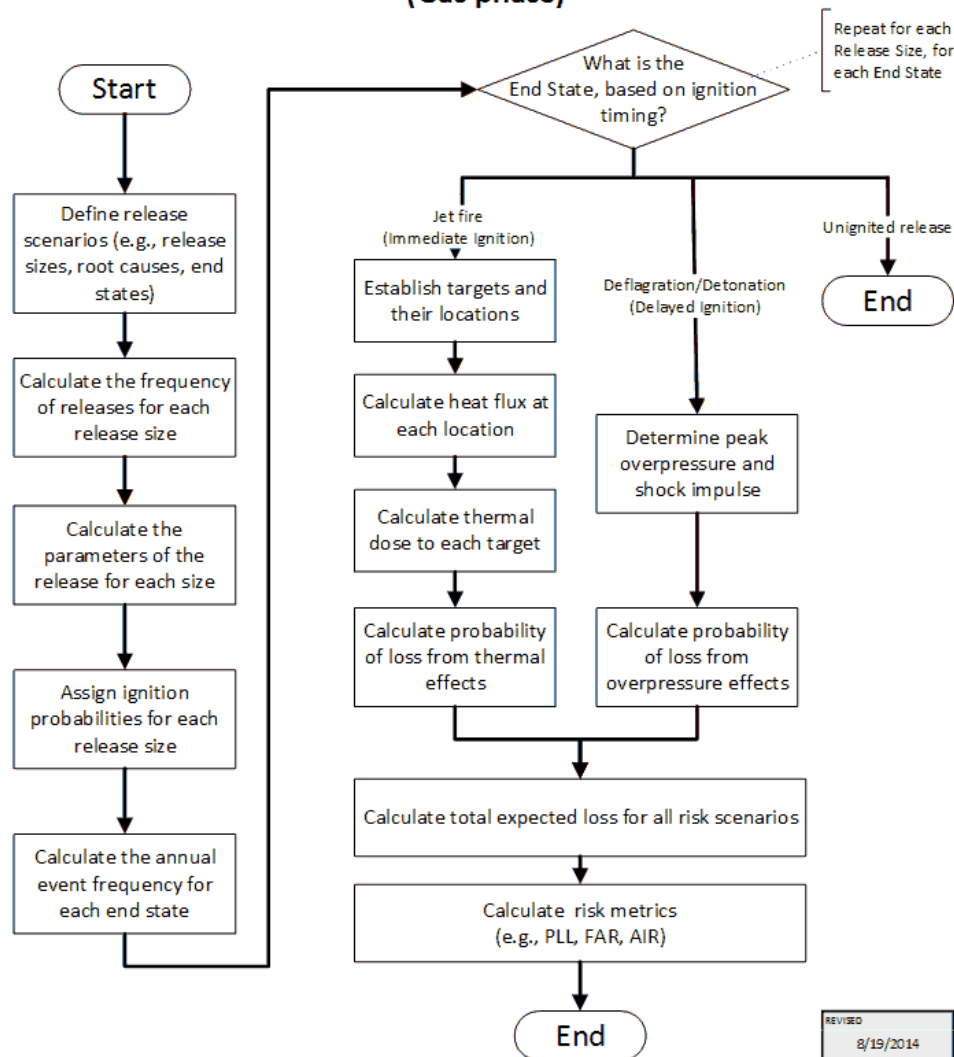## Process Flow Chart for Hydrogen QRA
(Gas phase)

FIGURE 1. Flowchart of modules contained in the HyRAM toolkit. Modules can be used end-to-end, as illustrated in this figure, or in stand-alone calculations.

relevant to releases from liquid hydrogen storage systems similar to those located at commercial fueling stations. This will enable development and experimental validation of cold-plume release models that can be integrated into QRA and safety assessments to enable deployment of liquid hydrogen infrastructure.

