R&D for Safety, Codes and Standards: Hydrogen Behavior

Project ID: SCS010

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Overview

Timeline
• Project start date: Oct. 2003
• Project end date: Sept. 2017*
  * Project continuation and direction determined by DOE annually

Budget
• FY16 DOE Funding: $510 k
• Planned FY17 DOE Funding: $500 k
• Partner funding:
  • $175k committed stakeholder funds (CaFCP Auto OEM Group, Linde, Shell)

Barriers
A. Safety Data and Information: Limited Access and Availability
G. Insufficient technical data to revise standards

Partners
• Stakeholder CRADA
  • Bki (contractor for California Fuel Cell Partnership)
  • Fire Protection Research Foundation (research affiliate of NFPA)
• Industry & Research
  • NFPA 2 code committee
  • HySAFE
Relevance

Objectives:

• Perform R&D to provide the science & engineering basis for the release, ignition, and combustion behavior of hydrogen across its range of use (including high pressure and cryogenic)

• Develop models and tools to facilitate the assessment of the safety (risk) of H₂ systems and enable use of that information for revising RCS and permitting stations

<table>
<thead>
<tr>
<th>Barrier from 2015 SCS MYRDD</th>
<th>Goal</th>
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<tbody>
<tr>
<td>A. Safety Data and Information:</td>
<td>Build validated H₂ behavior physics models that enable industry-led C&amp;S revision and Quantitative Risk Assessment</td>
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<td>Limited Access and Availability</td>
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<td>G. Insufficient technical data to revise standards</td>
<td>Perform experiments to address targeted gaps in the understanding of H₂ behavior physics</td>
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Relevance: Current separation distances for liquid hydrogen are based on consensus, not science

- Previous work by this group led to science-based, reduced, gaseous $H_2$ separation distances.
- Higher energy density of liquid hydrogen over compressed $H_2$ makes it more economically favorable for larger fueling stations.
- Even with credits for insulation and fire-rated barrier wall 75 ft. offset to building intakes and parking make footprint large.
Approach (Sandia H₂ SCS): Coordinated activities that facilitate deployment of hydrogen technologies

- **Hydrogen Behavior (this project, SCS010)**
  - Develop and validate scientific models to accurately predict hazards and harm from liquid releases, flames, etc.

- **Quantitative Risk Assessment, tools R&D (SCS011)**
  - Develop integrated methods and algorithms enabling consistent, traceable, and rigorous QRA (Quantitative Risk Assessment) for H₂ facilities and vehicles

- **Enable Hydrogen Infrastructure through Science-based Codes and Standards (SCS025)**
  - Apply QRA and behavior models to real problems in hydrogen infrastructure and emerging technology
Approach: Develop and execute experiments to enable predictive modeling across H₂’s range of use

Issue: Cryogenic H₂ releases have been outdoors and/or instrumented with low fidelity sensors, with experimental uncertainty too high for model validation

• SNL Approach (FY17 goals):
  – Perform lab-scale cryogenic hydrogen dispersion validation experiments with precise control of boundary conditions and high-fidelity imaging diagnostics (described in next slides)
  – Design large indoor experiments to enable the modeling of pooling and vaporization of liquid hydrogen (described in remaining challenges)

Issue: Low fidelity sensors and very specific vent geometries in previous accumulation experiments

• SNL Approach (FY17 goal): Design an experimental platform with flexible vent/source geometry and high-fidelity, accurate concentration measurements (task to begin in Q4)
Approach (FY17 Hydrogen Behavior): Validate model for cryogenic hydrogen dispersion

• Previously developed model requires validation data
  – Several model parameters based on empirical data
  – Data only from warm hydrogen or other warm gases
  – Are more physics required?

• Use experimental platform commissioned in FY16 to generate cryogenic hydrogen releases

➢ Milestone (FY17Q2): Measure dispersion field of < 40 K hydrogen (milestone complete) and incorporate validated model into HyRAM (FY18 milestone)
Accomplishment: Developed and implemented Raman imaging technique to measure cryogenic plumes

- Conventional Rayleigh signal overwhelmed by Mie scattering off of condensed water vapor in jet
- Filtered Rayleigh had insufficient Mie scattering light suppression (OD≈3)
- Raman scattering enables higher optical density filters
  - 10 nm FWHM bandpass filters at wavelengths of interest
  - OD of 12 @ all wavelengths
  - OD of 18 @ 532 nm

➢ Enables simultaneous measurement of concentration and temperature in 2D
Accomplishment: Measured concentration and temperature fields of cryogenic hydrogen releases

