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Hydrogen Quantitative Risk Assessment

Project ID: SCS011

DOE Project Award #: WBS 6.2.0.801 PI: Benjamin Schroeder

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DOE Hydrogen Program

2023 Annual Merit Review and Peer Evaluation Meeting

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Project Goals

Develop a rigorous scientific & engineering basis for assessing safety risk of H₂ systems and facilitate the use of that information for revising safety regulations, codes, and standards (RCS) for emerging hydrogen technologies.

- Address significant issues relevant to code requirements through the consistent, logical, and sciencebased use of QRA and other risk-informed approaches.
- Create and maintain reduced-order models and tools in an integrated framework (HyRAM+) to support a safer deployment of new hydrogen technologies.
- Generate new data and advanced risk-informed approaches needed to evaluate emerging H2@Scale applications.
- Demonstrate leadership in the international harmonization of standards for LH₂ and hydrogen infrastructure, including tunnels.

Overview

Timeline and Budget

- Project Start Date: 10/01/2003
- FY22 DOE Funding: \$500,000
- FY23 Planned DOE Funding: \$767,000

Barriers

- Risk informed codes and standards
- Safe deployment of new hydrogen technologies
- Harmonization of hydrogen standards

Partners

- Benjamin Schroeder (PI, Sandia National Laboratories)
- Industry & Research Collaborators:
 - Wabtec, Chart Industries, Hexagon, Hexagon Digital Wave, Air Products, PNNL, NREL, ANL, HySafe, Sims Industries, 40+ organizations using HyRAM+
- Codes and Standards Development:
 - NFPA 2/55, DOT Tunnel Jurisdictions
- International Engagement:
 - IPHE, IEC, ISO, IEA

Potential Impact

Goal: Develop a rigorous scientific & engineering basis for assessing safety risk of H₂ systems and facilitate the use of that information for revising safety RCS for emerging hydrogen technologies.

Goals of HFTO SCS Subprogram	Project Goal and Impact
Facilitating the creation, adoption, and harmonization of regulations, codes, and standards (RCS) for hydrogen and fuel cell technologies	Develop H₂-specific QRA tools, data , & methods which support RCS requirements.
Conducting research to generate the valid bases needed to define requirements in developing RCS	Build validated H2 behavior physics models that enable industry-led C&S revision and Quantitative Risk Assessment (QRA) methodologies.
Developing and enabling widespread dissemination of safety related information resources and lessons learned	Provide validated models in free, open source, and publicly available toolkit. Provide documentation of risk informed basis for code revisions.

Approach (Sandia H₂ SCS) *Coordinated Activities* to Enable Consistent, Rigorous, and Accepted Safety Analysis



Approach: FY22-23 Milestones

Impact Areas	Status				
Liquid Hydrogen QRA Methodology Development					
Implement LH2 pooling modeling	On track (Sept 2023)				
Enabling Fuel Cell Electric Vehicles in Tunnels					
 Develop generalized tunnel safety assessment framework Work with FHWA, other stakeholders to address all US tunnels 	On track (Sept 2023) Ongoing				
Improve SCS through Risk Assessments					
 Document NFPA 2 setback distance technical basis Distribute HyRAM+ as Python package (v4.1.1) 	Complete (Feb 2023) Complete (Sept 2022)				
Hydrogen/Natural Gas Blends QRA					
 Support blends in HyRAM+ (v5.0) Determine QRA defaults appropriate for blends 	Complete (Dec 2022) On track (Sept 2023)				
Uncertainty Quantification / Sensitivity for Hydrogen QRA					
Demonstrate sensitivity study on hydrogen QRA study	On track (Sept 2023)				
Establish sensitivity study capability within HyRAM+	On track (Sept 2023)				

Accomplishment: NFPA 2 Liquid Storage Setback Revisions

Technical justification supporting revisions to NFPA 2 liquid bulk storage setback distances **formally documented** in *SAND2023-12548*

NFPA 2 2023 has been published with updated bulk liquid storage setback distance requirements

Risk informed approach changed setbacks from being based on stored quantity to **pipe size** and **pressure**

Effort included technical review of HyRAM+ capabilities by **external parties**

- Industry representatives reviewed technical approach
- Verified physics and QRA models predictions and implementations against industry software

Documentation ensures supporting analyses are **repeatable** in the future

Technical justification for revisions to NFPA 2 liquid bulk storage setback distances published Sensitivity study results comparing equivalent fractional hole sizes over a range of pipe diameters



