SCS011: Hydrogen behavior and Quantitative Risk Assessment

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Sandia National Laboratories

DOE Hydrogen and Fuel Cells Program Annual Merit Review

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SCS011

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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Overview

Timeline

- Project start date: Oct. 2003
- Project end date: Sept. 2014*

* Project continuation and direction determined by DOE annually.

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
L. Usage and Access Restrictions – parking structures, tunnels and other usage areas

Budget

- FY13 DOE Funding: $0.7M
- Planned FY14 DOE Funding: $0.9 M
- Total DOE Project Value: $20.9M

(Funding numbers include SCS#010 and SCS#011: Behavior and Risk program elements)

Partners

Industry & research collaborators:
Air Products and Chemicals Inc., HySafe, Linde, Tsinghua University,

SDO/CDO participation:
CGA, ISO TC197, NFPA2, CSA HGV4.9

International engagement:
HySafe, HyIndoor, IEA HIA Task 31

Relevance and Objectives

Provide a **science & engineerin**g basis for assessing safety (risk) of H2 systems and **facilitate use of that information** for revising RCS and permitting stations

Barrier from 2013 SCS MYRDD	**Project Goal**
A. Safety Data and Information: Limited Access and Availability	Develop & validate H2 behavior physics models to address targeted gaps in knowledge
F. Enabling national and international markets requires consistent RCS G. Insufficient technical data to revise standards	Build tools to enable industry-led C&S revision and safety analyses to be based on a strong science & engineering basis.
L. Usage and Access Restrictions – parking structures, tunnels and other usage areas	Develop H2-specific QRA [Quantitative Risk Assessment] tools & methods to support RCS decisions and to enable Performance Based Design (PBD) code-compliance option.

Program Approach

The Safety, Codes and Standards program coordinates critical stakeholders and research to remove technology deployment barriers

Partnerships with industry, labs, academia

Identify R&D needs → *Perform High-Priority R&D* → *Impact Codes and Standards*

Harmonize Internationally

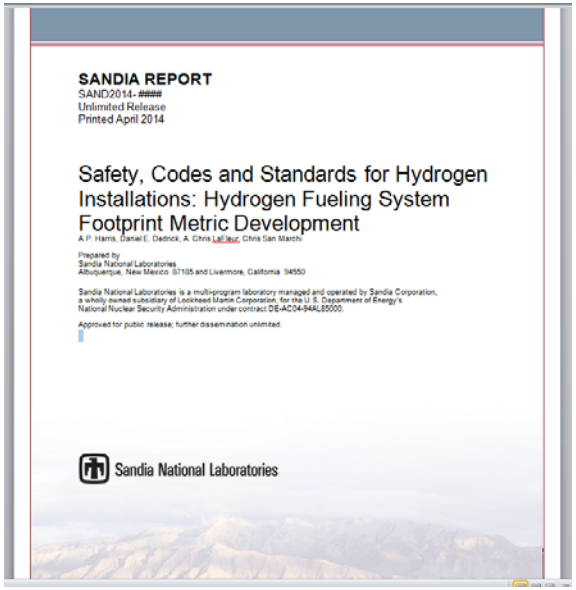
Regulations, Codes and Standards [RCS]

International Standards (ISO)

International Agreements (IEA, IPHE)

Program Accomplishment: Metric Benchmark Development

- Objective: Develop a meaningful metric for the Safety Codes & Standards Program that is able to:
  - show evidence of supporting market growth
  - guide future R&D investments
- A new metric has been defined as the **"Number of sites which can readily accept hydrogen"**
- Benchmark results showed initial SNL contributions to NFPA2 code work resulted in an increase from 0% to 18% of H2 targeted sites in CA can now accept hydrogen
- Metric details and benchmark results published as a SAND Report



SANDIA REPORT
SAND2014-####
Unlimited Release
Printed April 2014

Safety, Codes and Standards for Hydrogen Installations: Hydrogen Fueling System Footprint Metric Development

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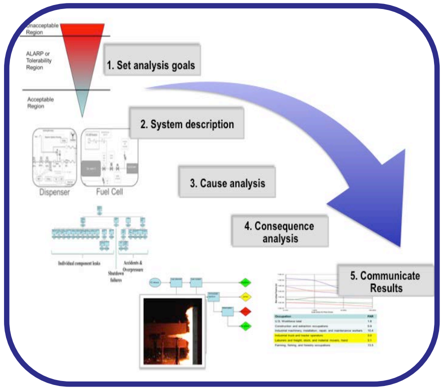
This metric addresses the primary barrier to the commercial success of fuel cell electric vehicles: fuel availability

Project Approach: Three coordinated activities

Apply R&D in RCS

Apply risk assessment techniques in step-out hydrogen technologies

QRA methods, tools R&D



Develop integrated algorithms for conducting QRA (Quantitative Risk Assessment) for H_2 facilities and vehicles

H2 behavior R&D

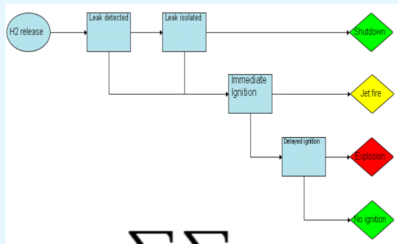
Develop and validate scientific models to provide reduced-order information for accurate depiction of releases, flames, etc.

