VIII.1 Hydrogen Behavior and Quantitative Risk Assessment

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

Overall Objectives

- Build tools to enable industry-led codes and standards 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 code compliance option

Fiscal Year (FY) 2015 Objectives

- Develop prototype Version 1.0 of the HyRAM toolkit/platform to facilitate use of hydrogen safety research in industry-led safety analyses
- Initiate HyRAM testing activities with external stakeholders by distributing the alpha version of the software to partners from industry, research, and government
- Design and construct laboratory for cold hydrogen release experiments by specifying the modifications needed for the Turbulent Combustion Lab and identifying and purchasing needed equipment
- Experimentally validate an equivalent source model for high pressure hydrogen by conducting release experiments in the Turbulent Combustion Lab

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 & 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 2.10: 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 2015 Accomplishments

- Developed and copyrighted HyRAM Version 1.0
- Initiated HyRAM user testing by inviting 22 external stakeholders

- Developed detailed design and purchased major equipment needed for lab modifications necessary to conduct experiments on cryogenic hydrogen releases
- Conducted high pressure hydrogen release experiments by conducting experiments with releases up to 60 bar and developed empirical correlations that give boundary conditions to a reduced-order equivalent source model

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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 regulations, codes, and standards. 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

HyRAM Toolkit Development

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 an engineering tool called HyRAM.

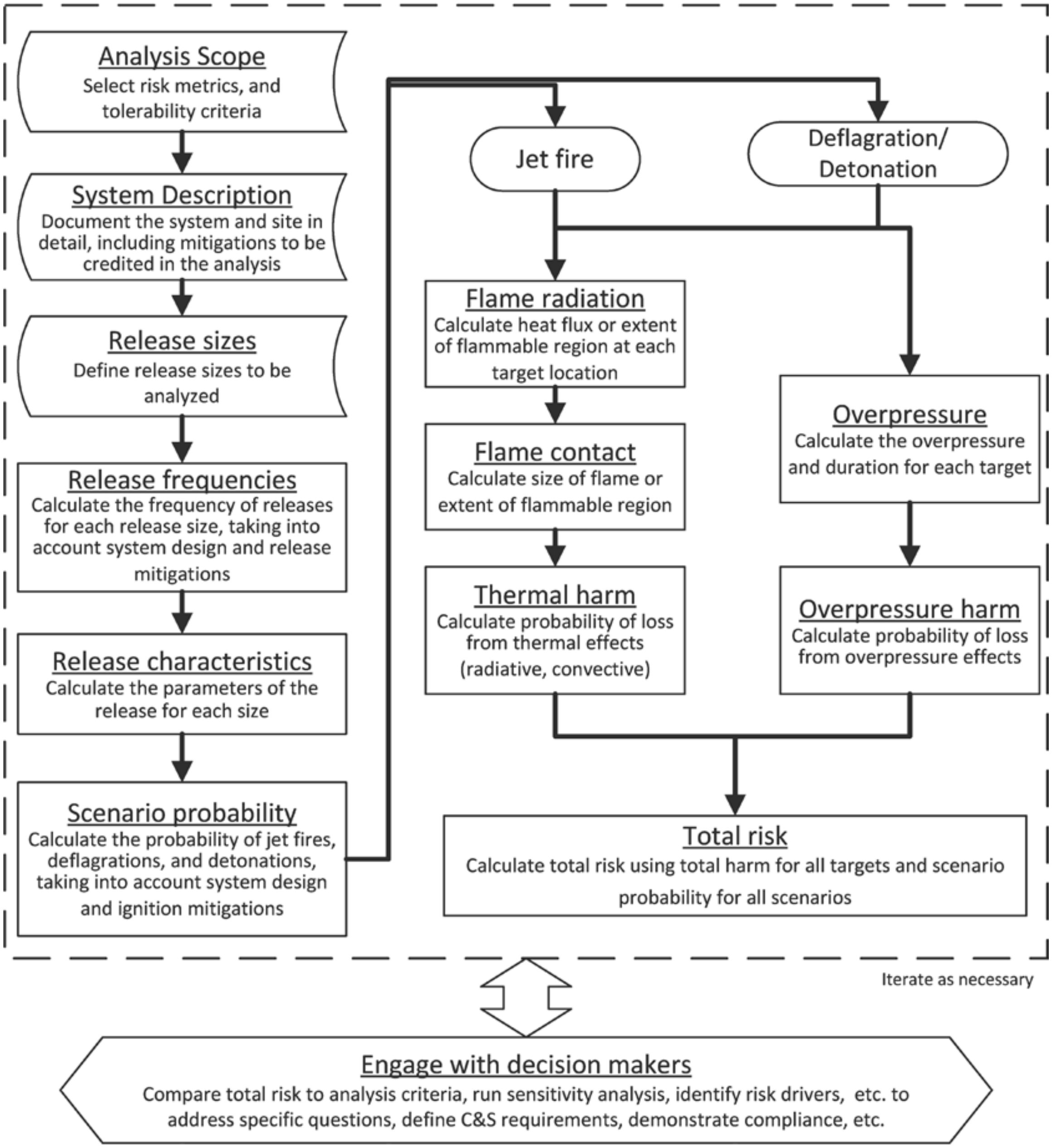
The HyRAM package will enable installation designers, and code and standards development organizations to conduct consequence modeling and QRA with state-of-the-art, validated science and engineering models (see Figure 1). Near-term uses of HyRAM are focused on the needs of codes and standards developers (e.g., National Fire Protection Association [NFPA] 2 and International Organization for Standardization [ISO]-TR-19880). HyRAM can be used to support the establishment of safety distances and other mitigation credits, and furthermore can be used to enable a performance-based compliance option within these codes and standards. Longer-term, HyRAM is anticipated to support development of safety cases and design decisions for user-defined hydrogen installations, and can also be used to demonstrate improvements in facility safety.