<table>
<thead>
<tr>
<th>$T_{\text{noz}}$ [K]</th>
<th>$P_{\text{noz}}$ [bar$_{\text{abs}}$]</th>
<th>$d$ [mm]</th>
<th>$T_{\text{throat}}$ [K]</th>
<th>$n_{\text{hts}}$</th>
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<tbody>
<tr>
<td>58</td>
<td>2</td>
<td>1</td>
<td>43.5</td>
<td>4</td>
</tr>
<tr>
<td>56</td>
<td>3</td>
<td>1</td>
<td>41.9</td>
<td>4</td>
</tr>
<tr>
<td>53</td>
<td>4</td>
<td>1</td>
<td>39.6</td>
<td>4</td>
</tr>
<tr>
<td>50</td>
<td>5</td>
<td>1</td>
<td>37.4</td>
<td>5</td>
</tr>
<tr>
<td>61</td>
<td>2</td>
<td>1.25</td>
<td>45.7</td>
<td>6</td>
</tr>
<tr>
<td>51</td>
<td>2.5</td>
<td>1.25</td>
<td>38.2</td>
<td>2</td>
</tr>
<tr>
<td>51</td>
<td>3</td>
<td>1.25</td>
<td>38.2</td>
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<tr>
<td>55</td>
<td>3.5</td>
<td>1.25</td>
<td>41.2</td>
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</tr>
<tr>
<td>54</td>
<td>4</td>
<td>1.25</td>
<td>40.4</td>
<td>2</td>
</tr>
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- Two-dimensional images are superior to centerline only measurements for model validation
Accomplishment: Measured temperatures as low as 85 K, 38 mm from the release point

- $d_{\text{noz}} = 1 \text{ mm}$
  - 2 bar, 58 K
  - 3 bar, 56 K
  - 4 bar, 53 K
  - 5 bar, 50 K

- $d_{\text{noz}} = 1.25 \text{ mm}$
  - 2 bar, 61 K
  - 2.5 bar, 51 K
  - 3.5 bar, 55 K
  - 4 bar, 54 K
  - 3 bar, 51 K

➢ Control of pressure, and measurement of temperature at nozzle enables data to be used for model validation
Accomplishment: When normalized properly, centerline and half-width decay rates scale linearly.

• Literature inverse mass-fraction decay rate: 0.21–0.271
• Literature mass-fraction half-width spreading rate: 0.1–0.11 mm

First ever measurements of temperature needed for model energy balance.
Accomplishment: Radial profiles are self-similar, but wider than literature data of warm releases.

Different profiles imply different modeling parameters from warm releases.

\[ \eta = \frac{r}{z} \]
Accomplishment: Radial profiles of temperature are also self-similar, and wider than mass fraction.

Data can be used to validate relative spreading ratio in model.
Progress: Initial comparisons to model show slower centerline mole-fraction decay rate than predictions

- Expansion model and/or entrainment rate may need to be adjusted.
Progress: Initial comparisons to model show good agreement in terms of temperature

Improved data analysis may yield reduced noise
Response to last year’s Reviewer’s comments

- The project needs more emphasis on adding liquid hydrogen capability. It would be helpful if the project could address releases in a container that did not trap hydrogen under a roof, thereby limiting the concentration.
  - We recognize the ability to predictively model liquid hydrogen releases as being a critical barrier to code revisions; this work focuses directly on model validation. We are close to having a valid model for some aspects of liquid hydrogen stations. We are also planning some enclosure experiments to improve our simulations of scenarios with walls.

- The proposed work to evaluate cold/liquid releases does not appear adequate to meet the needs of the project if the intent is to address large-scale releases.
  - The large-scale releases being planned (described in the following slides) will address the shortcomings of the lab-scale experiments, enabling modeling of larger releases.

- The project should add benchmarking against other fuels.
  - We are planning on running similar (cryogenic release) experiments with methane (as a surrogate for natural gas), with funding from the vehicle technologies office.

Note: While this work was presented during the 2016 AMR, it was not independently reviewed. Since there are such close ties to SCS-011: Hydrogen behavior and Quantitative Risk Assessment, some relevant comments were taken from there.
Collaborations have enabled this research and expanded impact

**H₂ behavior (SCS010) collaborations**

- **CRADA with BKi** to fund experiments
  - Commitments from Shell, Linde, CaFCP Auto OEM group
  - Inquires out to other industry organizations and local government agencies

- **NFPA 2 Technical Code Committee**
  - Regular attendance with expert advisory role

- **HySafe**
  - Panelist for HySAFE Research Priority workshop on Hydrogen Safety