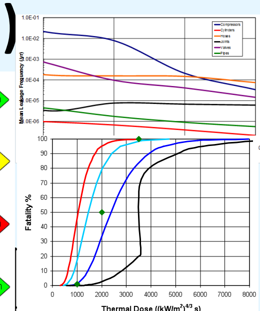
Enabling methods, data, tools for H2 safety & RCS community

Previous SNL accomplishments: Develop, validate & integrate models

QRA method, data & models (FY08-11)

- Hazards
- Accident sequences
- Release frequencies
- Ignition probabilities
- Harm/damage



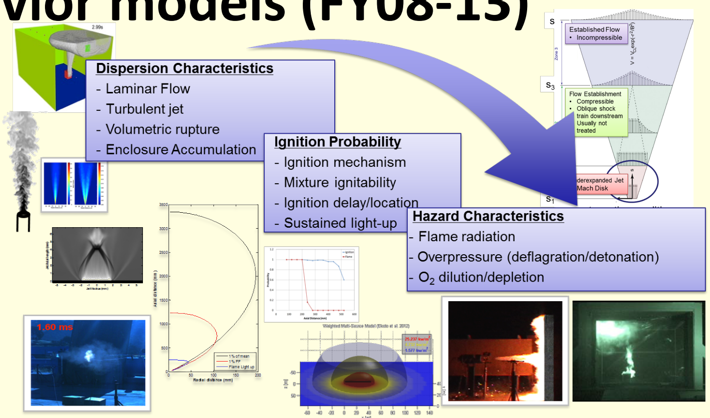


$$Risk \sim \sum_n \sum_j (f_{nj} \cdot c_{nj})$$

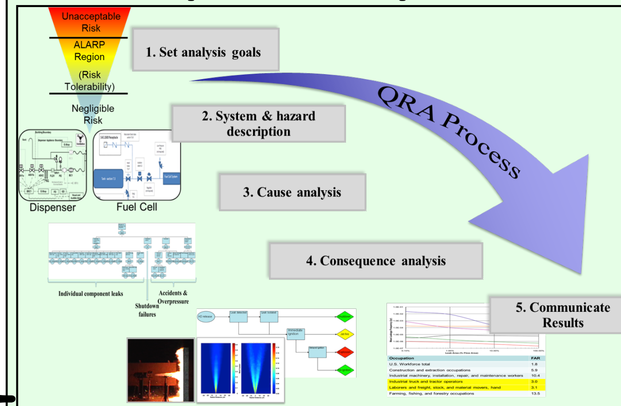
<0.125	0.008	0.004
0.125 – 6.25	0.053	0.027

Physics-based behavior models (FY08-13)

- GH2 release
- Ignition
- Reduced-order jet flame models
- Deflagration simulation



