Project SCS5

SAND2008-2597P

Hydrogen Release Behavior

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Livermore, CA

June 12, 2008

DOE Hydrogen Program

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Overview

Timeline

- Project start date Oct 2003
- Project end date Sep 2015
- Percent complete 42%

Barriers

- 2007 Targets:
  - Provide expertise and technical data on hydrogen behavior, and hydrogen and fuel cell technologies
- 2007 Barriers:
  - N. Insufficient technical data to revise standards
  - P. Large footprint requirements for hydrogen fueling stations

Budget

- Total project funding (to date)
  - DOE share: \$9.7M (\$8.2M*)
- FY07 Funding: \$1.8M (\$1.7M*)
- FY08 Funding: \$3.3M (\$3.0M*)

(* R&D core, no IEA contracts)

Partners

- SRI: combustion experiments
- Princeton / U. Alabama: ignition
- Enersol / Penn St. U.: odorants
- IEA Contractors: W. Hoagland, and Longitude 122 West
- CSTT, ICC, NFPA, HIPOC, NHA, NIST, CTFCA

Objectives

- Hydrogen codes and standards need a traceable technical basis:
  - perform physical and numerical experiments to quantify fluid mechanics, combustion, heat transfer, cloud dispersion behavior
  - develop validated engineering models and CFD models for consequence analysis
  - use quantitative risk assessment for risk-informed decision making and identification of risk mitigation strategies
- Provide advocacy and technical support for the codes and standards change process:
  - consequence and risk: HIPOC and NFPA (2, 55)
  - international engagement: HYPER (EU 6th Framework Program), *Installation Permitting Guidance for Hydrogen and Fuel Cell Stationary Applications*

Milestones

9/07	Milestone: Parameter study with small leak buoyant model -- IJHE 33(4) 2008, SAE 2007 Trans.
12/07	Milestone: Develop generic QRA models and data for hydrogen gas components – SAND report, NHA 2008, WHEC 2008
3/08	Milestone: Complete walled storage tests for advanced barrier configurations and correlate data – HYPER 2007, NHA 2008, WHEC 2008; second round of tests are planned and will occur in Spring 2008
3/08	Milestone: Develop one-dimensional models for tank filling using Powertech fueling station and client fuel systems -- multi-client, fast-fill fueling consortium project is 6 months behind schedule
6/08	Milestone: Design turbulent flame lean-limit ignition experiment and diagnostics -- task ahead of schedule by 3 months, hardware is built and currently taking data

- green – completed
- orange – in progress
- red – behind schedule

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Approach

- Introduce more risk-informed decision making in the codes and standards development process using quantitative risk assessment (QRA); provide a traceable technical basis for new codes.
- Characterize mitigation effectiveness of barriers/deflectors for hydrogen releases using experiments and models; validate Navier-Stokes calculations (CFD) of hydrogen jet flames and simulations of jet deflection; partner with HYPER project on combustion hazards.
- Quantify hydrogen ignition behavior: 1) lean limits in turbulent flow, and 2) auto-ignition in high-pressure releases; perform benchmark experiments and develop predictive models for risk assessment.
- Develop fueling model to characterize the 70 MPa fast-fill process; apply model to identify optimal fuel strategy for the SAE J2601 interface standard.