Hydrogen Behavior Modeling and Experimental Validation

Ongoing research occurring over the past decade at Sandia has resulted in the development and validation of numerous scientific models of the behavior of gaseous hydrogen releases. During FY 2014, the jet flame model was updated to account for downstream buoyancy behavior that was observed during experimental validation activities. This and other physical models (products of several years of research in this program) are being consolidated, modularized, and documented for integration into the HyRAM toolkit. Gaseous hydrogen jet dispersion models and jet flame models (along with the required sub-models, e.g., notional nozzle models) were formalized and integrated into HyRAM during FY 2014. Ongoing activity includes a first-order overpressure model suitable for integrating into HyRAM in the FY 2015 timeframe. Several of these models and their sub-models require additional validation data and further refinement, including the overpressure model, the notional nozzle model, and models of liquid hydrogen behavior. Additionally, we are planning experiments to reduce the ambiguity in the notional nozzle (under-expanded jet) model in collaboration with a student from Tsinghua University.
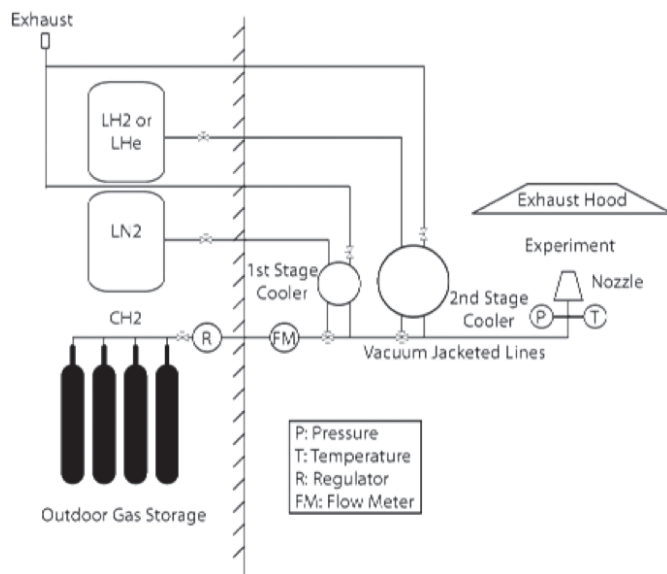
FIGURE 2. Cryogenic release laboratory design—gaseous hydrogen is cooled in two stages, by liquid nitrogen and then liquid hydrogen, before release.

Develop Design Brief to Enable Performance-Based Compliance Option

NFPA 2, Hydrogen Technologies Code, allows for the use of PBD for hydrogen facilities as a means of complying with the code without strict adherence to the prescriptive code requirements. While HyRAM can be used as a means of evaluating the risk of alternate designs, it can also be used to quantitatively evaluate risks associated PBD options. The establishment and demonstration of PBD option will directly increase the availability of locations for hydrogen fueling stations, reduce the effort required by industry to use the PBD approach and lay the groundwork for similar QRA-backed design processes for other alternative fuels. In order to initiate real-world application of science-based risk analysis, a Cooperative Research and Development Agreement was initiated with a major hydrogen fueling station provider.

Figure 3 depicts the approach of the application of QRA to the design of both a representative commercial hydrogen refueling station and a real-world station. The HyRAM software will be used to calculate the risk metrics for a station that is fully compliant with the prescriptive code requirements in order to establish a baseline for these metrics for a specific station configuration. In the next phase of work, a station design with key modifications to the prescriptive requirements will be evaluated with input from the industry partner. This mock PBD will then be vetted with in the fire protection and hydrogen industries with the aim of identifying best practices for implementing PBD methods. Following this, a real-world station with a key modification backed by a performance-based design will be processed

through the permitting process for a hydrogen station in California.

Codes and Standards Participation

- CSA Group HGV 4.9 – Hydrogen fueling station guidelines have been edited and reorganized and are ready for industry review before they become a CSA Group standard.

- Hydrogen Safety Panel – Sandia participated in several hydrogen safety plan reviews for innovative industrial hydrogen implementations as well as participating in the revision of the hydrogen event data collection fields.

- NFPA 2 – Sandia participated in the second draft meeting of the 2016 version of NFPA 2 Hydrogen Technologies Code. Sandia also actively participated in the reactivation of the NFPA 2 liquid hydrogen separation distances task group, which began work on revision of the prescriptive requirements for the next revision cycle of the code.

CONCLUSIONS AND FUTURE DIRECTIONS

- Project impact is demonstrated by benchmarking metric: "Number of sites that can readily accept hydrogen"
  - (future) Re-evaluate benchmark to evaluate R&D investments at key project milestones and to ensure continued alignment with program goals.

- A template for implementing the performance-based approach in NFPA2 Chapter 5 is the next step for increasing the number of sites that can readily accept hydrogen.
  - (future) Demonstrate PBD option and work the PBD brief through a permitting process to demonstrate acceptance of a PBD approach by an authority having jurisdiction.

