Development, Validation, and Benchmarking of Quantitative Risk Assessment Tools for Hydrogen Refueling Stations

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2020 DOE Hydrogen and Fuel Cells Annual Merit Review

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Overview

Timeline
- Project start date: Jan 2019
- Project end date: Dec 2020

Budget
- FY19 DOE Funding: $250k
- FY19 Air Liquide Funding: $250k
- FY19 Air Liquide In-Kind Contribution: $75k
- Total DOE Funds Received to Date: $250k
- FY20 Carryover/planned spending: $360k

Barriers
- A. Safety Data and Information: Limited Access and Availability
- F. Enabling National and International Markets Requires Consistent RCS
- G. Insufficient Technical Data to Revise Standards

Partners
- Air Liquide
- NFPA H2 Storage Task Group
- CGA G-5.5 Testing Task Force
Objective: Utilize SNL’s hydrogen behavior models and quantitative risk assessment (QRA) methodology to defensibly revise safety codes and standards.

<table>
<thead>
<tr>
<th>Barrier from 2015 SCS MYRDD</th>
<th>SNL Goal</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. Safety Data and Information: Limited Access and Availability</td>
<td>Build validated H₂ behavior physics models that enable industry-led C&amp;S revision and Quantitative Risk Assessment (QRA).</td>
</tr>
<tr>
<td>F. Enabling national and international markets requires consistent RCS</td>
<td>Develop H₂-specific QRA tools &amp; methods which support SCS decisions.</td>
</tr>
<tr>
<td>G. Insufficient Technical Data to Revise Standards</td>
<td>Provide tools and validated models to enable better informed codes and standards revisions.</td>
</tr>
</tbody>
</table>
Approach: Benchmark HyRAM software

1. Select station designs to analyze
2. Perform risk analysis of stations using HyRAM while AL performs analysis using their models
3. Analyze and characterize differences between HyRAM and AL internal risk tool (ALDEA) results
4. Document results
Approach: Make quantitative measurements from large LH$_2$ experiments that enable defensible codes/QRA

• Support CGA G-5.5 testing task force measurements of LH$_2$ vent stack flames
  – Hardware support (providing Sandia owned sensors to support the work)
  – Analysis support (Sandia expertise in data analysis and documentation)

• Experimentally measure unignited hydrogen dispersion from LH$_2$ vent stacks
  – Develop a diagnostic tool for capturing high-fidelity quantitative data for large scale unignited LH$_2$ experiments
    • non-intrusive (optical diagnostic)
    • Measure concentration in at least 2-dimensions with good temporal resolution
  – Measure vent stack dispersion for a range of flow rates and weather conditions
Approach: Scale-up our lab scale Raman imaging technique

- Use high-speed (low f-number) optics to collect as much light as possible with large field of view to measure entire plume
- High-powered light source required to excite as many molecules as possible
  - High-power laser scanning in space
  - Concentrations measured along a series of lines
- Effective background light suppression is key (both sunlight and illumination source that reflects off of condensed water vapor)
  - Time gating
  - Spectral gating
Accomplishment: Scenarios were identified for comparison of HyRAM to internal Air Liquide models

- **Free jets/flames:**
  - Low pressure (40 bar)
  - Medium pressure (100 bar)
  - High pressure (700 bar)

- **Vessels:**
  - Vessel blowdown
  - Vessel burst
  - Fragments formation
  - Pipeline blast

- **Vented explosion:**
  - Small scale
  - Medium scale

- **H₂ build up in a room:**
  - Closed unventilated
  - Naturally ventilated

- **Liquid hydrogen accident scenarios:**
  - Rupture before pump
  - Rupture after pump

Comparison of:

- Mass flow rate
- Distance to 4, 10% concentration
- Flame length
- Distance to 3, 5, 8 kW/m² heat flux
- Blowdown time as function of leak size
- HyRAM unable to calculate vessel burst, fragments or blast wave
- HyRAM unable to calculate vented explosions
- Concentrations over time
- Preliminary comparisons to ColdPLUME to assist in validation and development
Accomplishment: Good agreement between HyRAM and ALDEA for free jets and flames