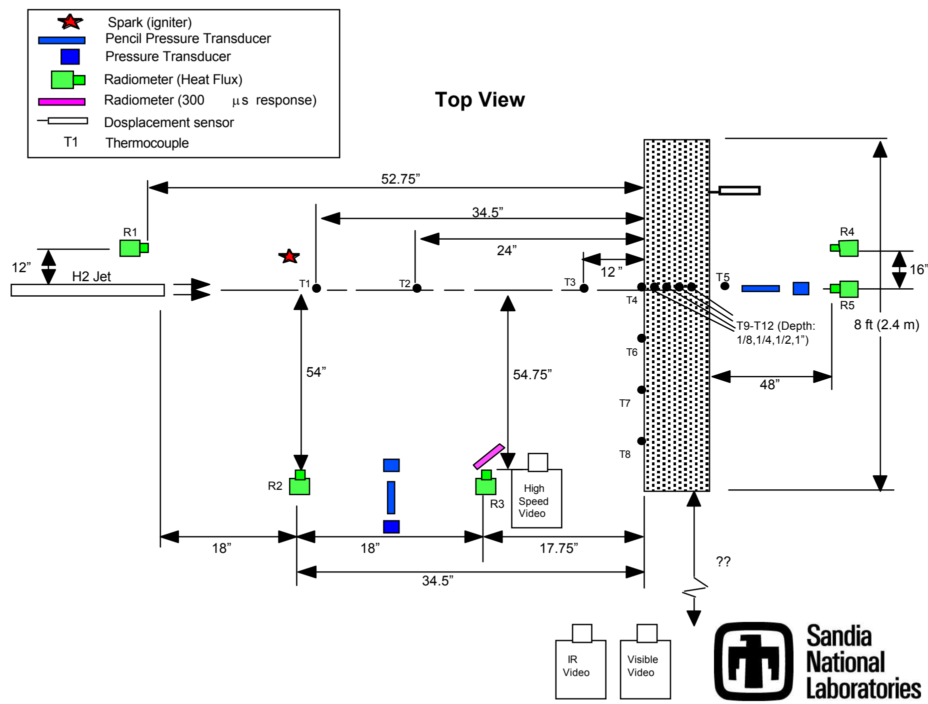
Barrier wall jet flame tests are complete

Characterize effectiveness of four barrier configurations for mitigation of over-pressure and jet flame hazards.


Tests completed at SRI Corral Hollow Experimental Station on XXXXXX


Next steps:

- barrier wall over-pressure tests with ignition timing study.
- combine data and validated CFD analyses with quantitative risk assessment for barrier design and configuration guidance.



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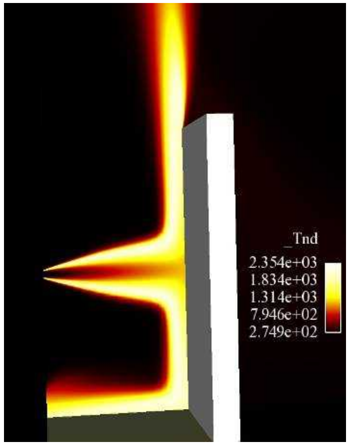
Jet flame simulations have been validated against test data

Jet centerline aligned with center of barrier

Experiment

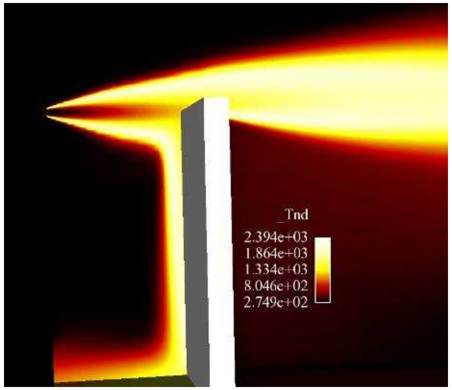
Simulation



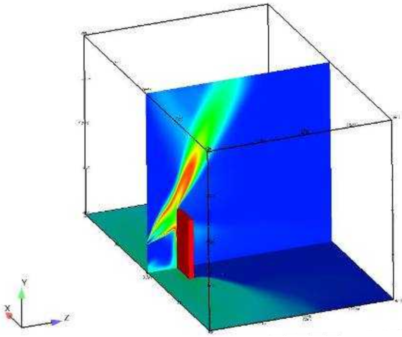
Jet centerline aligned with top of barrier

Experiment

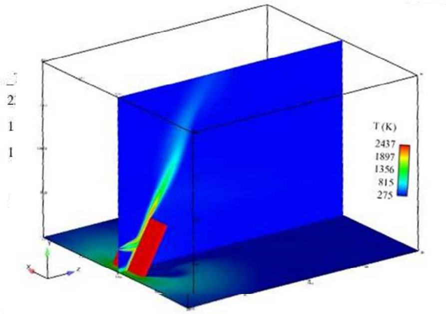
Simulation



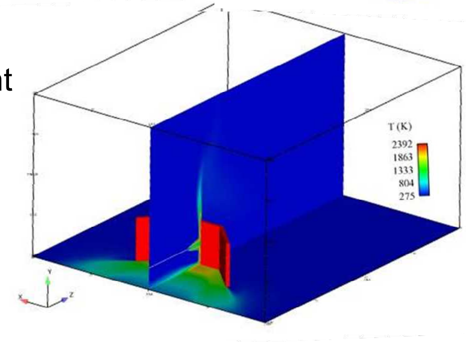
- CFD model captures qualitative trends
- no flame stabilization (hot gas recirc.) behind barrier in top of wall configuration
- flame radiation CFD model required emission model calibration to match test data (modeled emission was too high)



vertical wall +45° impingement



60° tilted wall



3-wall configuration (135° between walls)