HyRAM development was initiated in FY 2014, and during FY 2015 we completed and copyrighted HyRAM Version 1.0 (build number 1.0.0.280). The HyRAM 1.0 toolkit integrates deterministic and probabilistic models for quantifying scenario likelihood, predicting physical effects, and characterizing the impact of hydrogen hazards on people and structures. The current build of HyRAM incorporates generic probabilities for leaks from nine types of hydrogen equipment, generic probabilities for hydrogen ignition, expressions for calculating scenario likelihood and individual risk, probabilistic models for the impact of heat flux on humans and structures, and experimentally validated models of hydrogen jet flames and gaseous hydrogen releases (notional nozzle models and plumes). New modules developed in FY 2015 include the curved flame model (developed and experimentally validated by SNL in 2013) to replace the previous "straight flame" model (developed by SNL in 2007). During FY 2015 work began on integrating the necessary modules to enable calculation of deflagration overpressures resulting from confined hydrogen releases. This overpressure module is being tested internally and is expected to be stable by the end of 2015.

The flexible architecture of the HyRAM framework enables the incorporation of additional physical models, including liquid hydrogen release and dispersion. On the physical model side, future modifications will provide ability to calculate physical effects of liquid hydrogen releases and subsequent ignitions. The models will also be updated to include the effects of a cross wind on plume and flame trajectories, and the submodels (e.g., the jet flame model) will be kept current as scientific consensus changes. For QRA outputs, future modifications will provide cut-sets for Fault Trees and reliability importance measures for risk scenarios.

Initiate HyRAM Testing and Documentation

User feedback is a critical aspect of creating enabling tools and guidance. During FY 2015 we initiated usability



C&S--codes and standards

FIGURE 1. Quantitative risk assessment methodology implemented in HyRAM toolkit

testing on HyRAM 1.0.0.280 with a small number of external stakeholders from various aspects of the hydrogen community. Currently, seven stakeholders have signed non-disclosure agreements to gain access to HyRAM 1.0 versions, and Sandia is in various stages of the license process with 15 additional stakeholders. The current alpha testing activities are focused on obtaining unstructured user feedback on the look and feel of the HyRAM prototype. Future external testing activities will include planning for more formal user feedback.