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<tr>
<th>Expanded impact through HyRAM (SCS011) and C&amp;S participation (SCS025)</th>
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<td><strong>HyRAM users</strong> – including ITM Power, Paul Scherrer Inst., ZCES, AVT, ...</td>
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<td><strong>Gexcon</strong> - Technical exchanges on validation activities for physics models, integration of safety methodology approaches; In-kind support - provided FLACS research license</td>
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<td><strong>PNNL</strong> - Technical exchanges on PBD; QRA; Hydrogen Safety Panel</td>
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<td><strong>NREL</strong> - Technical exchanges on PBD; QRA</td>
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<td><strong>HySafe</strong> - Technical exchanges on safety methodology; QRA toolkits</td>
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<td><strong>ISO TC197 WG24</strong> - SNL co-leads sub-team on safety methodology</td>
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<tr>
<td><strong>IEA HIA Task 37</strong> - SNL leads sub-task on Safety Integration Toolkits</td>
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<td><strong>H2USA</strong> - Various working groups</td>
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Remaining challenges: Phenomena from large-scale releases are not well understood

Need experiments to characterize:

- Pooling
- Evaporation from LH₂ pools

Planning underway for experiments at Sandia (Albuquerque) facilities:

- Thermal test complex
  - Flame cell
    - Up to 3m diameter pool
    - 18.3 m dia. x 12.2 m high
    - Well characterized conditions for model validation
  - Crosswind test facility
    - Dispersion in controlled crosswind
    - Single-direction flow
    - Well-characterized ambient conditions
- Severe Accident Phenomena/Analysis (Surtsey)
  - 100 m³ pressure vessel with 6 levels of instrumentation ports
Proposed future work

• Remainder of FY17
  – Complete Raman imaging characterization of cryogenic hydrogen releases
  – Conclude development/validation of the ColdPLUME model for predictive dispersion modeling
  – Develop R&D plans for large-scale experiments
  – Develop research plans and design enclosure/accumulation experiments

• FY18
  – Integrate validated ColdPLUME model into publicly released HyRAM
  – Conduct large-scale release experiments to characterize hydrogen pooling, evaporation, and interaction with atmosphere
  – Complete enclosure/accumulation experiments and develop predictive models of risk for unintended releases of hydrogen in containers

• Out years
  – Simulate scenarios driving separation distances in NFPA 2 and enable the science-based revision of the liquid hydrogen separation distances in the 2022 version of NFPA 2

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

- **Relevance:** Address lack of safety data, technical information relevant to development of Codes & Standards.

- **Approach:** Develop and validate scientific models to accurately predict hazards and harm from liquid releases, flames, etc. Generate validation data where it is lacking.

- **Technical Accomplishments:**
  - Raman imaging used to characterize concentration and temperature profiles of cryogenic hydrogen releases
  - Preliminary analysis suggests that mixing of cryogenic hydrogen jets is different from warm hydrogen jets, requiring new empirical model parameters
  - Experiments on-going
    - Push to even lower temperatures

- **Future work:**
  - Modify ColdPLUME model as validation data dictates
  - Implement ColdPLUME into HyRAM
  - Perform large-scale experiments and develop models for pooling and evaporation
  - Use models to advise NFPA 2 code committee on hazards and harm for high priority scenarios (to inform 2022 edition of NFPA 2)
TECHNICAL BACKUP SLIDES
A conceptual model needs to further validation

- Conservation of mass, momentum, species, energy
- 5-zones:
  - Zone 0: accelerating flow
  - Zone 1: underexpanded jet
  - Zone 2: initial entrainment and heating
  - Zone 3: flow establishment
  - Zone 4: self-similar, established flow
- 1-dimensional along streamline, can curve due to buoyancy
(Air) icing at the nozzle likely improves mixing for temperatures < 50K
Ignition distance and radiant fraction were mapped out last FY.
Two high priority scenarios identified by the NFPA 2 code committee are initially targeted for modeling

✔ Flow from vent of ultra-cold hydrogen (e.g. trailer venting excess pressure after normal LH₂ delivery or burst disk rupture)
  – Are vent stacks appropriately designed?
  – Separation distance from air intakes and overhead utilities
  – Vertical discharge, 3” diameter pipe, 20-140 psig

❑ Release from pipe containing liquid H₂ (e.g. leading from tank to vaporizer or vaporizer itself - caused by thermal cycles or ice falling from vaporizers)
  – Requires ability to model flashing, pooling and evaporation from pools
  – Need to model concentration plume and heat flux from a subsequent fire
  – Horizontal discharge, ¾”-2” diameter pipe, 20-140 psig
We are running an experiment, releasing ultra-cold hydrogen in the laboratory

Accurate control/measurement of boundary conditions