Example results for free jet and flame models

<table>
<thead>
<tr>
<th></th>
<th>AL results</th>
<th>AL tool</th>
<th>HyRAM results</th>
<th>HyRAM module</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass release (g/sec)</td>
<td>607</td>
<td>ALDEA-HP</td>
<td>682</td>
<td>Eng. Toolkit</td>
</tr>
<tr>
<td>Axial distance at 4% (m)</td>
<td>35</td>
<td>ALDEA-HP</td>
<td>33</td>
<td>Gas Plume Disp.</td>
</tr>
<tr>
<td>Axial distance at 10% (m)</td>
<td>14</td>
<td>ALDEA-HP</td>
<td>12.5</td>
<td>Gas Plume Disp.</td>
</tr>
<tr>
<td>Flammable mass (4-75%) (kg)</td>
<td>1.2</td>
<td>ALDEA-HP</td>
<td>Not calculated in HyRAM GUI</td>
<td></td>
</tr>
<tr>
<td>Flammable mass (10-75%) (kg)</td>
<td>0.176</td>
<td>ALDEA-HP</td>
<td>Not calculated in HyRAM GUI</td>
<td></td>
</tr>
<tr>
<td>$R_{\text{max}}(4%)$</td>
<td>2</td>
<td>ALDEA-HP</td>
<td>2</td>
<td>Gas Plume Disp.</td>
</tr>
<tr>
<td>$R_{\text{max}}(10%)$</td>
<td>0.8</td>
<td>ALDEA-HP</td>
<td>1</td>
<td>Gas Plume Disp.</td>
</tr>
<tr>
<td>Distance (200 mbar) (m)</td>
<td>10</td>
<td>ALDEA-ME (5)</td>
<td>Unconfined overpressures not calculated in HyRAM</td>
<td></td>
</tr>
<tr>
<td>Distance (140 mbar) (m)</td>
<td>12</td>
<td>ALDEA-ME (5)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Distance (50 mbar) (m)</td>
<td>22</td>
<td>ALDEA-ME (5)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$L(\text{flame})$ (m)</td>
<td>15</td>
<td>ALDEA-Rad</td>
<td>15</td>
<td>Jet Flame</td>
</tr>
<tr>
<td>Distance (3 kW/m²)</td>
<td>10</td>
<td>ALDEA-Rad</td>
<td>10.6</td>
<td>Jet Flame</td>
</tr>
<tr>
<td>Distance (5 kW/m²)</td>
<td>8</td>
<td>ALDEA-Rad</td>
<td>7.2</td>
<td>Jet Flame</td>
</tr>
<tr>
<td>Distance (8 kW/m²)</td>
<td>6</td>
<td>ALDEA-Rad</td>
<td>4.9</td>
<td>12 mm / 100 bar</td>
</tr>
</tbody>
</table>
Progress: Final report has been drafted; final analysis of differences and best approach underway

- Report references literature description and validation of models
- Preliminary results:
  - Consequences from free jets and flames are similarly predicted HyRAM and ALDEA
  - HyRAM predicts longer blowdown time than ALDEA – reasons for differences being investigated
  - ALDEA models for vessel burst, fragments, blast from vented explosions may be able to be incorporated into HyRAM – assessing feasibility
  - ALDEA predicts higher concentrations at a given time in the case of leaks within enclosures – reasons for differences being investigated
  - Differences in cryogenic hydrogen models are being evaluated

Example results for vessel blowdown models

<table>
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<tr>
<th>H2 140 L, 700 bar</th>
<th>AL results</th>
<th>AL tool</th>
<th>HyRAM results</th>
<th>HyRAM module</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mm / time (s)</td>
<td>848</td>
<td>ALDEA-Blowdown</td>
<td>1073</td>
<td>Eng. Toolkit</td>
</tr>
<tr>
<td>2.4 mm / time (s)</td>
<td>147</td>
<td>ALDEA-Blowdown</td>
<td>186</td>
<td>Eng. Toolkit</td>
</tr>
<tr>
<td>4 mm / time (s)</td>
<td>53</td>
<td>ALDEA-Blowdown</td>
<td>67</td>
<td>Eng. Toolkit</td>
</tr>
</tbody>
</table>
Progress: A mobile laser scanning system has been developed, built and deployed (but not yet used)

Current status:
- All equipment onsite
- LH$_2$ tank filled
- Equipment (LH$_2$ pump, laser and diagnostic equipment at site) tested and operational
- Awaiting final safety signoff

Technology:
- Line-imaging of Raman scatter
- Laser to be rastered throughout plume to generate 3D picture of dispersion
Progress: A series of tests are planned, representative of a range of operations

Notes: maximum pump flow rate: 120 kg/hr = 2 kg/min = 33 g/s, normal boil-off is 4-8 kg/day