- HyRAM provides a standardized platform for developing and integrating hydrogen QRA and consequence models into codes and standards.
  - (future) Add reduced order overpressure model and features to enable PBD.
  - (future) Formalize rules for user-defined models and international harmonization of methodology.

- Improved physics-based models of hydrogen behaviors (e.g., jet flame model, multi-source radiation model) improves the fidelity of risk calculations.
  - (future) Improve the accuracy of the sub-models, particularly the notional nozzle model, through targeted experiments.
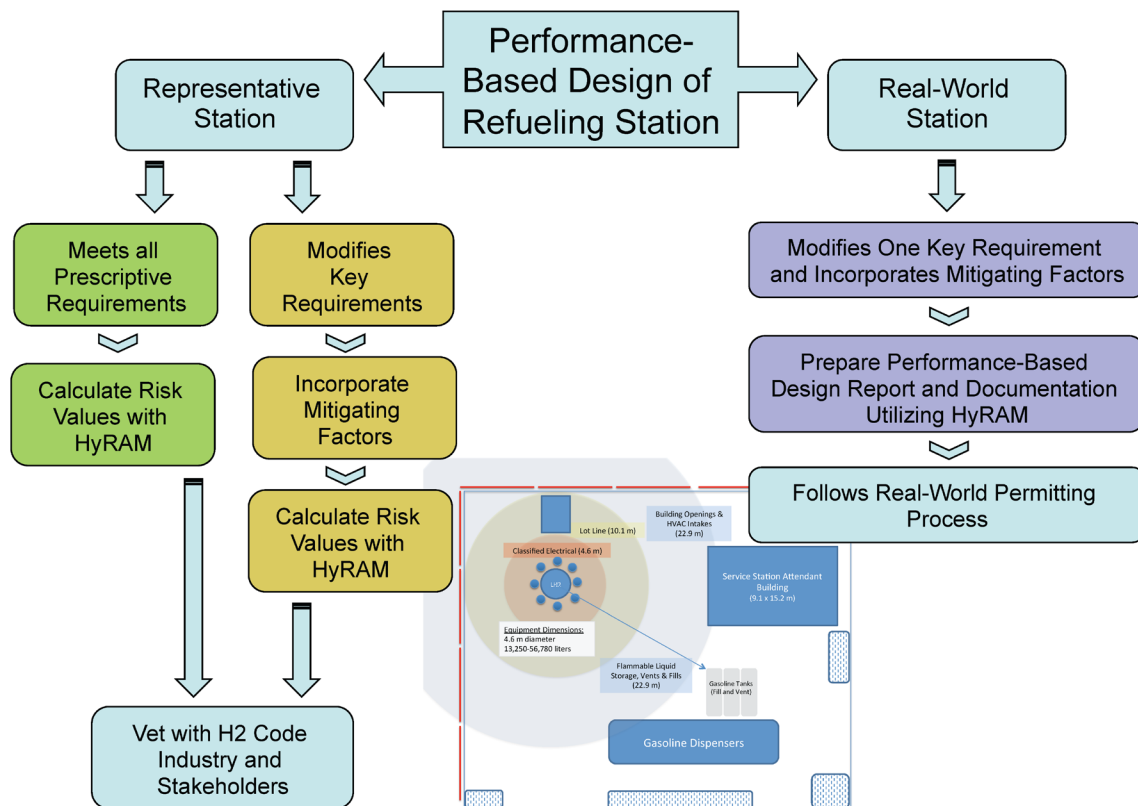
FIGURE 3. Overview of PBD Application of QRA

- An integrated, reduced-order overpressure model enables the calculation of overpressure in HyRAM and fills a key gap in modeling hydrogen deflagrations.
  - (future) Add overpressure model into HyRAM in the early FY 2015 timeframe.
  - (future) Validate model accuracy and make improvements as needed.
- The storage of liquefied hydrogen is limited by the existing code requirements and predictive behavior models for liquefied hydrogen releases.
  - (future) Construct experimental platform for characterizing the unintended release of liquid-vapor mixed-phase hydrogen releases (with support from industry).

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FY 2014 PUBLICATIONS/PRESENTATIONS

1. A.C. LaFleur, K. Groth, A.B. Muna. "Application of Quantitative Risk Assessment (QRA) to Hydrogen Fueling Infrastructure for FCEVs." Presentation at the 2014 ASME 12th Fuel Cell Science, Engineering and Technology Conference, Boston, MA, July 2014.