Integrated algorithm & v0 toolkit (Matlab®) (FY12-13)




```
    Y=-77.1 + 6.91*log(P_s);
case 'Lung_HSE'
    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    %HSE - Lung hemorrhage
    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    Y=1.47+1.371*log(P_s);
case 'Head_impact'
    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    %TNO - Head impact
    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
    Y=5-8.49*log((2430./P_s)+4e8./(P_s.*impulse));
case'Collapse'
    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

QRA-informed C&S (FY11-13)

- Indoor fueling (NFPA2 Ch. 10)
- Station separation distances (NFPA2 Ch.7)

Gaps/Needs: 1) User-friendly toolkit to enable CDO-led QRAs, industry-led PBD siting option 2) Reduced-order deflagration models 3) downstream jet flame physics 4) Models for LH2 releases

Approach: FY13/14 milestones

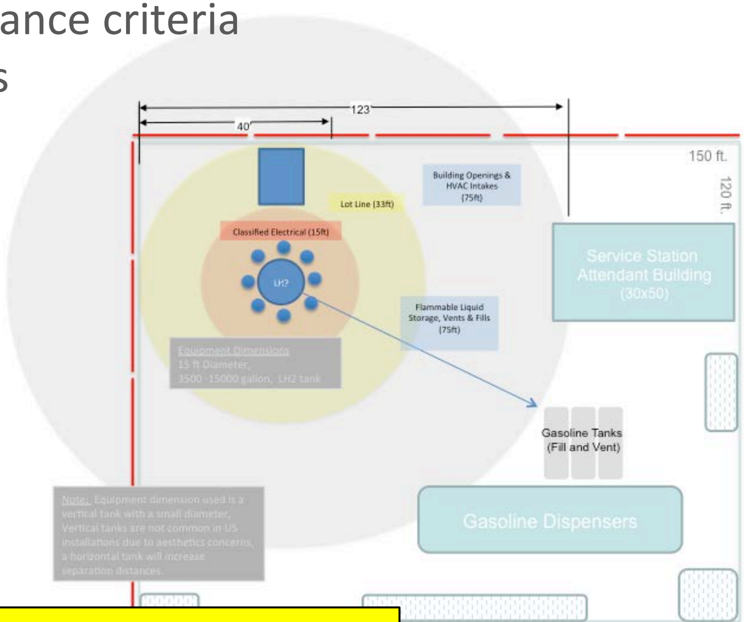
C&S activities	**Performance-Based Design (PBD) NFPA 2:** Develop a detailed project plan to validate the performance based approach of NFPA 2 Chapter 5 by performing analysis on a selected part (i.e., parking space separation distance) of a proposed station.
	C&S/QRA user workshop: Conduct workshop to help build stakeholder awareness of risk and to get C&S user feedback on QRA activities to reduce risk.
QRA methods & tools	**QRA toolkit R&D:** Complete and publish version 1 of an integrated hydrogen specific risk assessment toolkit. *Go/No-Go: Receive in-kind contribution of time or materials from industrial gas or H2 station partner*
Behavior physics	**Overpressure R&D**: Develop and validate simplified overpressure model for transient release
	Liquid behavior R&D: Develop a detailed project plan to research and model the behavior of unintended releases of hydrogen at cold and cryogenic temperatures. *Go/No-Go: Coordinate a consortium of industrial gas and hydrogen station partners.*
	Flame Radiation R&D: Update existing models with large scale, downstream flame radiation behavior

Approach: FY13/14 milestones

Milestone / Deliverable	Status
Performance based-design	- Project plan completed (Dec. 2013) - Station design selection ongoing w/ Linde, H2FIRST
C&S/QRA user workshop	Conducted June 2013; Proceedings published Sept. 2013
QRA toolkit R&D	- On track for Sep. 2014 alpha release - **Demonstration offered tomorrow (4:30-6pm EDT)** - *Go/ No-Go met: 20 workshop attendees*
Liquid behavior R&D	- Project plan on track for June 2014 completion *- Go/No-go: Actively pursuing agreements with major industrial gas companies through NFPA and CGA.*
Overpressure R&D	- 90% (model complete; writing documentation)
Flame Radiation R&D	Curved-flame model completed (Sep. 2013)

Accomplishment: Initiated performance-based design of H2 Fueling station

- **Goal: Demonstrate the use of the QRA toolkit to develop and analyze a Performance-Based Design (PBD)**
  - A PBD is an alternative compliance option for fire codes
