RESEARCH PRIORITIES WORKSHOP – 26/27 SEPTEMBER 2016
JRC IET PETTEN, NETHERLANDS

Session: Integrated Computational Tools

The Focal Point on Integrated Research and Information for Hydrogen Safety

Chair: Andrei V. Tchouvelev
Panelists: Katrina Groth (SNL),
Frank Markert (DTU),
Thomas Jordan (KIT),
Dmitriy Makarov (UU)

Agenda and Format

- ❑ Introduction and Stage Setting – Andrei (10 min)
- ❑ Topics overview (5 min each):
  - ❑ Quantitative risk assessment (QRA) – Katrina
  - ❑ Alternative risk assessment via dynamic modeling – Frank
  - ❑ Consequence modeling tools – Thomas, Dmitriy, Andrei
- ❑ Conclusion: Summary / Gaps / Next Steps & Priorities – transition to panel discussion (chair and panelists) (20 min)
- ❑ Panel discussion continued – Q&A (20 min)

Timeframe: 11:30 – 12:45

Integrated Computational Tools – Introduction and Stage Setting

RPW2014 Ranking of Research Areas:

1. QRA Tools (23%)
2. Reduced Model Tools (15%)
3. Indoor (13%)
4. Unintended Release-Liquid (11%)
5. Unintended Release-Gas (8%)
6. Storage (8%)
7. Integration Platforms (7%)
8. Hydrogen Safety Training (7%)
9. Materials Compatibility/Sensors (7%)
10. Applications (2%)

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RPW2014 Ranking of Research Areas:

Tools and resources for QRA were identified as the highest priority topic among the ten research areas presented at the workshop (23%)

Topic Number	Topic	Number of Votes	% of Votes Received
1.1	User-friendly, industry-focused software tools to enable risk-informed decision making	21	22%
1.2	Guidance on the use of risk insights in decision making	17	18%
1.6	Validated probability models and consequence scenarios including: overpressure, cryo-release, barrier walls, and detonation/ignition probability	16	17%
1.4	Comprehensive incident databases and guidelines for estimating the probability of events	14	15%
1.7	Development of static and dynamical QRA systems to facilitate reproducible risk assessments for a variety of scenarios	13	14%
1.3	Hydrogen-specific data for updating probability models	11	11%
1.5	Statistics on initiation data	4	4%

Andrei V. Tchouvelev, AVT 26/27 September 2016

Integrated Computational Tools –
Introduction and Stage Setting

RPW2014 Ranking of Research Areas:

Reduced model tools were recognized as a significant need to address a technical gap in hydrogen safety R&D activities worldwide (15%). This represents a direct link to the QRA Tools, wherein the Reduced Model Tools shall be implemented.

Topic Number	Topic	Number of Votes	% of Votes Received
2.2	Model of barrier wall effects on flame and overpressure behavior	22	22%
2.7	Collect tools published in peer reviewed journals and develop/ support an online tool for hydrogen safety research & engineering	20	20%
2.1	Cryogenic release behavior prediction	16	16%
2.3	Validated two-zone notional nozzle model and notional nozzle model for non-circular orifice	11	11%
2.4	Integration of tools to provide a systematic approach	10	10%
2.5	Deflagration overpressure prediction	10	10%
2.8	Transient models	10	10%

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DRAFT Definition:

Integrated Computational Tools for hydrogen safety – a suite of ***engineering*** probabilistic and / or physical effects (consequence) validated models ***integrated*** into a user-friendly interface allowing the user to input user-specific information and boundary conditions and capable of generating risk and / or hazard assessment data within reasonably short time (up to 3 min).