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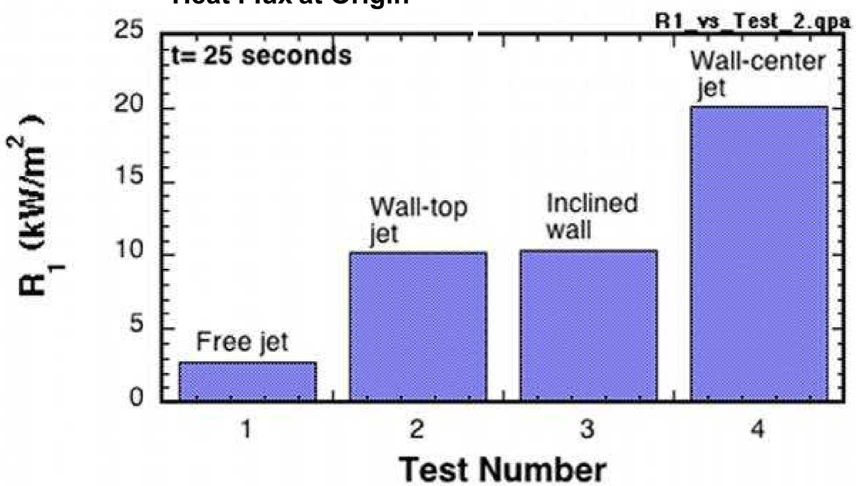
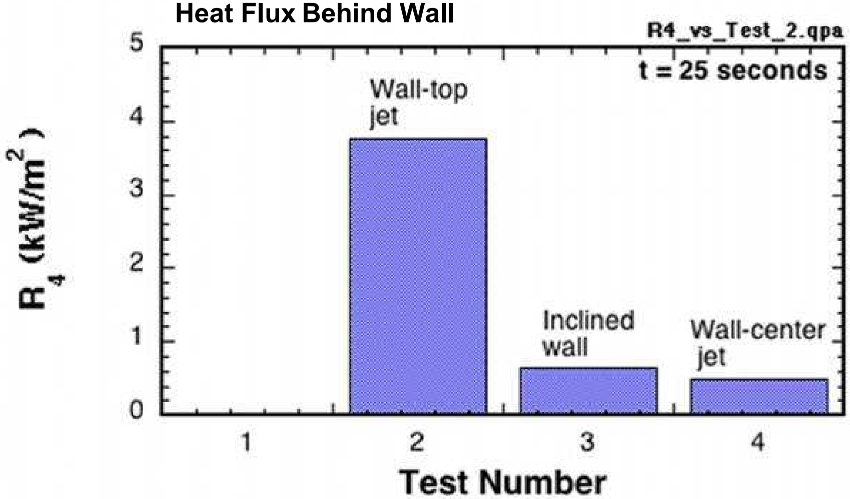
Barrier walls increase front-side thermal exposure