  - PBD promotes safety through use of performance criteria rather than explicit prescriptive requirements
  - Allows a *risk-informed* compliance option
- A PBD Brief has been prepared for a representative refueling station
  - Approach will be vetted in hydrogen industry and AHJ's covering stations in California



Developing a template & tools for PBD approach facilitates industry use, AHJ acceptance, and leads to improved PBD requirements in the codes

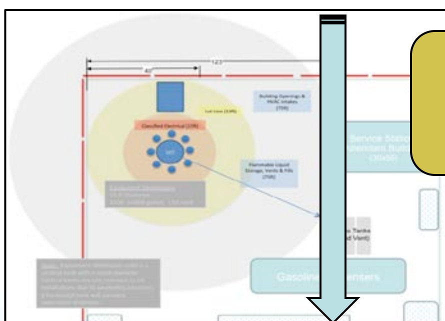
Demonstrating successful use of PBD option may significantly increase number of available sites - **if** industry can use PBD option in a cost-effective manner

Approach: Application of QRA to Performance-Based Design

Performance-Based Design of Refueling Station

Representative Station

- Meets all Prescriptive Requirements
  - Calculate Risk Values with QRA Toolkit
- Modifies Key Requirements
  - Incorporate Mitigating Factors
  - Calculate Risk Values with QRA Toolkit



Vet with H2 Code Industry and Stakeholders

Real-World Station

- Modifies One Key Requirement and Incorporates Mitigating Factors
- Prepare Performance-Based Design Report and Documentation Utilizing QRA Toolkit
- Follows Real-World Permitting Process

Accomplishment: Organized H2 C&S QRA user workshop

- **Objectives:** Understand C&S user needs; Set QRA R&D priorities
- **Organized by SNL, co-hosted by SNL & HySafe** -- Washington DC, June, 2013
  - **20 Participants from**: SNL, HySafe, DOE FCTO, US DOT, HSP, FM Global, Air Products, UMD, CVEF, AVT, Kryogenifix, ZCES, CSA Group, ISO and NFPA committees,
  - **Supportive responses from**: GE, Air Liquide, Linde, DNV, CARB, NREL, PowerTech, FP2Fire, GM Canada, Daimler, BMW, Honda, CAFCP, TAMU, KIT, UQTR, UC, DTU
- **Key Results**:
  - Application of QRA/physics for H2 infrastructure is limited by:
    - Lack of hydrogen-specific models for current QRA tools
    - Lack of integrated QRA/physics tools for all hazard scenarios
  - Users interested in multiple types of analyses:
    - High level, generic insights (e.g., for C&S developers, regulators)
    - Detailed, site-specific insights (e.g., for AHJs, station designers)

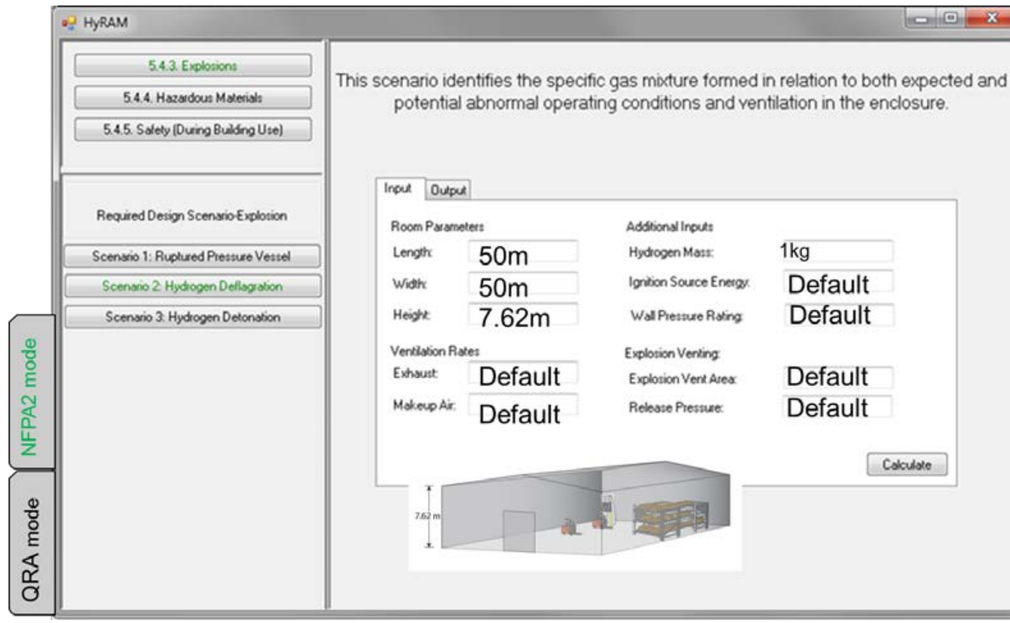
C&S and industry want to use QRA, but need enabling tools

Main R&D priorities: Develop a single toolkit that addresses all of the potential hazards – based on comprehensive science- and data-informed models.

Final report: *Groth & Harris (Sept, 2013). Hydrogen Quantitative Risk Assessment Workshop Proceedings.* ***SAND2013-7888***.

Accomplishment: HyRAM (QRA Toolkit "v1") HyRAM = Hydrogen Risk Assessment Models

- **Goal**: Develop toolkit to enable integrated probabilistic and deterministic modeling
  - All relevant hazards (thermal, mechanical, tenability)
  - Probabilistic models & data
  - H2 phenomena (gas release, ignition, heat flux, overpressure)



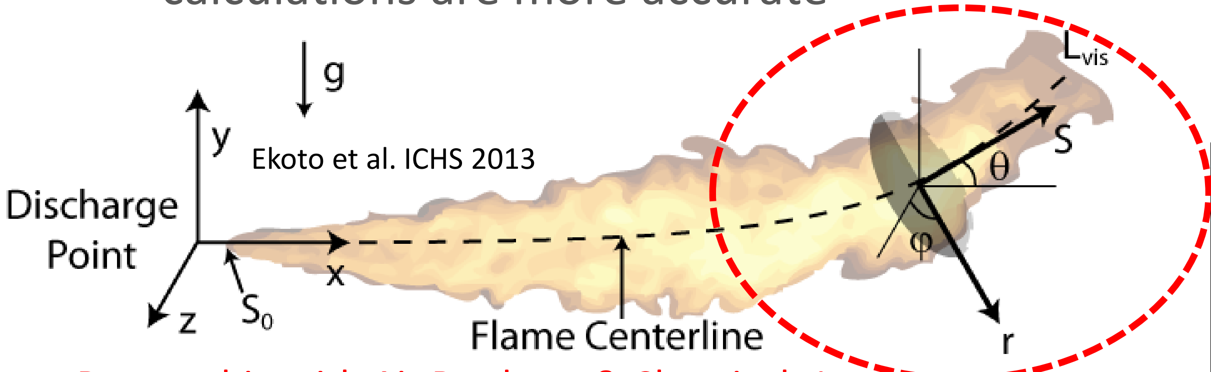
- Windows GUIs, planning HTML
- Currently, two interfaces (views):