Quantitative Risk Assessment is enabling infrastructure deployment

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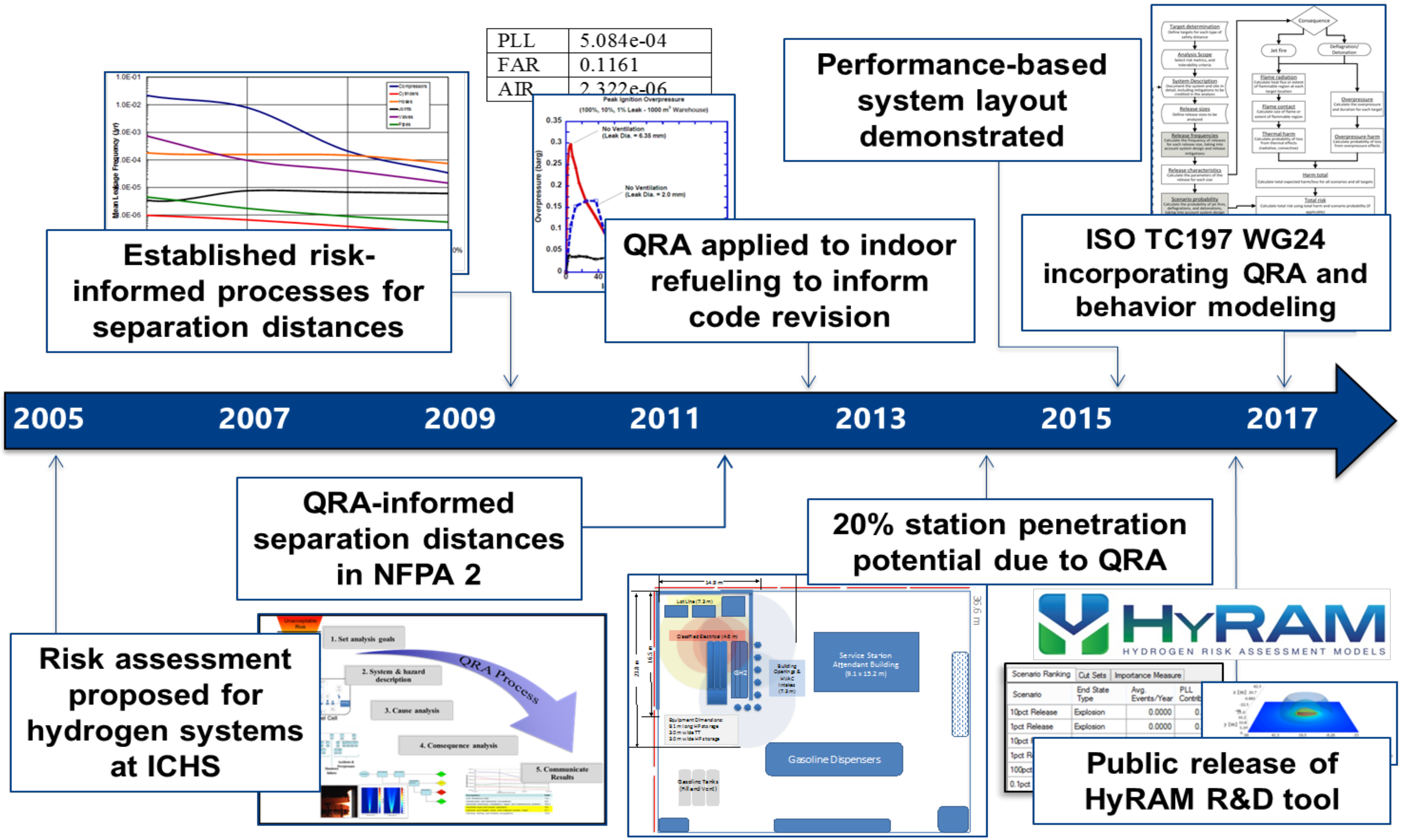
Sandia *Quantitative Risk Assessment* activities



Katrina Groth, SNL

HyRAM: Making hydrogen safety science accessible through integrated tools

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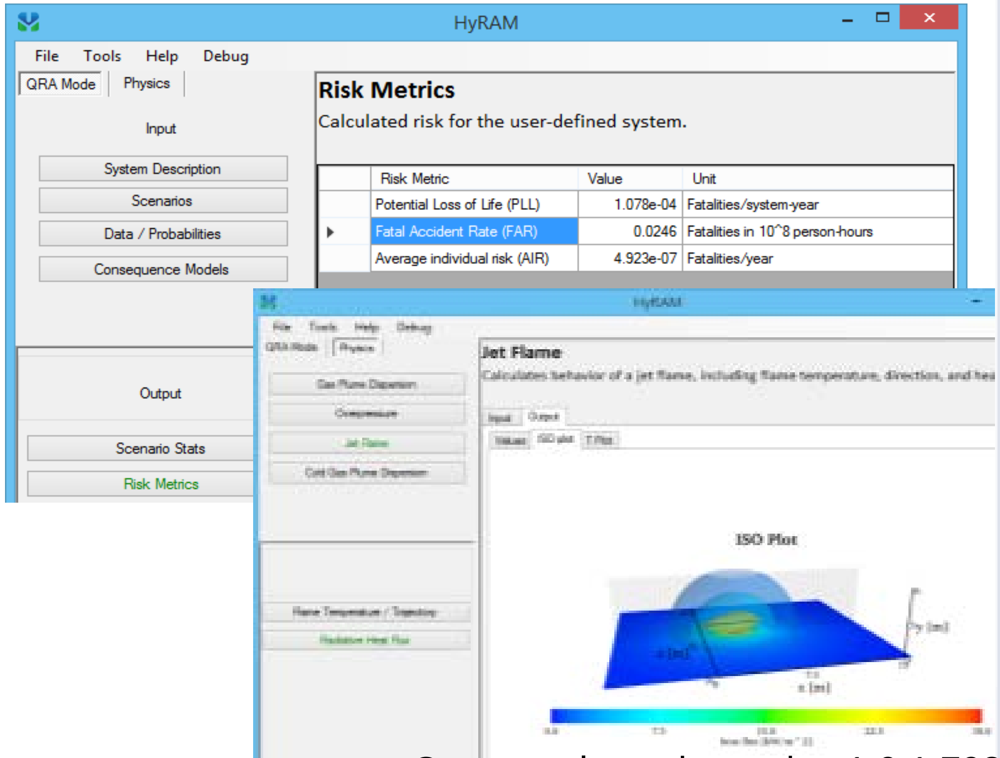
First-of-its-kind integration platform for state-of-the-art hydrogen safety models & data - **built to put the R&D into the hands of hydrogen safety experts**