<table>
<thead>
<tr>
<th>description</th>
<th>flow rate (g/s)</th>
<th>duration (mins)</th>
<th>total H2 (kg)</th>
<th>Wind</th>
<th>Humidity</th>
<th>Purpose</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>high-flow warm plume dispersion</td>
<td>16.67</td>
<td>30</td>
<td>30</td>
<td>low (&lt; 5 MPH)</td>
<td>any</td>
<td>validate diagnostic (high flow-rate/concentration, no condensation)</td>
<td>Warm H2 to as high a T as possible, repeat until diagnostic deemed ready</td>
</tr>
<tr>
<td>high flow cold dispersion</td>
<td>16.67</td>
<td>30</td>
<td>30</td>
<td>low (&lt; 5 MPH)</td>
<td>low</td>
<td>simulate vent release during transfer</td>
<td>Possibly repeat with high and low ambient temperatures</td>
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<tr>
<td>simulated high-boiloff</td>
<td>0.56</td>
<td>30</td>
<td>1</td>
<td>low (&lt; 5 MPH)</td>
<td>low</td>
<td>simulate high level of boiloff</td>
<td>possibly repeat with high and low ambient temperatures</td>
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<td>high</td>
<td>simulate high level of boiloff</td>
<td>possibly repeat with high and low ambient temperatures</td>
</tr>
<tr>
<td>normal boiloff</td>
<td>0.07</td>
<td>30</td>
<td>0.125</td>
<td>low (&lt; 5 MPH)</td>
<td>any</td>
<td>normal boiloff measured by meter</td>
<td>May need to scrap if diagnostic not sensitive enough</td>
</tr>
<tr>
<td>normal boiloff</td>
<td>0.07</td>
<td>30</td>
<td>0.125</td>
<td>high (&gt; 5 MPH)</td>
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4 weather conditions: high and low wind, high and low humidity. Each day when the weather is right, can perform 4 experiments: high-flow cold dispersion, simulated high boil-off, and normal boil-off. This means there are 4 actual days of testing (8 if we do high and low ambient temperatures). If everything goes right, we need approximately 160 kg/H2.
Progress: We will be able to answer key questions at the end of the campaign

- Does wind cause channeling and increase the distance to the LFL, or improve mixing to decrease the distance to the LFL?
- Does high humidity cause increased buoyancy due to the energy transfer from the condensation of moisture, or does the condensed moisture drag the hydrogen down so it’s less buoyant?
- Is the hydrogen concurrent with the condensed moisture? Does concurrency depend on the humidity?
- Is our model accurate enough for risk calculations for larger releases?
Response to previous year reviewer’s comments

• This project was not reviewed last year
Collaboration & coordination

For the benchmarking HyRAM task:

- **AL:** Select up to 10 scenarios, use internal risk tool to analyze scenarios, compare with HyRAM results, review final report.
- **SNL:** Analyze up to 10 scenarios with HyRAM and compare results, develop final report.

For the experimental tasks:

- **AL:** Support experimental design by providing industry experience, conduct periodic advisory panel meetings, review final report.
- **CGA G-5.5 testing task force:** Coordinate LH2 vent stack flame experiments with industrial and national laboratory partners.
- **SNL:** Develop optical diagnostic to measure dispersion of cold gaseous hydrogen from a LH2 release plume in at least 2-dimensions, design validation testing, develop final report.
Remaining challenges & barriers

Task 1 - Benchmarking HyRAM:

- Cryogenic hydrogen models are not validated well enough to warrant presenting results publically

Task 2 - Experimental work:

- Final safety approval for experiments at LLNL are imminent
- CGA G-5.5 led ignited releases have been indefinitely delayed due to pandemic
- Challenge to translate experimental results into proposal(s) for NFPA 2
Proposed future work

- Finalize and publish report on HyRAM - ALDEA comparison
- Update HyRAM with lessons-learned from comparisons
- Perform planned vent-stack dispersion experiments at LLNL liquid hydrogen pad
- Provide measurement and analysis support of CGA G-5.5 testing task force data collection on H2 vent stack flame experiments
- Refine characterization of LH2 releases with validated cold plume release and provide sound, scientifically based revised bulk LH2 separation distances in NFPA 2/55

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

- Technology transfer strategies are tied to the accessibility of HyRAM QRA tool kit to other users (AHJs, station designers, etc.) to analyze station risks or consequences-only

- Free HyRAM download at http://hyram.sandia.gov

Current release is version 2.0
Summary

Relevance: Build validated H$_2$ behavior physics models and QRA tools that enable industry-led C&S revision

Approach:
- Benchmark HyRAM against Air Liquide models (ALDEA) and update models where issues are seen
- Measure unignited dispersion at LLNL LH$_2$ research facility using custom diagnostic and support CGA G-5.5 testing task force experiments measuring LH$_2$ vent stack flames and, using results to validate models
- Generate proposal(s) for science based LH$_2$ setback distances in NFPA 2/55

Progress & Accomplishments:
- Common scenarios were identified and simulated with ALDEA and HyRAM
- Good agreement was seen for free jets and flames
- Differences in blowdown and other models being investigated
- Report drafted
- Diagnostic designed, constructed and deployed
- Test plan in place for unignited dispersion measurements

Future work:
- Finalize and publish report on modeling comparison
- Perform experiments and report on results
- Provide proposal(s) to NFPA 2/55 for liquid hydrogen separation distances
Technical Back-Up Slides
HyRAM: Making hydrogen safety science accessible through integrated tools

First-of-its-kind integration platform for state-of-the-art hydrogen safety models & data - built to put the R&D into the hands of industry safety experts

Core functionality:
• Quantitative risk assessment (QRA) methodology
• Frequency & probability data for hydrogen component failures
• Fast-running models of hydrogen gas and flame behaviors

Key features:
• GUI & Mathematics Middleware
• Documented approach, models, algorithms
• Flexible and expandable framework; supported by active R&D

Current release is version 1.1.0.1047

Free download at http://hyram.sandia.gov