  - **"QRA mode"** and **"NFPA2 mode"**
  - Planned "standalone physics model" mode

First-of-its-kind software tool for integrating H2 consequence models w/ QRA models

Includes behavior models & data developed through FY12.

Accomplishment: Curved flame model

- Updated flame radiation model to account for buoyancy behavior (curvature) in the far field
  - By taking into account flame curvature behavior, downstream heat flux calculations are more accurate



Partnership with Air Products & Chemicals Inc.

Flame curvature *reduces* downstream heat flux at ground level; improving this prediction has **implications for exposure risk, separation distances**

Notional Nozzle Model	Flame length [m]	Heat Flux (Straight) [kW/m^2]	Heat Flux (Curved) [kW/m^2]
Experimental	45.9	–	23.9
Birch et al. (1984) w/ Abel-Noble	49.3	97.3	29.9
Yüceil & Ötügen (2002) w/ A-N	44.6	34.8	23.8

Better match w/experimental data than straight-flame model

Needs to be updated to include wind corrections, plus validation activities

Accomplishment: Integrated overpressure model

Model pieces integrated by SNL in FY13 (SCS010)

Overpressure Model
Bauwens & Dorofeev, ICHS, 2013.

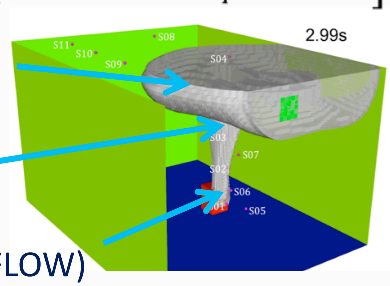
- p_0: Ambient pressure
- V_T: Facility volume
- V_{H2}: Expanded volume of pure H2
- V_{stoich}: Stoichiometric consumed H2 volume
- σ: Stoichiometric H2 expansion ratio
- γ: Air specific heat ratio (1.4)

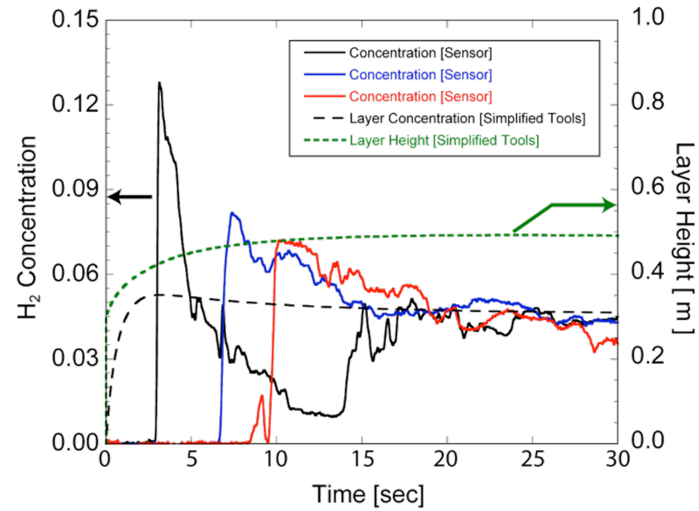
$$\Delta p = p_0 \left\{ \left[\frac{V_T + V_{H2}}{V_T} \frac{V_T + V_{stoich}(\sigma - 1)}{V_T} \right]^{\gamma} - 1 \right\}$$

H2 Layer Accumulation Model
Lowesmith et al. IJHE 2009

SNL H2 Jet/Plume Model
Houf & Schefer, IJHE 2008

SNL Network Flow Model (NETFLOW)
Winters, SAND 2001-8422





Model predictions (dotted lines) show good agreement with experiments/simulation results (solid lines)

Data in illustration from: SNL H2 indoor refueling experiments (Ekoto et al. IJHE 2012, Houf et al. IJHE 2013)

Addresses two user needs: Model completeness (integrated overpressure model addresses modeling gap in QRA toolkit) and model confidence (validation of model)

- Still needs to be programmed into QRA toolkit.
- More work needed to account for ventilation & wall heat loss for impulse prediction

Collaborations

Partner	FY 13 - FY14 Role
Air Products and Chemicals Inc. (Allentown, PA) - Jimmy Li, Leonard Creitz, Derek Miller	**Major** - In-kind support, data exchange for jet flame experiments and modeling
Linde (Hayward, CA) Nitin Natesan, Jennifer Yan	**Major** - In-kind support, data exchange for QRA tool and QRA demonstration activities, liquid modeling
HySafe (International) Andrei Tchouvelev	**Major -** Technical exchanges, workshop hosting, parallel/complementary development of QRA toolkits
Tsinghua University (China) David Christopher	**Major** – Visiting academic researcher at SNL to develop two-zone notional nozzle model