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

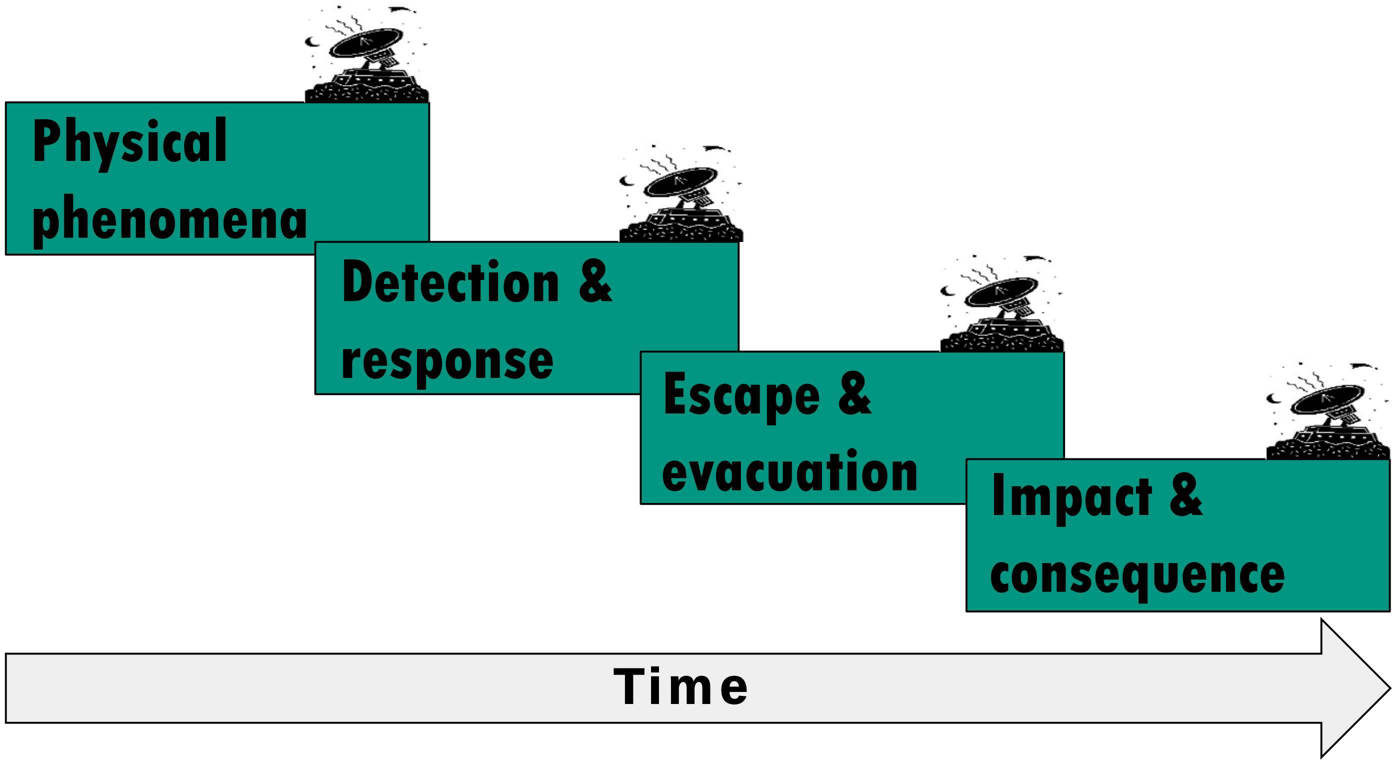


Current release is version 1.0.1.798

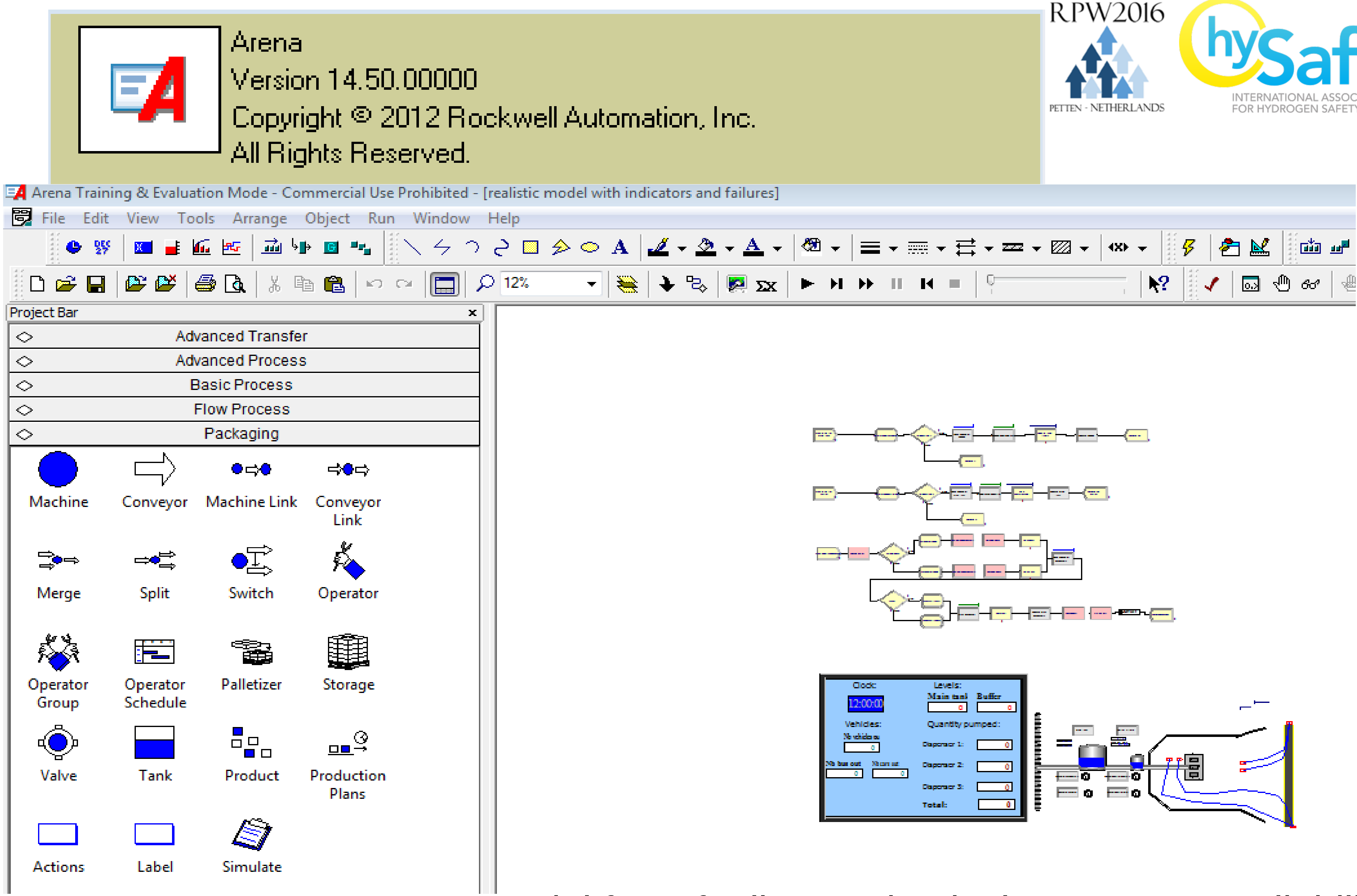
Free download for Windows
http://hyram.sandia.gov