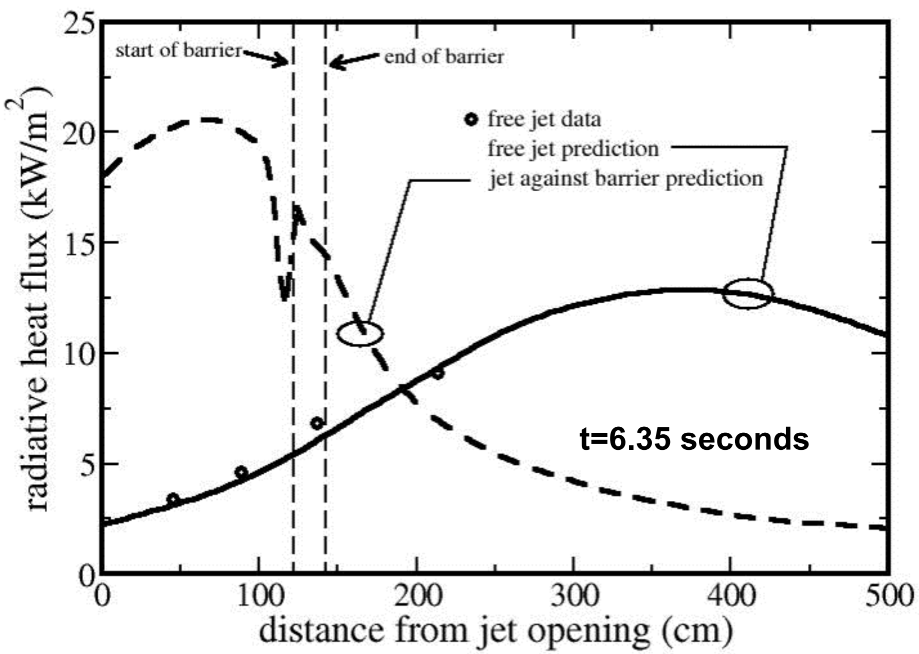
Heat Flux at Origin



Heat Flux Behind Wall



comparison of experiment and simulation for free jet and wall-centered jet flames



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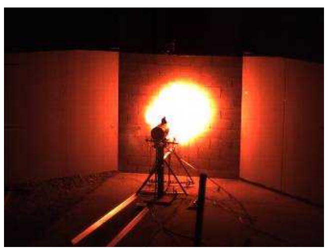
Barrier wall over-pressure mitigation

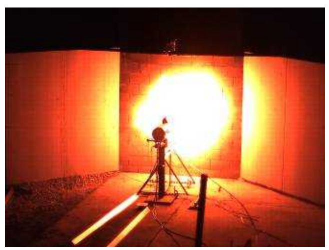
Frame 1 (t = 137 msec)
Spark ignition

Frame 5 (t = 145 msec)

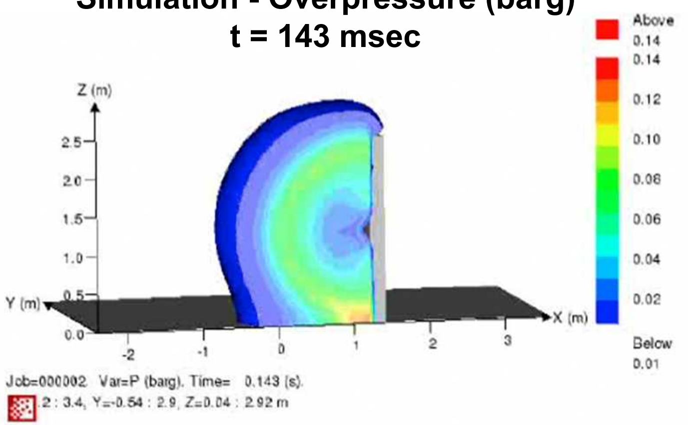
Frame 10 (t = 155 msec)



Frame 15 (t = 165 msec)