Technical justification report SAND2023-12548



Technical Justifications for Liquid Hydrogen Exposure Distances

Brian D. Ehrhart, Ethan S. Hecht, Benjamin B. Schroeder

Progress: Generalized Tunnel Safety Analysis

Developing **generalized** tunnel safety analysis framework

- Assessing hydrogen vehicles in terms of meeting current tunnel safety standards
- Individual tunnel analyses **not scalable** for tunnel general population
- Reduced-fidelity modeling enables exploration of time dependence and **multiple accident scenarios**

Engagement with Massachusetts Department of Transportation (MassDOT) continues to inform legislation on light-duty hydrogen vehicles in Boston's tunnels

- Fully coupled thermal-mechanical analysis of H₂ vehicle jet fire scenario allows determination of mechanical response
- Studying multiple tunnel ceiling geometries to support different tunnels in MassDOT's jurisdiction
 - Steel I-beams, box-beams, suspended ceiling panels

Visible flame length estimates from tank release calculations when varying tank parameters

Basecase: 70 MPa, 2.25 mm orifice, 125 L



Thermal heating profile on tunnel ceiling model with support beams



Expanding modeling results to consider additional tunnel types and characteristics to assess tunnels more generally

Process: Hydrogen Blends

Physics model support for hydrogen/natural gas blends included in HyRAM+ v5.0

QRA parameter defaults for blends under development

- Ignition probabilities
- Component leak frequencies
- Hazard models

Blends consequences will **need validation** data spanning composition range

SCS-035 CRADA with PRCI investigating leak frequencies for components in hydrogen/natural gas blends

HyRAM+ blends specification menu in graphical user interface

	Fu	el (overrides tal	ble)	Blend (manual)
Active	Fuel	Formula	Pe	rcent (vol-%)
\checkmark	Hydrogen	H2		20.000
\checkmark	Methane	CH4		80.000
	Propane	C3H8		0.000
	Nitrogen	N2		0.000
	Carbon Dioxide	CO2		0.000
	Ethane	C2H6		0.000
	n-Butane	N-C4H10		0.000
	Isobutane	ISOBUTANE		0.000
	n-Pentane	N-C5H12		0.000
	Isopentane	ISOPENTANE		0.000
	n-Hexane	N-C6H14		0.000
		To	otal	100.000
Allocate	e remainder:	Methane	~	Allocate



HyRAM+ QRA will soon support hydrogen/natural gas blends

Progress: QRA Sensitivity Analysis

Sampling of **uncertain QRA parameters** will allow determination of relative impact on risk predictions

- System specification
- Environment characterization
- Modeling parameters
- Analysis assumptions

Enable **uncertainty quantification** in risk predictions to quantify expected variability or prediction confidence

Sensitivity rankings help inform risk mitigation prioritization

Value of sensitivity studies previously shown in NFPA 2 bulk liquid storage **revisions**

Sensitivity study will be **demonstrated** for QRA H2 application

Tornado plot representation of sensitivity of risk-based distances calculated with HyRAM+, representing the distance away from the system at which a selected risk metric is met.





Achievement: HyRAM+ Standalone Python Package

HyRAM+ v4.1.1 release provided users direct access to Python backend Risk (PLL) [fatalties/year]

- Enabling parameter studies
- Easing individualizing result plotting
- Ability to modify risk calculations

Distributed as standalone Python package through popular code repositories

- Python Package Inde (וחיים)
- Conda-Forge

	hyram 5.0.0
	pip install hyram==5.0.0 🗗
nporting HyRAM upyter Noteboo	1+ for use in a QRA study within a k



Risk calculated for a range of distances from the system compared to a risk metric

> Flammable masses from tank release calculations when varying H₂ tank size



Progress: Liquid Hydrogen Pooling Modeling

Liquid pooling model being implemented in **HyRAM+** for future release

Current modeling **assumption** is liquid hydrogen leaks vaporize instantly

- May not be realistic for larger leaks
- Pooling model to capture pool size and rate of vaporization

Liquid hydrogen **pooling experiments** (SCS-010) occurring this year will be used for **validation** of the implemented model

Liquid pooling modeling capability will enable risk assessments of large scale liquid hydrogen storage



Development version of pooing model in HyRAM+





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Responses to Previous Year Reviewers' Comments

A greater emphasis on work to predict and calculate the impact of explosions based on releases with delayed ignition, as well as jet explosions from large releases, would be helpful in fully evaluating the safety and risk at a given site.