Why is an alternative QRA method useful?

Application of dynamic & dependent models

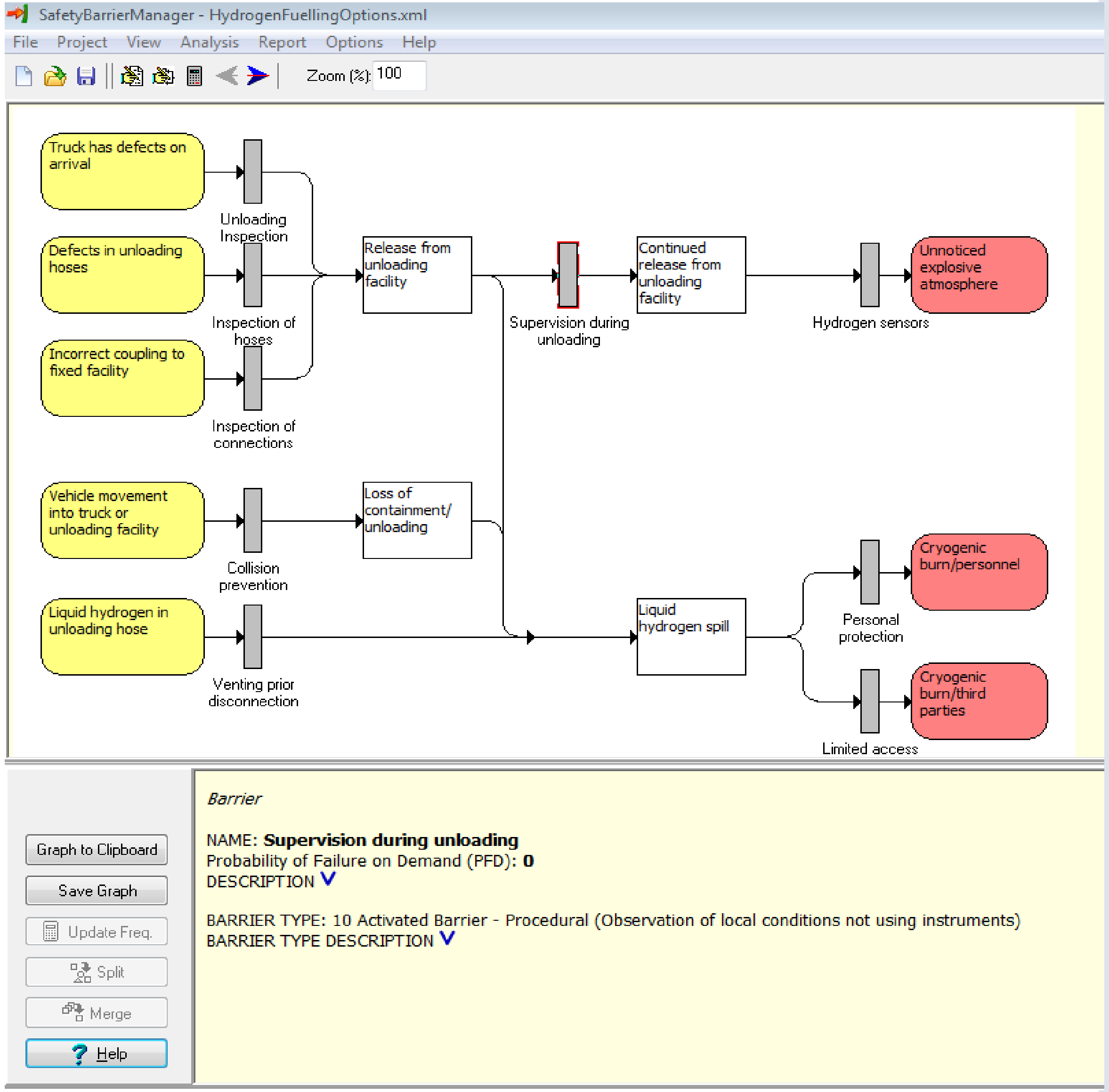


- The event sequences trigger each other and are simulated concurrently.
- Events taking place in one sequence change the conditions in the other sequences (dynamic interaction)