Design and Construct Laboratory for Cold Hydrogen Release Experiments

Stations that have liquid hydrogen delivered and/or store hydrogen cryogenically can serve a larger number of customers per day, and can have favorable economics over stations that have high pressure gas delivered. However, the codes and standards that govern the siting of cryogenic hydrogen have separation distances that are often prohibitively large (e.g., public assembly areas and building openings or air intakes that must be 75 ft away from the

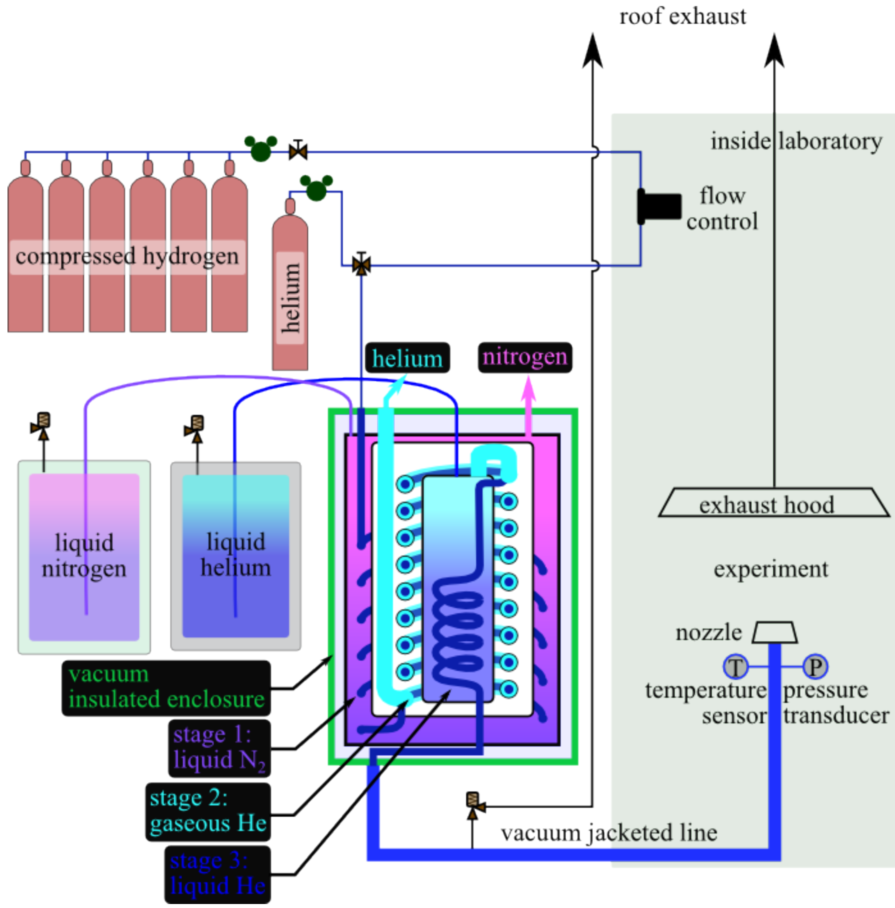


FIGURE 2. Sketch of the planned cryogenic hydrogen release experiment. Compressed hydrogen is cooled in a unique three-stage heat exchanger by liquid nitrogen, cold gaseous helium, and liquid helium.

liquid hydrogen storage). To address this issue, an experiment in the Turbulent Combustion Laboratory has been designed to characterize the dispersion characteristics of cryogenic hydrogen. The experiment will have well controlled releases (i.e., hydrogen temperature, pressure, ambient conditions) characterized by high fidelity diagnostics (e.g., planar laser Rayleigh scattering, Schlieren imaging). This data will be used to develop and validate models for cryogenic hydrogen releases, enabling revision of the safety, codes and standards for cryogenic hydrogen.

