Hydrogen Safety, Risk Assessment, and Material Compatibility R&D

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Defensible safety standards for the built environment

Goal
Facilitate the safe use of hydrogen technologies by understanding and mitigating risk

Demonstrated Impact

- Enabling the deployment of refueling stations by developing science-based, risk-informed decision making processes for specification of safety distances.
- Sandia's analysis has enabled the indoor use of fuel cell powered vehicles.
Risk framework incorporates science basis for safety

**Hydrogen Behavior Models**

**Validated mathematical models** to accurately predict hazards and harm from liquid releases, flames, etc.

**Quantitative Risk Assessment**

**Develop integrated methods and algorithms** enabling consistent, traceable, and rigorous QRA (Quantitative Risk Assessment) for hydrogen facilities and vehicles.

**Decision Support for Standards Development**

**Provide physics models and risk calculations** to address real problems in hydrogen infrastructure and emerging technology.
Current separation distances for bulk liquefied hydrogen are based on consensus, not science

- Previous work by this group led to science-based, reduced, gaseous $\text{H}_2$ separation distances
- Higher energy density of liquid hydrogen over compressed $\text{H}_2$ makes it more economically favorable for larger fueling stations
- Even with credits for fire-rated barrier wall, 75 ft. offset to building intakes and parking make footprint large
Phenomena from large-scale liquid 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 m$^3$ pressure vessel with 6 levels of instrumentation ports
Leadership in materials and components for hydrogen service

Goals

• Develop and characterize high-performance, hydrogen containment materials and structures to lower capital cost of hydrogen infrastructure, systems and components

• Understand fundamentals of hydrogen interactions with metals and polymers to enable materials selection and mitigation strategies for hydrogen-enhanced degradation

Demonstrated Impact

• Enabled worldwide deployment of hydrogen and fuel cell systems by developing test methodologies for science-based standards
In order to develop a more complete mesoscale model of the interfacial behaviour, an analytical model of boundary energy and hydrogen segregation which relies on modelling is limited by how the enthalpy of segregation is a function of inclination. However, the explanatory power of the structural unit model applied to segregation compared to the calculated variation of excess hydrogen concentration with inclination was examined. Existing literature was reviewed to explain the differences in structure and potential energy histogram of the low inclination boundary in Figure 10.

This work examined the case of a separated junctions to hydrogen in bulk octahedral sites (see the discussion of adsorption to the coherent twin in Section 3.3). Now it is conclusively demonstrated that the separated junctions provide the isolated junctions. Hydrogen concentrations due to breakup of LTB facets and the resulting generation of lower energy sites (near $-6 \text{ eV}$) that are more populated in grain boundaries with higher hydrogen concentrations.

Conclusions

To separate the LTB facets that form in the absence of hydrogen (a) into $-0.6 \text{ eV}$, which corresponds to segregation to the junctions while the peak centred on $-2 \text{ eV}$ corresponds to segregation to the individual junctions, resulting in (c) a more planar structure. Inspecting the segregation histogram of the low inclination boundary in Figure 10, the hydrogen potential energy histogram is evidently related to the tendency of the structure, $\langle 110 \rangle_{\sigma_1}$, $\langle 111 \rangle_{\phi_1}$.

The effect of hydrogen on the structure of a 48-atom unit was discussed in relation to closely related MD models of inclined grain boundaries coupled to a GCMC model and applied to determine the degree of hydrogen segregation. In order to facilitate the application of the excess enthalpies of facets, the deviation of the calculated enthalpy predicted from a simplified model using superposition was examined.

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$\phi_1 \leq 90^\circ$
Evaluation of *Materials Compatibility* enables hydrogen technology innovation

**ASME article KD-10**
Input on test methodology

**Platform for material testing**
Testing in GH$_2$ at high pressure

**Critical assessment of**
Statically loaded cracks

**CSA CHMC1**
Test methods and material qualification

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**2005**  **2007**  **2009**  **2011**  **2013**  **2015**  **2017**

**First qualification data**
For high-pressure ASME vessels

**Technical Reference established**

**Full-scale tank testing**
CSA HPIT1 SAE J2579

**Platform for high-pressure GH$_2$**
Over temperature range (-40°C to +85°C)

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**Design space**

**Evaluation of Materials Compatibility** enables hydrogen technology innovation
Safety, Codes and Standards needs for H2@Scale

- Protocols for distributed production and power systems integration
- Oxygen management in distributed systems
- Metrology at scale (metering for geologic storage and pipelines)
- Purity requirements and purification
- Gas segregation in mixed gas systems
- Leakage in geologic storage and pipeline systems
- Materials compatibility in existing infrastructure (PVC, cast iron, etc.)
- Combustion requirements (e.g., burners)
- Safety requirements for underground storage at point of use
- Maritime standards for international shipping and transport over waterways
- Safety standards for conveyance of LH₂
BACKUP SLIDES
Evolution of quantitative risk assessment in standards

Established risk-informed processes for separation distances

QRA applied to indoor refueling to inform code revision

ISO TC197 WG24 incorporating QRA and behavior modeling


QRA-informed separation distances in NFPA 2

20% station penetration potential due to QRA

Risk assessment proposed for hydrogen systems at ICHS

Public release of HyRAM
Developing risk models for liquid hydrogen storage

Temperature of LH$_2$ = 20K (-253°C)

Laboratory experiments and validated models of cryogenic hydrogen releases inform safety requirements for LH$_2$ storage
International testing collaboration to develop common material qualification protocols

- Developing shared experience on capability deployment in Europe, Asia and North America for fatigue testing in high-pressure hydrogen (>700 bar) and low temperature (≤233K)
- Goals: (1) international consensus within SAE Fuel Cell Safety Task Force on materials test methods and performance metrics for FCEV fuel systems; and (2) proposal for Phase II of UN GTR no. 13a