ARENA: DES model for refueling station incl. component reliability

Safety Barrier Manager



http://safetybarriermanager.duijm.dk

TBD during panel discussion (Frank)

Integrated Computational Tools – Consequence Modeling Tools

Status at the time of previous workshop

- Consequence Modeling Tools partially addressed in 2014 via „Integration Platforms“ low ranked on position 7 with 15%
- Within „Integration Platforms“ the following ranking of sub-topics was derived:

Topic Number	Topic	Number of Votes	% of Votes Received
7.2	Model verification and validation	22	55%
7.1	Platform completeness	10	25%
7.3	Software testing	8	20%

- However, effectively Consequence Modeling Tools are rather split up in “Engineering tools” and “CFD”

Integrated Computational Tools – Consequence Modeling Tools

Work-in-Progress / Closed gaps

- **Engineering tools**:
  - H2FC Cyberlab SAGE Network had issues – TBD during panel discussion (Thomas)
  - NETTOOLS project application under FCH JU 2.0 succesful. Work package will translate the PmWiki based BRHS/ Hydrogen Safety Handbook to Jupyter notebooks (see jupyter.org) to be used as a more **open framework for the scientific community** and as an academic **educational tool**
  - HyRAM was launched! (Katrina)
  - UU and Canadian projects advancements (Dmitriy and Andrei)
- **CFD**:
  - SUSANA project provided the basis for CFD **validation**
  - FireFOAM user basis is growing
  - GexCon has been working on an integrated approach for FLACS

Hydrogen Behavior studies are at the foundation of HyRAM's consequence modeling capabilities

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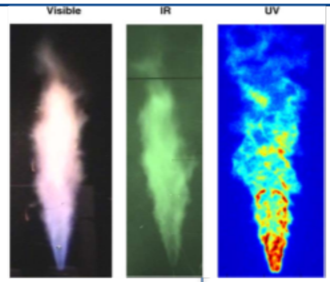
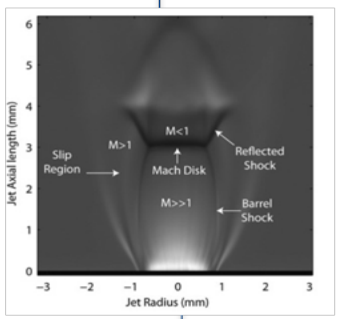
Sandia *Hydrogen Behavior* studies

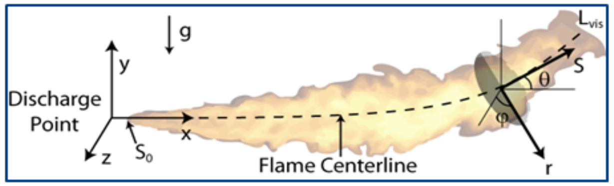
Radiative properties of H2 flames quantified



Barrier walls for risk reduction

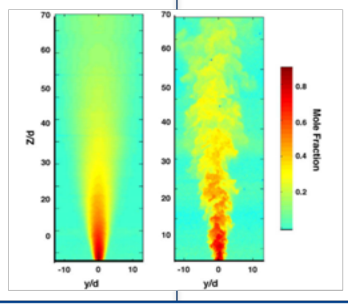
Ignition of under-expanded H2 jets





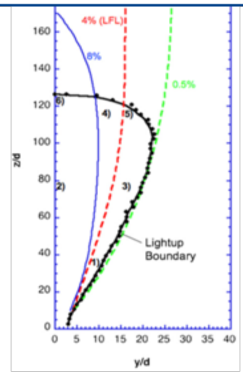
Buoyant jet flame model with multi-source radiation

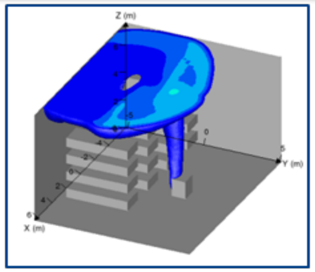
2005 | 2007 | 2009 | 2011 | 2013 | 2015 | 2017



Advanced laser diagnostics applied to turbulent H2 combustion

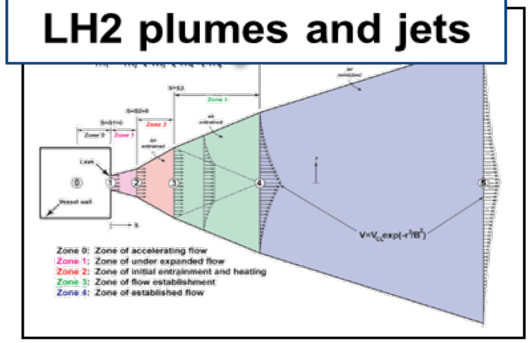
Ignition limits of turbulent H2 flows





Experiment and simulation of indoor H2 releases

Laboratory-scale characterization of LH2 plumes and jets



Ulster engineering tools

- Developed and validated models
  - Under-expanded CGH2 jet parameters (in real and notional nozzles)
  - The similarity law for CGH2 concentration decay and hazard distances in axisymmetric expanded and under-expanded jets
  - Tank blowdown dynamics as a function of volume, pressure, and leak diameter: adiabatic and isothermal releases
  - Pressure peaking phenomenon for unignited release for: constant mass flow rate release and tank blowdown
  - Flame length and three hazard distances (no-harm, injury, fatality) for jet fires
  - Passive ventilation in an enclosure with one vent
  - Blast wave decay from high-pressure GH2 tank storage
  - Vent sizing correlation for deflagration mitigations
  - Nomogram for effect of buoyancy on hazard distances