2. K. Groth "Hydrogen behavior and Quantitative Risk Assessment." Presentation at the 2014 DOE Hydrogen Fuel Cell Technologies Program Annual Merit Review, Washington, DC. June 2014.

3. K. Groth. "Hydrogen QRA & HyRAM Toolkit Introduction" Presentation at side-meeting on Hydrogen Risk Assessment at DOE Hydrogen Fuel Cell Technologies Program Annual Merit Review, Washington, DC. June 2014.

4. A.C. LaFleur, A.B. Muna, "Hydrogen Fueling Station Performance-Based Approach." Presented at 20th Hydrogen Safety Panel (HSP) meeting, Golden, CO, May 2014.

5. K.M. Groth. "Hydrogen QRA & HyRAM Toolkit Introduction" Presented at 20th Hydrogen Safety Panel (HSP) meeting, Golden, CO, May 2014.

6. A.V. Tchouvelev, K.M. Groth, P. Benard, T Jordan. "A Hazard Assessment Toolkit For Hydrogen Applications." *Proc World Hydrogen Energy Conference* (WHEC 2014), 2014.

7. K.M. Groth, A.V. Tchouvelev, "A toolkit for integrated deterministic and probabilistic risk assessment for hydrogen infrastructure*." Proc Int Conf Probabilistic Safety Assessment and Management (PSAM 12)*, June 2014.

8. I.W. Ekoto, A.J. Ruggles, L.W. Creitz, J.X. Li. "Updated Jet Flame Radiation Modeling with Corrections for Buoyancy". *Int. J. of Hydrogen Energy*, Accepted in 2014.

9. A.J. Ruggles, I.W. Ekoto. "Experimental investigation of nozzle aspect ratio effects on underexpanded hydrogen jet release characteristics*," International Journal of Hydrogen Energy*, Accepted March 2014.

10. K.M. Groth, J.L. LaChance, A.P. Harris. "Design-stage QRA for indoor vehicular hydrogen fueling systems". *Proc of the European Society for Reliability Annual Meeting (ESREL 2013).*

11. A.P. Harris, D.E. Dedrick, A.C. LaFleur and C. San Marchi, "Safety, Codes and Standards for Hydrogen Installations: Hydrogen Fueling System Footprint Metric Development." SAND2014-3416, Sandia National Laboratories, April 2014.

12. A.C. LaFleur, "Risk and Reliability Analysis" presented at AIST-SNL workshop on High Pressure Hydrogen Storage Systems, January 24, 2014.

13. K.M. Groth, "Sandia H2 Quantitative risk assessment (QRA) activities." Presented to DOE H2 CSTT, December 19, 2013.

14. A. Harris. "Survey of Materials Selection Information for Hydrogen Service" Presented to US DOE Hydrogen Safety Panel meeting, December 11, 2013.

15. A. Harris. "Leak Rate Standard Working document" Presented to US DOE Hydrogen Safety Panel meeting, December 11, 2013.

16. A. Harris. "Results from a case study of separation distances in support of program performance metric development for US DOE EERE FCTO" Presented to California Fuel Cell Partnership, December 4, 2013.

17. K.M. Groth, "SNL QRA toolkit and SNL-HySafe workshop." Presented to International Energy Agency Hydrogen Implementing Agreement Task 31 experts workshop (IEA HIA), October 15, 2013.

18. I.W. Ekoto, A.J. Ruggles, L.W. Creitz, J.X. L. "Updated Jet Flame Radiation Modeling with Corrections for Buoyancy." Proc Int Conf Hydrogen Safety, Brussels, Belgium, September 2013.

19. A.J. Ruggles, I.W. Ekoto. "Experimental investigation of nozzle aspect ratio effects on underexpanded hydrogen jet release characteristics." *Proc Int Conf Hydrogen Safety*, Brussels, Belgium, September 2013.

20. I.W. Ekoto. "Hydrogen release and deflagration experiments within a scaled, ventilated warehouse." Presented at HyIndoor Advanced Research Workshop, Brussels, Belgium, September 12, 2013.

21. I.W. Ekoto, "Simulation of hydrogen-air deflagrations within ventilated warehouse enclosures." Presented at HyIndoor Advanced Research Workshop, Brussels, Belgium, September 12, 2013.

22. K.M. Groth, "Design-stage QRA for indoor vehicular hydrogen fueling systems." Presented at the European Society for Reliability Annual Meeting (ESREL 2013), Amsterdam, 2013.