Unconfined overpressure models to estimate effects of delayed ignition of jets and plumes have been added to HyRAM+ physics and QRA capabilities.

More commentary on assumptions applied to achieve C&S values is needed, especially where risk analysis results are based upon the high likelihood for 1% release orifice size.

- A report detailing the technical basis for the NFPA 2 liquid storage setback distance revisions, including significant exploration and discussion of assumptions made when applying HyRAM+'s QRA methods to a C&S application, was recently published SAND2023-12548.
- Sensitivity study capabilities are being integrated into HyRAM+ to allow users to quickly assess the impact of assumptions.

It would be good to seek a third-party review to provide validation to the process. These calculations are complex and may not be fully understood by most who review them, so an independent report would provide additional confidence that this important work is consistent with industry-wide risk analysis.

• Both physics model and QRA method implementations were independently assessed during the recent NFPA 2 liquid storage setback distance task group work through comparisons to tools used by industry representatives.

It is unclear what experimental data will be used to support the [LH2 pooling] modeling.

• This highlights a clear need for detailed experimental data. This effort will be supported by in-house experiments at Sandia National Laboratories later this FY (see SCS010).

Collaboration and Coordination

Relationship	Category	Collaborator	Role	
CRADA Partner	Industry	Wabtec	Detailed relevant application for HyRAM+	
CRADA Partner	Industry	PRCI	Application motivating validation of HyRAM+ capabilities	
Committee Members	Codes and Standards Organizations	NFPA 2, 55	Task group support for separation distances, vent pipes, balloons	
Committee Members	Codes and Standards Organizations	ISO TC 197, IEA Task 43	Promoting harmonization of international standards	
Collaborator	National Lab	Pacific Northwest National Laboratory	Hydrogen tools portal, Hydrogen Safety Panel, Center for Hydrogen Safety, multiple CRADAs	
Collaborator	National Lab	National Renewable Energy Laboratory	Technical exchanges on QRA, safety codes and standards committees and task groups	
Collaborator	Industry	Air Products		
Collaborator	Industry	Chart Industries		

Remaining Challenges and Barriers

Science-Based Codes & Standards Improvements

- Acceptance criteria for hydrogen vehicles in tunnels is not well defined
- Need more complete data for liquid hydrogen system component failures and leaks
- Liquid hydrogen pooling difficult to model without complex and computationally expensive CFD; even then, little validation data
- Hydrogen QRA depends on ignition probabilities that do not account for project-specific parameters
- Few science-based requirements for hydrogen/natural gas blends

Hydrogen in Other Applications

- Bulk storage and transportation risk for H2@Scale applications need to be better assessed
- Non-transportation storage and use (e.g., energy storage buffers and pipelines) also have different safety considerations
- Larger potential release quantities need specific consideration for supporting infrastructure
- Geological storage safety presents new release environments for consideration

Proposed Future Work

Rest of FY23:

- Implement liquid pooling modeling capability in HyRAM+
- Perform sensitivity study for hydrogen QRA
- Apply generalized tunnel safety analysis framework to multiple crash scenarios
- Implement default QRA specifications for hydrogen/natural gas blends

Proposed Work for FY24:

- Incorporate uncertainty quantification methods into HyRAM+ to allow users to quantify risk uncertainties and sensitivities
- Document unconfined overpressure and liquid pooling model validation
- Baseline reduced-order model predictions for tunnel safety scenarios with high-fidelity comparisons
- Explore use of heat-flux effects versus temperature for quantification of risk from hydrogen flames

Any proposed future work is subject to change based on funding levels

Goal: Provide science & engineering basis for assessing safety (risk) of H₂ systems and facilitate use of that information in SCS and permitting

Relevance: Reducing barriers related to limited availability and access to safety data and assessments for SCS revision

Approach: Coordinated activities ensures accelerated transfer of R&D results into codes and standards and R&D focused on high-impact stakeholder problems

Accomplishments:

- Published report on technical basis for NFPA2 LH₂ storage siting revisions
- Released HyRAM+ 4.1.1 providing users with direct access to Python backend
- Released HyRAM+ 5.0 supporting hydrogen/natural gas blends

Progress:

- Supporting analyses for hydrogen vehicles in tunnels
- Developing generalized tunnel safety analysis framework
- Incorporating liquid pooling modeling and blends QRA in HyRAM+
- Demonstrating sensitivity analysis on hydrogen QRA