CFD tools for safety engineering

- Vision for open source CFD code

- License-free CFD code “HyFOAM” for academic research and industrial safety engineering design (financial support is required) based on OpenFOAM
- Legacy of EC FP7 H2FC project
- Collection of case studies, demos and tutorials:
  - Releases
  - Fires
  - Deflagrations
  - Detonations
  - etc.
- Current progress
  - CGH2 axisymmetric jet
  - Deflagration in open atmosphere

Integrated Computational Tools – Consequence Modeling Tools

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Canadian (UQTR/AVT) Toolkit Project

Hydrogen Toolkit - Under Development

UQTR Savoir. Surprendre.

Dispersion | Overpressure effects | Thermal effects | LH2 | LNG | Workbench

Jet extent | Enclosures | Confined Areas

Jet extent

Choose your models

Jet extent: Comparative results ?

Equation of State: Abel Noble ?

Gas: Hydrogen

Select

This project made possible with funding from Natural Resources Canada

Canadian (UQTR/AVT) Toolkit Project

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Vertical Free jet centerline extent

Hydrogen	Equation of State	Effective Diameter (m)	Centerline extent (m)
Birch 1984	Ideal Gas	0.07999	40.9423
Birch 1987	Ideal Gas	0.05399	27.6319
Chen & Rodi	Abel Noble	0.00400	33.6027
Chen & Rodi	Ideal Gas	0.00400	41.2917
Ewan and Moodie	Ideal Gas	0.07635	39.0774
Houf et. al.	Abel Noble	0.05436	27.8227
Houf et. al.	Ideal Gas	0.06414	32.8297
Molkov et. al. using Chen & Rodi	Abel Noble	0.06749	36.5027

Equations

Maximum jet Extent (ME) at 1 m from the surface
Lower Flammability Limit only (4%)
Valid for h/deff <= 55, current value of h/deff=10

Hydrogen	Effective Diameter (m)	Vertical Jet Surface extent (m)	Horizontal Jet Surface extent (m)	Side Wall Jet Surface extent (m)	Zero Gravity Jet Surface extent (m)
Surface Jets	0.10521	72.3375	33.5655	52.5021	98.4999

Definitions Equations

Surface effect:
Leak d = 4 mm
P = 70 Mpa
H = 1 m

Canadian (UQTR/AVT) Toolkit Project

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Molkov et. al. using Chen & Rodi	Abel Noble	0.06749	36.5027

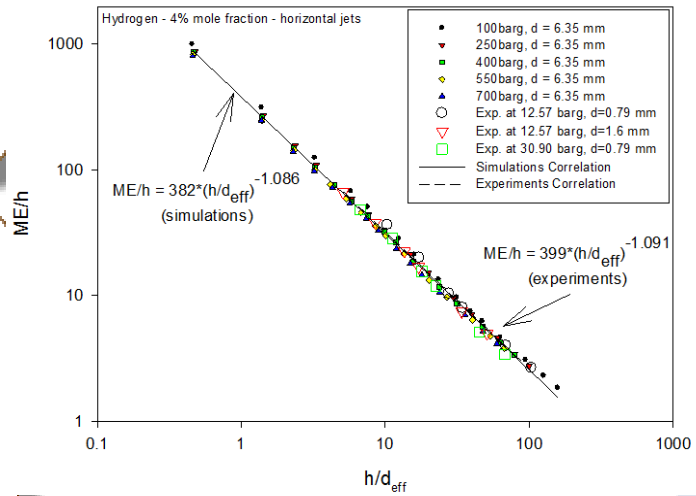
Equations

Maximum jet Extent (ME) at 3 m from the surface
Lower Flammability Limit only (4%)
Valid for h/deff <= 55, current value of h/deff=29

Hydrogen	Effective Diameter (m)	Vertical Jet Surface extent (m)	Horizontal Jet Surface extent (m)	Side Wall Jet Surface extent (m)	Zero Gravity Jet Surface extent (m)
Surface Jets	0.10521	67.7230	30.7414	51.3611	90.2123

Definitions Equations

Surface effect:
Leak d = 4 mm
P = 70 Mpa
H = 3 m



Comparison of engineering correlations with experiment

Andrei V. Tchouvelev, AVT

Integrated Computational Tools – Conclusions

Summary of Challenges, Limitations and Gaps

Transition to Panel Discussion

QRA Tools
Remaining challenges & barriers

- **Ongoing need for safety data and models:**
  - **Validated physics models for hydrogen behaviors**, including: liquid/cryogenic release behavior; deflagration (unconfined) and detonation models, flow/flame surface interactions, barrier walls, ignition,
  - **Operating experience or other information to generate data/probabilities** for hydrogen system component failures, leak frequencies, detection effectiveness, etc.
- **Need for additional features and models** to enable deeper system-specific insights to enable overcoming station-siting barriers
  - **Uncertainty & sensitivity analysis capabilities**
  - **Higher fidelity and depth of QRA models** (e.g., Fault Trees, Event Sequence Diagrams, importance measures) - Capabilities to allow users to edit scenarios, root cause models
- **Opportunities to partner** to support formal software activities, validation, testing, training, design decision making….