In continuation of previous efforts to achieve cryogenic release capabilities, the cryogenic hydrogen release experiment was designed, equipment was ordered, and assembly in the laboratory began in FY 2015. A sketch of the design is shown in Figure 2. A gaseous hydrogen flow will be controlled in the lab using a mass flow controller or pressure drop across a critical flow orifice. This metered gaseous hydrogen will then flow back outside the lab to be cooled in a unique three-stage heat exchanger, first with liquid nitrogen, then with cold gaseous helium, and finally, with liquid helium to near its saturation point. The cold hydrogen will then flow back into the laboratory through a vacuum jacketed line. The temperature and pressure of the hydrogen will be monitored near the release point, and interchangeable orifices, with a range of diameters (around 1 mm) will allow jets/plumes of hydrogen to be studied in the laboratory. Initial experiments will focus on the dispersion characteristics, with other experiments planned to study ignition (using a well-controlled laser-spark) and the impact of barrier walls and other risk mitigation strategies.

Experimentally Validate Equivalent Source Model for High Pressure Hydrogen

When a pressurized gas flowing through a restriction (orifice) is above a critical pressure ratio (1.9 for hydrogen), the flow chokes at the restriction point, and the mass flow rate through the orifice is only dependent on the upstream (high pressure) conditions. Downstream of the flow restriction, this dense gas must expand to the atmospheric conditions. In this expansion region, there are often shocks and complex flow structures that are challenging to model (a high mesh resolution and significant computational resources are required for computational fluid dynamics). For reduced-

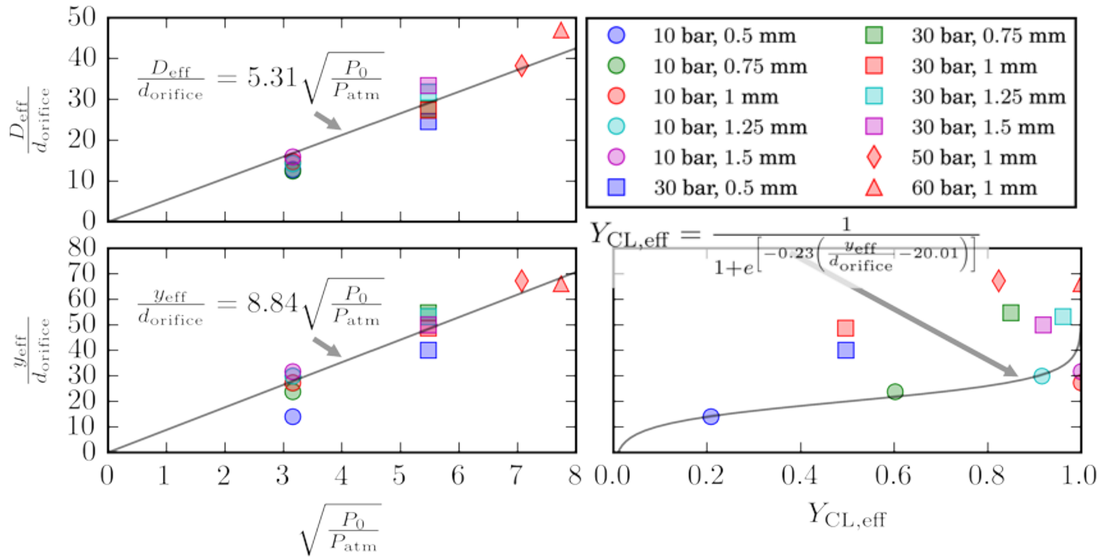


FIGURE 3. Effective leak diameter (upper left), starting point (lower left) and initial mole fraction hydrogen (lower right) for an under-expanded hydrogen jet. Fits to the data are also shown on the figure.

order models, where Gaussian shaped flow characteristics (e.g., mean velocity, mean concentration) are transported along a jet/plume streamline, a constant pressure is often assumed, and the conditions at the orifice cannot be used as inputs to the model. Therefore, in computation fluid dynamics and reduced-order models, an equivalent orifice is commonly used, giving the same downstream characteristics as the high pressure release, but the equivalent source (orifice) is at atmospheric pressure.