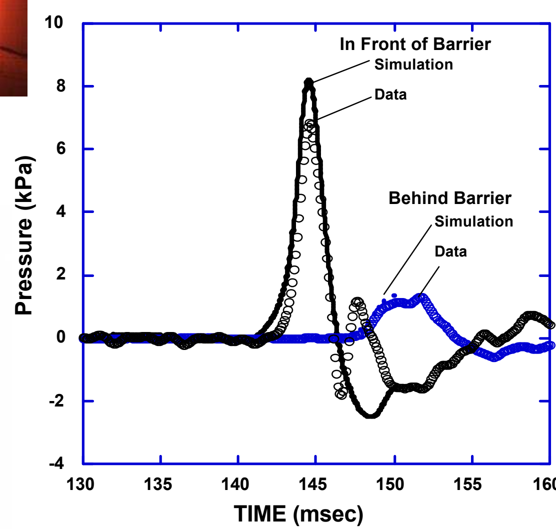


Single Wall Test
Simulation - Overpressure (barg)
t = 143 msec

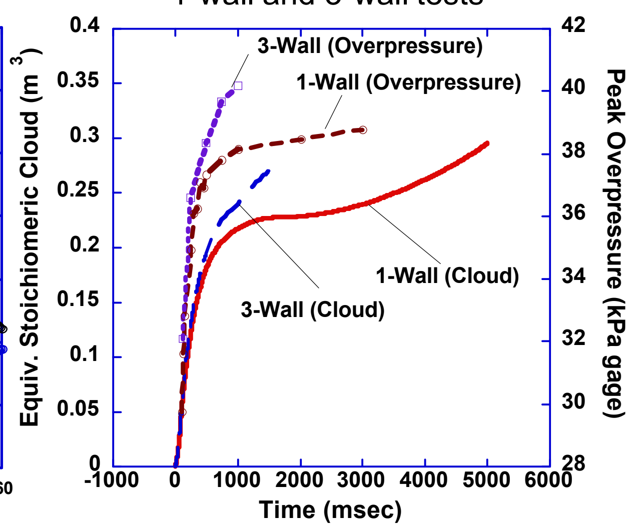


- Barrier wall test parameters:
  - over-pressure on front and back of barrier
  - barrier wall configuration geometry
  - time of release before ignition
  - point of ignition
- Simulations are guiding next set of large-scale experiments (Spring 2008)

Comparison of simulation and experiment for lateral over-pressure, 1-wall test



Simulation of peak over-pressures for different ignition times, 1-wall and 3-wall tests



Tests performed at SRI Corral Hollow test site

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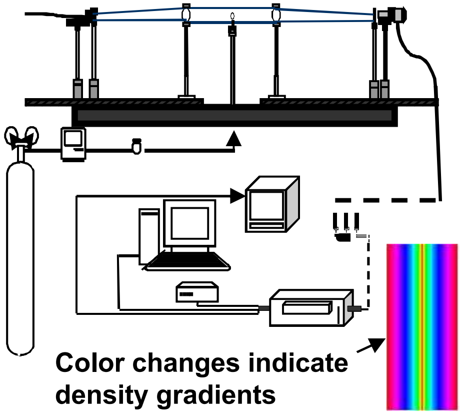
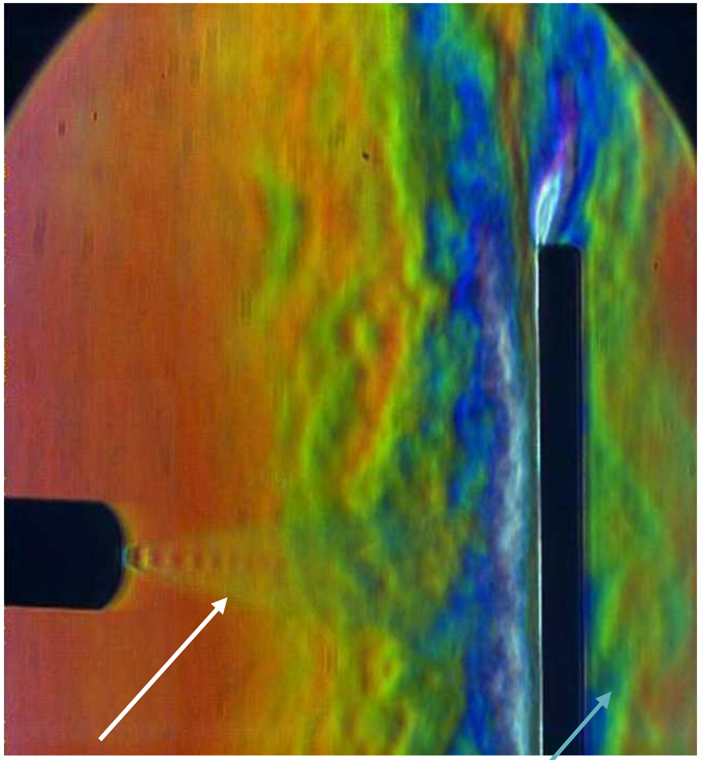
Near-wall concentrations are needed to understand ignition timing

Apparatus provides high-speed (2000 fps) imaging of fuel accumulation near barrier during transient jet startup.



Color changes indicate density gradients

Supersonic Helium Jet



Diamond shock structure

Fuel accumulation behind wall

- Collaboration with University of Alabama (Prof. Ajay Agrawal).
- Laboratory-scale experiments to characterize effect of barrier wall on transient fuel accumulation near wall.
- Provide data for transient flow and over-pressure model validation.
- Extend measurements to reacting H_2 jets interacting with walls.
- Provide guidance for large-scale test configurations for overpressure studies.