Katrina Groth, SNL

Case for DES Modeling
Limitations of conventional models

- conventional systems analysis tools
  as **fault** & **event trees, Bayesian networks, cause-consequence and barrier diagrams**
  - have proven to be very effective tools for reliability and risks analyses!

  But, they cannot capture a number of features accurately:
  - e.g. difficult to be applied to dynamic situations with:
    - dynamic demand: seasonal - daily changes
    - loss of partial performance
      - gas supply variations (amount gas delivered)
    - down times
      - residual time of gas delivery e.g. from line pack storage
    - gradual recovery after a failure

Integrated Computational Tools – Consequence Modeling Tools

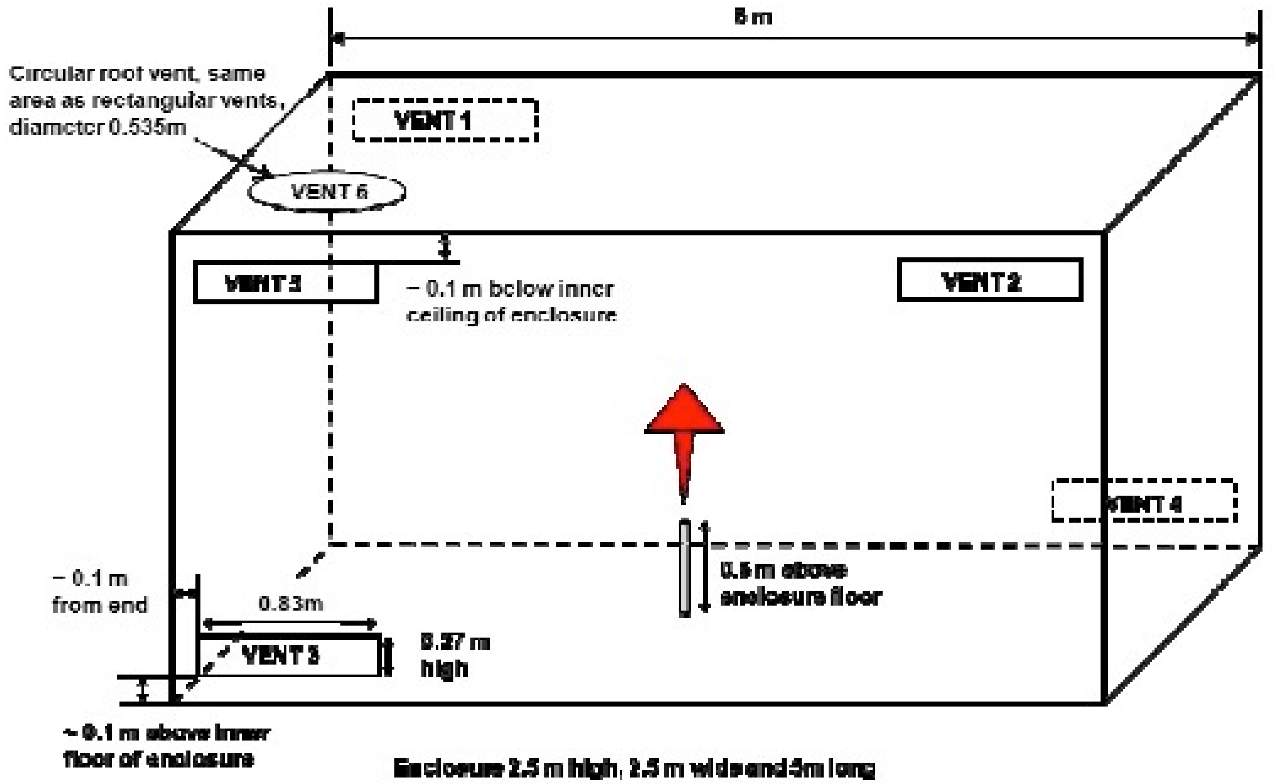
Important Findings

- **Engineering tools**:
  - SAGE based service got stuck after H2FC project stopped. Server was attacked, instable service. Lack of modularity (referencing one notebook from another did not work smoothly)