SRI International – Menlo Park, CA Mark Groethe, Erik Merilo	Minor – Technical feedback and peer review

SDO/CDO memberships
NFPA 2 ICC
ISO TC 197 WG24
CGA
CSA HGV4.9

Organization memberships*
HySafe
IEA HIA Task 31 H2USA Locations WG H2USA Stations WG
DOE CSTT

Technical exchanges, presentations & discussions
CaCFP, Texas A&M, UMD
DOE Hydrogen Safety Panel, DOT FRA
PNNL, NREL
AIST (Japan), HyIndoor (EU)

* Participation with these research initiatives enables sustained technical exchanges with Air Liquide, HSL (UK), Joint Research Centre (NL); KIT (DE), UQTR (CA), Univ. of Ulster (IE), and others

Remaining technical challenges: Sensitivity analysis (Indoor fueling, single param.)

Case	FAR
Baseline indoor fueling analysis	0.17
Uncertainty about modeled overpressures (Multiply by 10)	0.50
Uncertainty about ignition probability. (multiply by 100)	2.60
Uncertainty about ignition probability. (multiply by 10)	1.35
Uncertainty about the design (Multiplying number of components in the system by 10)	1.58
Uncertainty (under-prediction) about leak rate (use 95 percentile values).	0.51
Multiply number of vehicles by 10	0.27
Change leak detection probability to 0%	0.19
Change leak detection probability to 50%	0.093
Change thermal exposure time to 180s	0.21
Change thermal exposure time to 30s	0.15
Use Tsao instead of Eisenberg thermal probit model	0.20

Yellow denotes FAR that exceeds threshold (FAR = 0.3)

Critical uncertainties

- Completeness gaps: Lack of overpressure model, liquid model, barrier walls
- Ignition probability
- Variability in system design
- Uncertainty about leak rates

Less critical uncertainties

- Leak detection
- Thermal exposure time
- Choice of probit models

Red boxes denote Sandia FY14/15 priorities

Response to last year's Reviewer's comments

- *AMR2013 comment: "Future work for acquiring user feedback and improving the toolkit is an important step in getting the data in an easy-to-use form into the hands of users."*
  - The C&S user/QRA workshop (June 13) was a key outreach and engagement activity to address this. The resulting report aggregated stakeholder feedback and set priorities for improvements to the toolkit.
- *AMR2013 comment (on behavior work / SCS010): "Researchers still face challenges regarding equating this work into the codes, which is a driver for this work. This research cannot be used as a basis for code development – it is a good understanding of the physics."*
  - For FY14, the behavior work has been combined with the QRA/PBD work (SCS011) to address this. The integrated "HyRAM" toolkit is a key research activity to enable sustained use of physics models (along with probabilistic models) by RCS users, through a QRA/PBD approach.
- *AMR2013 comment: "The project team may want to consider some kind of affinity of sensitivity analysis to understand what factors have the greater impact on the models" (2 comments)*
  - We ran a sensitivity analysis (SA) on the indoor fueling QRA to explore the main risk drivers in the current algorithm (see results in reviewer-only slides)