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Experimental results and models are shared with international partners

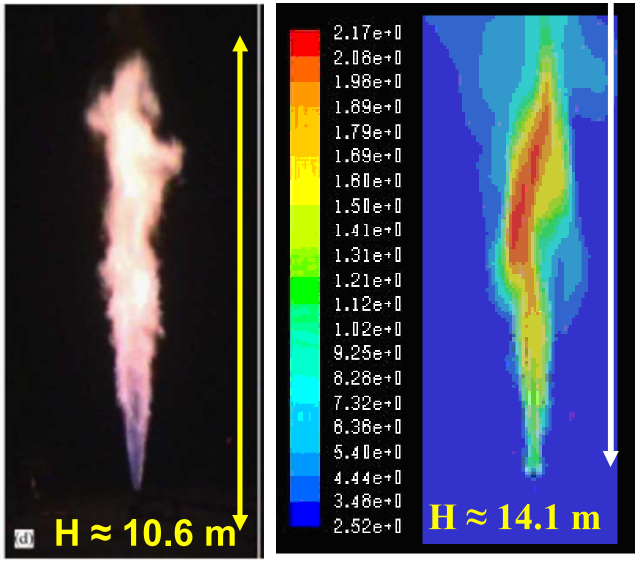
HYPER Project - EU project to create permitting guidance for stationary fuel cells

<u>Scenario A</u>: High pressure releases

- Provide previous free jet flame data and simulations
- HSE/HSL and INERIS performing additional large-scale high-pressure releases

<u>Scenario E</u>: Effects of barriers and walls on releases

- Sandia providing barrier simulations and experiments for barrier wall interactions
- HSL to perform additional tests on jet/flame barrier interaction
- Sandia/SRI large-scale free and impinging jet flame experiments modeled as part of HYSAFE (through FZK)



Comparison of visible flame length from Sandia/SRI large-scale H_2 test with LES CFD simulation from University of Ulster

IEA Task 19

- risk assessment guidelines and hydrogen-specific leak frequency data
- collaboration with HSL on auto-ignition work at Princeton
- sharing information on simplified under-expanded jet source models
- sharing information on ignition over-pressure around barriers (simulations and experiments)

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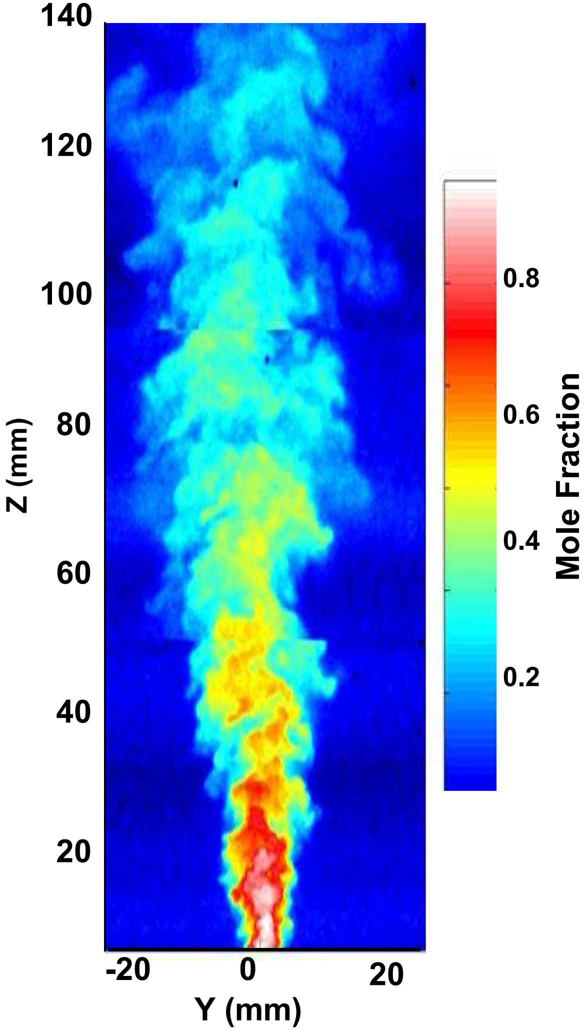
Ignition phenomena



- Characterize and quantify ignition probability in turbulent hydrogen releases (flowing system)
  - Experimentally determine flammability envelope in turbulent H_2 jets and plumes.
  - Utilize laboratory-scale releases where statistical data on H_2 distribution is available from FY07 studies.
  - Develop predictive theory for lean ignition limits for flames in typical H_2 release scenarios.
- Determine causes of auto-ignition phenomena and develop mitigation strategies (Princeton and SRI)
  - Perform experiments to identify mechanisms responsible for auto-ignition in H_2 releases.
  - Develop predictive capability for auto-ignition in H_2 release scenarios.