UU Closed Gaps Summary

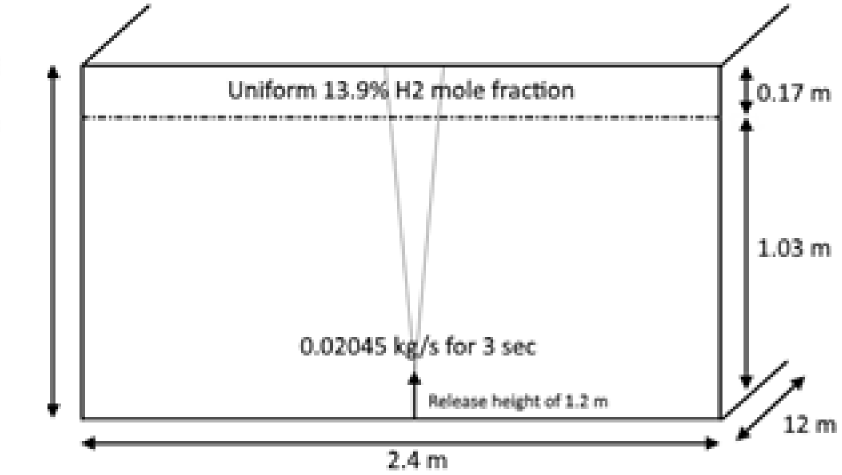
- **Wide range of published and validated models for consequence analysis available**
  - Releases and ventilation (8)
  - Fires (1)
  - Blasts (1)
  - Deflagration in closed and vented enclosures (3)

Need for validated relevant / realistic (for HP H2) models!

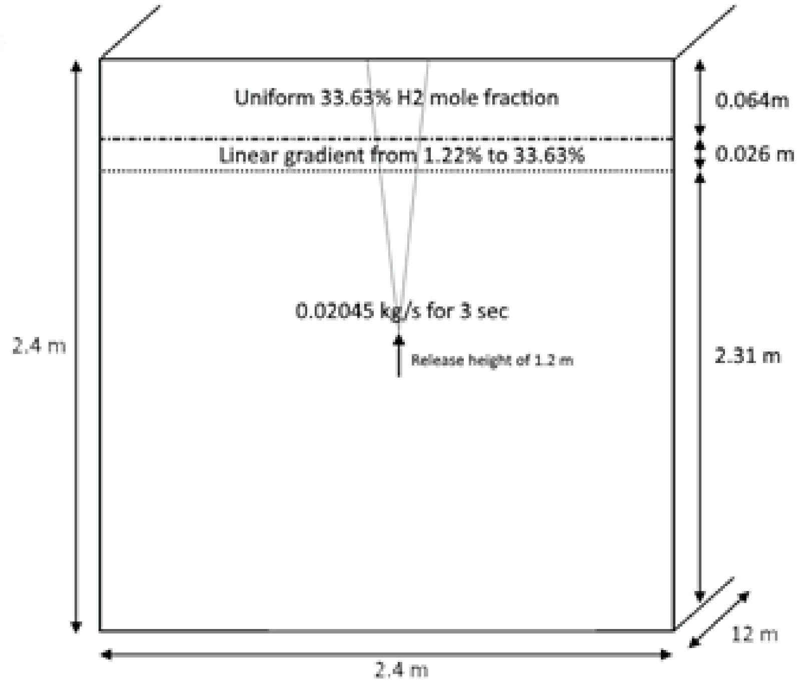


HyIndoor Experiments

Prasad



Cleaver



Available validated enclosure models are not relevant to realistic conditions of high pressure H2 systems

Panel Discussion on next steps and priorities

Next steps on hydrogen safety & risk at Sandia

Long-term vision – *Partner with stakeholders* to create a fully configurable, tested software product available for users to calculate hydrogen risk values and consequences; Able to support a wide range of activities within safety, codes, and standards.

- Upcoming extensions: HyRAM version 1.X
  - Version 1.X: Develop tests and scripts for software V&V.
  - Source code changes to bring overpressure model into QRA mode
  - Add validated model for liquid/cryogenic H_2 release (experimental work ongoing)
  - Stakeholder engagement
- Outyears: HyRAM 2.0++
  - Scoping algorithms for uncertainty analysis & dynamic QRA
  - Begin software changes to integrate IRIS software to allow users to edit Event Trees, Fault Trees & calculate importance measures
  - Establishing process to enable external R&D community to contribute models and data, i.e. as plug-ins

Approach of our choice: <u>D</u>iscrete <u>E</u>vent <u>S</u>imulation

1. Models processes and events
2. Models are dynamic (vs. static conventional models)
3. Data are sampled statistically, e.g. hole size, wind speed
4. Easy housekeeping of models and results
   – transparency of calculations
5. Animation and graphical scenarios contribute to understanding and confidence
6. Domain experts understand models and influence their development
7. Easy integration of the technical part and human performance
8. Multiple runs are performed to extract risk numbers for assessing Individual Risk, Potential Loss of Life, Group Risk)

Integrated Computational Tools – Consequence Modeling Tools

New gaps or directions

- Defining the validation basis in particular for engineering tools to be used for HRS and other H2 applications.
- Validating HyRAM
- Develop sound course material for HyRAM (possibly existing?) and offer courses to the community (potential activity of the HySafe educational committee to be set up, provided agreement by SNL)
- Introducing Uncertainty Quantification UQ for the CFD in the consequence analysis tools (although these type of uncertainties are small compared to the uncertainties in the statistical basis for QRA in general)
  There are new methods for UQ in CFD applied in particular for nuclear safety assessments

Ulster engineering tools – Next Steps

- Tools to be developed
- **Models available**
  - Forced ventilation system parameters
  - Upper limit of hydrogen inventory in closed space
  - Mitigation of localised non-uniform deflagration by venting
  - Blowdown time as a function of storage pressure, volume and TPRD diameter
- **Models not yet available**
  - Pressure peaking phenomenon for ignited releases
  - Radiation from hydrogen fireball after high-pressure CGH2 tank rapture in a fire
  - Effect of buoyancy on jet fire hazard distances