  - However, model gaps cannot be addressed by SA (e.g., lack of models for overpressures) these model gaps have greater impact on the results than the quantitative uncertainties addressed in SA. These larger gaps motivate SNL's FY14/15 work on overpressure and liquid-H2 behavior models.

Proposed future work

- FY14:
  - **Toolkit**: Demonstration and user interface revisions for HyRAM
  - **NFPA2 PBD**: Quantify baseline risk for NFPA2-prescriptive-compliant station design and PBD-compliant station (w/ Linde partner)
  - **Behavior**: Experimental work to develop two-zone notional nozzle model (w/Tsinghua University partner)
- FY15:
  - **Toolkit**: Incorporate new jet flame, overpressure models into HyRAM
  - **NFPA2 PBD**: Begin permitting process for PBD-compliant station (w/ Linde)
  - **Behavior**: Develop experimental capability for liquid/cryogenic H2 behavior (w/ financial support of industrial stakeholders)
- Out-years
  - Highly accessible (web-based / app) tool for enabling end-users to implement these algorithms
  - Fill gaps in hazard scenarios with science-based models

Summary

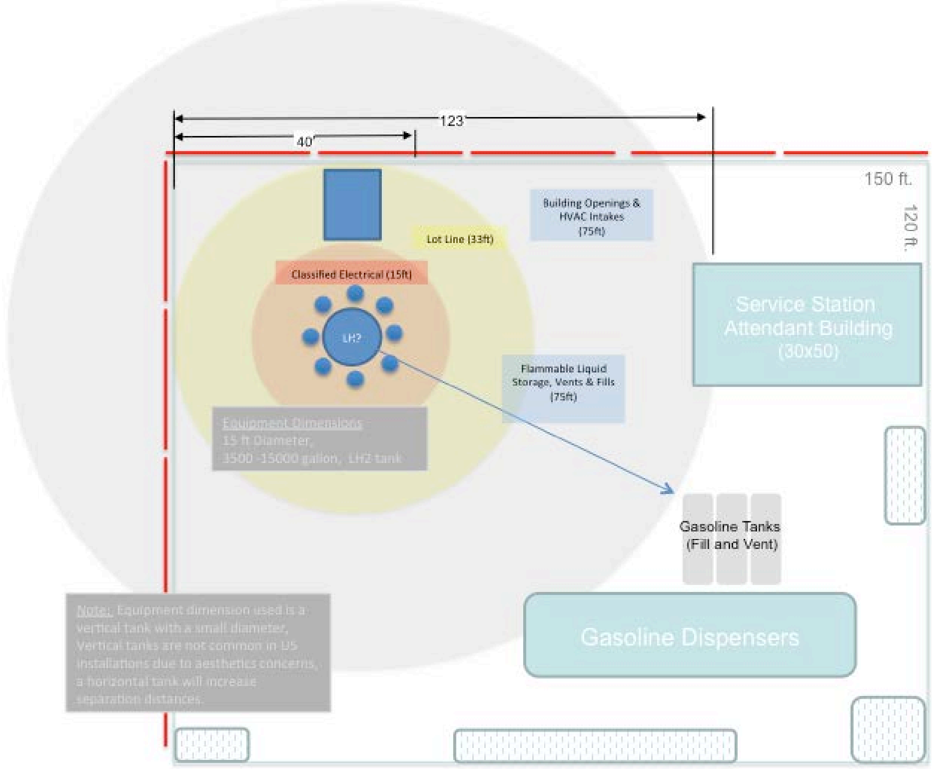
- **Relevance**: Address lack of safety data, technical data for RCS revision and compliance; reduce barriers to siting
- **Metric**: Increasing number of sites which can readily incorporate hydrogen
- **Approach**: Develop and apply science & quantitative risk assessment to reduce barriers to station siting
- **Technical Accomplishments:** C&S QRA User workshop, HyRAM toolkit, overpressure physics model, curved flame physics model,
- **Future Work**: Templated approach for PBD-compliance option; HyRAM toolkit; Liquid H2 behavior research

Technical Back-Up Slides

Survey of CEC preferred stations suggest LH2 separation distances would be prohibitive.

Separation Distances (NFPA 2-2011) **and Areas required for two station concepts**
(critical distances and areas emphasized)

Fueling System Description GH2: 12,500psi storage, 100kg, 0.4"ID tubing with a barrier wall LH2: 3500-15000 gallon (910-1300kg) with barrier wall and insulation	GH2	LH2
Lot lines (ft)	**24**	**33**
Public Streets, Alleys (ft)	24	33
Parking (public assembly) (ft)	13	**75**
Buildings (sprinkled, fire rated) (ft)	10	5
Building Openings or air intakes (ft)	**24**	**75**
Flammable and Combustible liquid storage, vents or fill ports (ft)	10	50
Parking from fill connections on bulk storage (ft)	13	25
Class 1 Div. 2 area diameter (ft)	15	15
Max Bulk Storage Dimensions with Sep. Distances (ft)	78	123
Min Bulk Storage Dimension with Sep. Distances (ft)	68	123
Max Bulk Storage Equipment Dimension with lot lines (ft)	54	40
Min Bulk Storage Equipment Dimension with lot lines (ft)	49	40
Reference Bulk Storage Equipment Area with lot lines (sqft)	2646	1600
Reference Storage Area with Sep. Distances (sqft)	**5304**	**15129**
Note: Add 5 feet for vehicle protection on vehicle facing sides of equipment		