Several authors have developed equivalent source models for hydrogen, with varying assumptions and conservation equations. In FY 2015, we took data on hydrogen releases up to 60 bar in collaboration with a visiting researcher from Tsinghua University. This data will enable Sandia to eliminate the ambiguity in these equivalent source models and develop a de facto model. We came up with empirical correlations that scale as the square root of the stagnation pressure to the ambient pressure, to give boundary conditions to a reduced-order model for high pressure releases of hydrogen. The correlations are shown in Figure 3. The data have led to questions regarding several uncertain parameters in the reduced-order model (such as the relative velocity to concentration spreading ratio) and the default values we have been using for these parameters.

CONCLUSIONS AND FUTURE DIRECTIONS

The prototype HyRAM software toolkit provides a platform for modeling the safety of hydrogen systems, which enables industry-led analyses with state-of-the-art hydrogen models. HyRAM development activities are focused on adding capabilities necessary to inform near-term regulations, codes, and standards needs, including those from NFPA 2 and ISO TC197 WG24.

- (future) Extend HyRAM prototype (internal version) to include capability to develop and modify fault trees
- (future) Add visualization capability for the overpressure, plume, and layering behavior models
- (future) Define modules to assess risk-informed separation distances for liquid hydrogen (LH_2)
- (future) Scope initial interface for web-based version of HyRAM for highly accessible (web-based/app) tool for enabling end-users to implement these algorithms

Experiment was designed to develop predictive behavior models for liquefied hydrogen releases which are necessary to improve code requirements limiting the deployment of LH_2 systems.

- (future) Conduct liquid/cryogenic hydrogen release experiments and develop validated LH_2 release model
- (future) Continue experimental work to generate needed validation data and develop new necessary science-based models (e.g., wall interactions)

FY 2015 PUBLICATIONS/PRESENTATIONS

1. K.M. Groth, "Hydrogen behavior and Quantitative Risk Assessment." Presented at the 2015 DOE Hydrogen and Fuel Cells Program Annual Merit Review, June 9, 2015.

2. K.M. Groth. "H2 safety integration toolkit: HyRAM." Presented at the IEA HIA Task 37 Kick-off meeting, Karlsruhe, Germany, April, 2015.

3. E. Hecht, C. LaFleur, I. Ekoto "Cryogenic Hydrogen Release Modeling Validation – Update for Hydrogen Safety Panel." Presentation at Hydrogen Safety Panel Public Meeting, Sacramento, CA, March 2015.

4. K.M. Groth and C. LaFleur "HyRAM demo." Presentation to Kathleen Almand, director of Fire Protection Research Foundation (FPRF), February 2015.

5. K.M. Groth "Hydrogen Quantitative Risk Assessment R&D Needs." Presentation to US DRIVE Hydrogen Codes & Standards Tech Team, February 2015.

6. John T. Reynolds. *HyRAM Testing Strategy and Quality Design Elements*. SAND2014-20676. Sandia National Laboratories, November 2014.

7. Owen T. Parkins. *HyRAM Testing Script*. SAND2014-20522. Sandia National Laboratories, November 2014.

8. E.S. Hecht, I.W. Ekoto. "Vision for validating the liquid hydrogen plume model at temperatures less than 80K." Presentation at HySAFE research priorities workshop, Washington DC, 11 November 2014.

9. K.M. Groth. "HyRAM model integration platform." Presentation at HySAFE research priorities workshop, Washington, DC, 10 November 2014.

10. K.M. Groth. "QRA Tools - Gaps, Methods, Models Tools." Presentation at HySAFE research priorities workshop, Washington, DC, 10 November 2014.

11. E.S. Hecht. "State of the art for gaseous release models." Presentation at HySAFE research priorities workshop, Washington DC, 10 November 2014.

12. C. San Marchi. "Trends in Hydrogen Research in the United States" Presentation at the Korean Society of Mechanical Engineers, GwangJu, Korea, November 2014

13. Ekoto, I.W., Hecht, E., San Marchi, C., Groth, K.M., LaFleur, A.C., Natesan, N., Ciotti, M. & Harris, A. *Liquid Hydrogen Release and Behavior Modeling: State-of-the-Art Knowledge Gaps and Research Needs for Refueling Infrastructure Safety*. SAND2014-18776. Sandia National Laboratories, October, 2014.