Of the 70 stations surveyed (out of 343), none met the separation distance requirements from NFPA 2 Ch. 6.

Harris, SAND-2014-XXXX

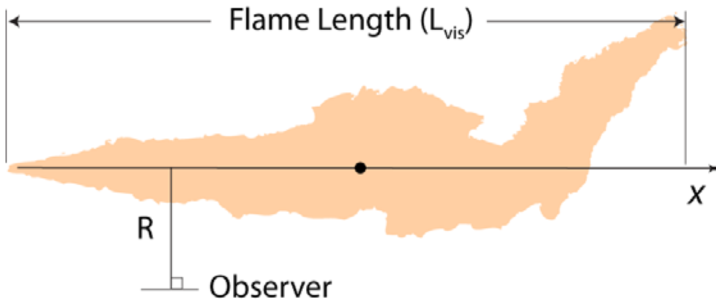
Improved LH2 modeling needed to <u>reduce separation distances</u> and <u>improve viability of risk informed certification processes</u> (NFPA 2 Ch. 5).

FY2013 Accomplishment

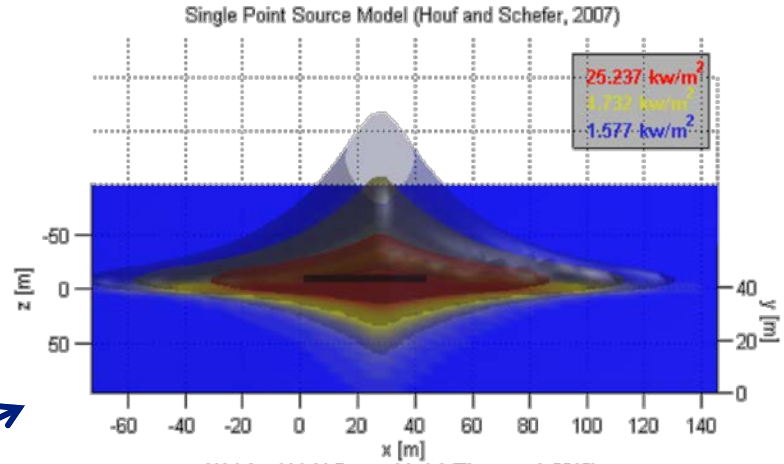
Large-scale flame data supplied by Air Products and Chemicals Inc.

d_j [mm]	[kg/s]	L_{vis} [m]	p_0 [barg]	T_0 [K]	T_{amb} [K]	p_{amb} [bar]
50.8	7.4	48.5	62.1	288	280	1.01

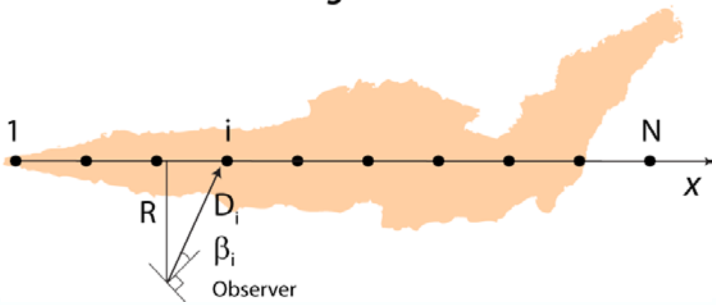
Single Point Source Model

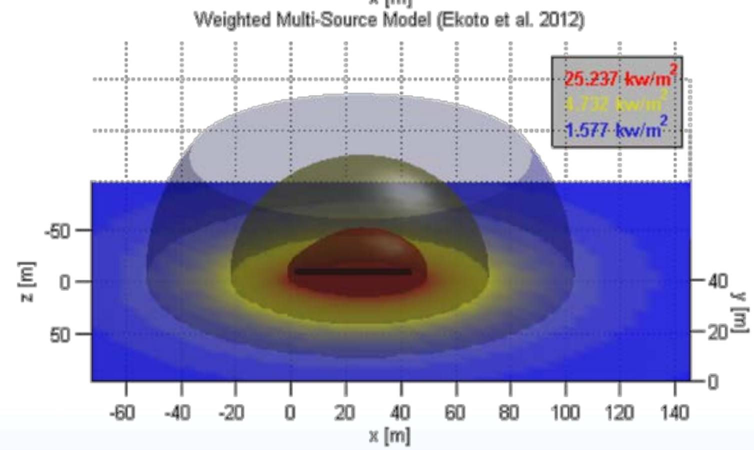


Old model used to inform NFPA 2/55



Weighted Multi Source Model



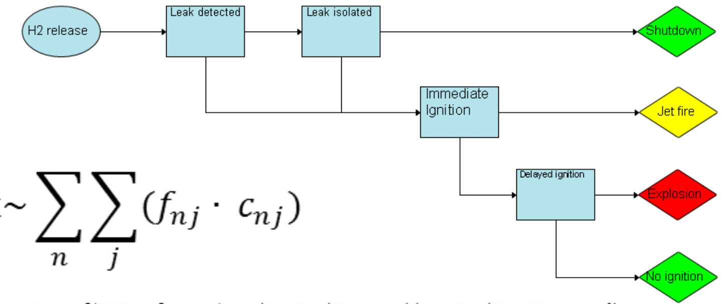


Improved radiative heat flux boundaries for more accurate harm and improved recommendations for reduced separation distances. **Model can be improved with a better prediction of flame trajectory to better reflect experimentally observed behavior**

HyRAM Modules: Cause & harm models

Accident sequences

- Hazards considered: Thermal effects (jet fire), overpressure (explosion/deflagration)



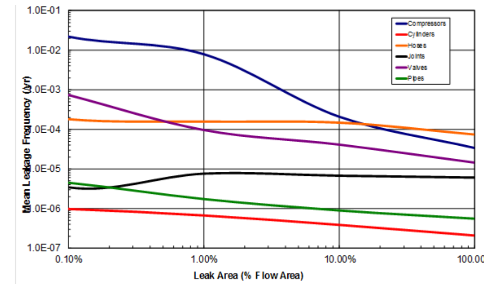
$$\text{Risk} \sim \sum_{n} \sum_{j} (f_{nj} \cdot c_{nj})$$

$$f(\text{JetFire}) = f(H2release) * (1 - \Pr(\text{Detect})) * \Pr(\text{IgnImmed})$$

Release frequency

- Expected annual leak freq. for each component type -- Data developed from limited H2 data combined w/ data from other industries.

$$f(H2release) = \sum_{i=9\ comps} n_i * E(f(Leak)_i) + E(Pr(accidents)) * n_{demands}$$



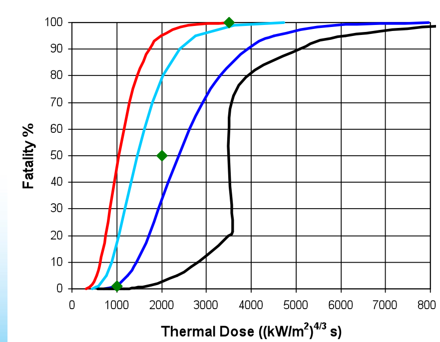
Ignition probability

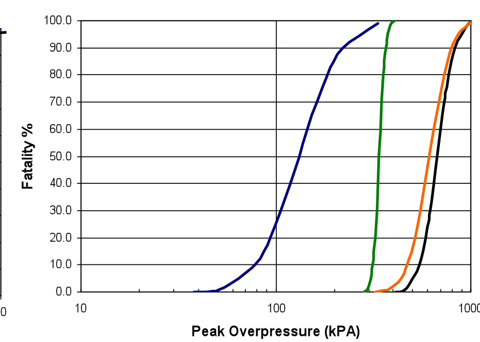
- Extrapolated from methane ignition probabilities
- Flow rate calculated using *Release Characteristics* module

Hydrogen Release Rate (kg/s)	Immediate Ignition Probability	Delayed Ignition Probability
<0.125	0.008	0.004
0.125 – 6.25	0.053	0.027
>6.25	0.23	0.12

Harm models

- Probability of fatality from exposure to heat flux and overpressures – multiple options

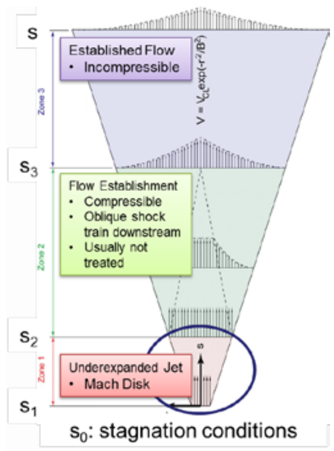


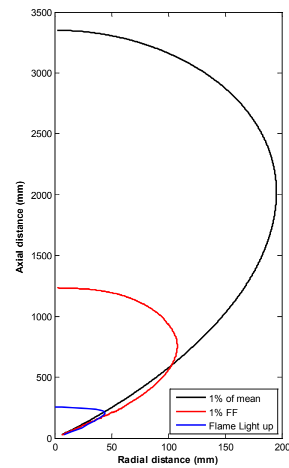


HyRAM Modules: Behavior & Consequence models

Release Characteristics

- H_2 jet integral model developed & validated
- Source models developed for LH2 & choked flow inputs





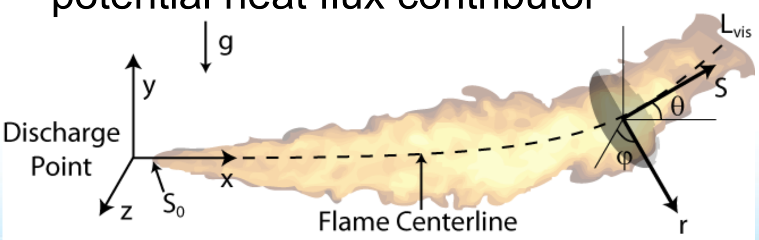
Ignition/Flame Light-up

(*pending addition*)

- Flammability Factor verified for ignition prediction
- Light-up boundaries identified
- Next: sustained flame prediction

Flame Radiation

- Flame integral model developed
- Multi-source models significantly improve heat flux prediction
- Surface reflection can be a major potential heat flux contributor



Deflagration within Enclosures

- Ventilated deflagration overpressure explored experimentally and computationally
- Current QRA module requires CFD results.
- Engineering model framework pending