Instantaneous H_2 concentration images reveal state of mixing that is critical to understanding ignition in H_2 leaks

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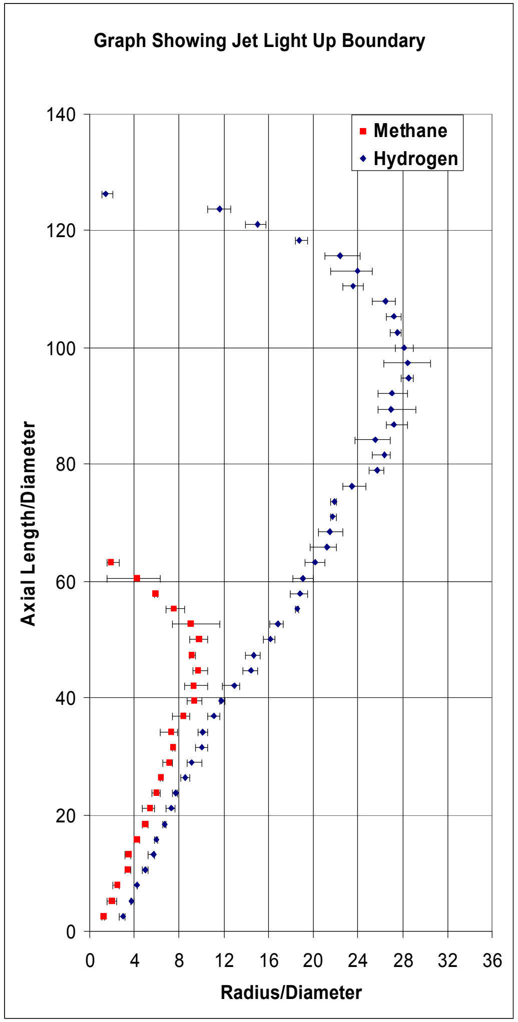
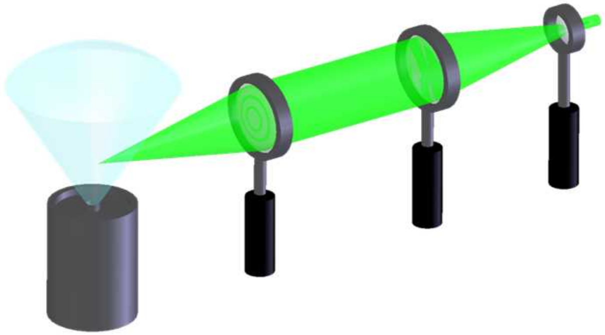
Jet ignition probability measurements





- Laser spark ignition system and software-controlled, translatable platform to allow automation of ignition location
- Jet Light-up boundary has been defined for methane and hydrogen jets
- Methane boundary plot agrees well with Birch *et al* (1981)
- Detailed investigation to determine ignition probability envelope for hydrogen

Determination of true ignitability envelope in flowing systems is important to the development and application of separation distances.

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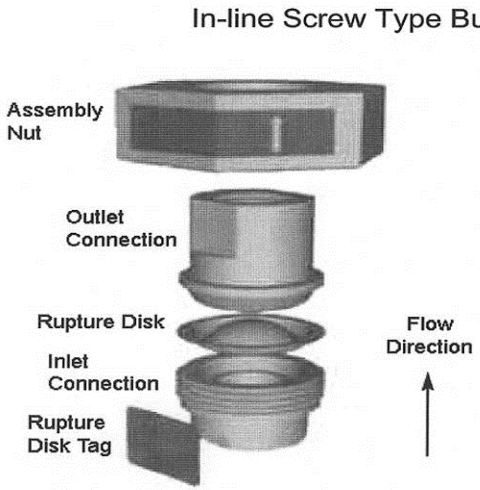
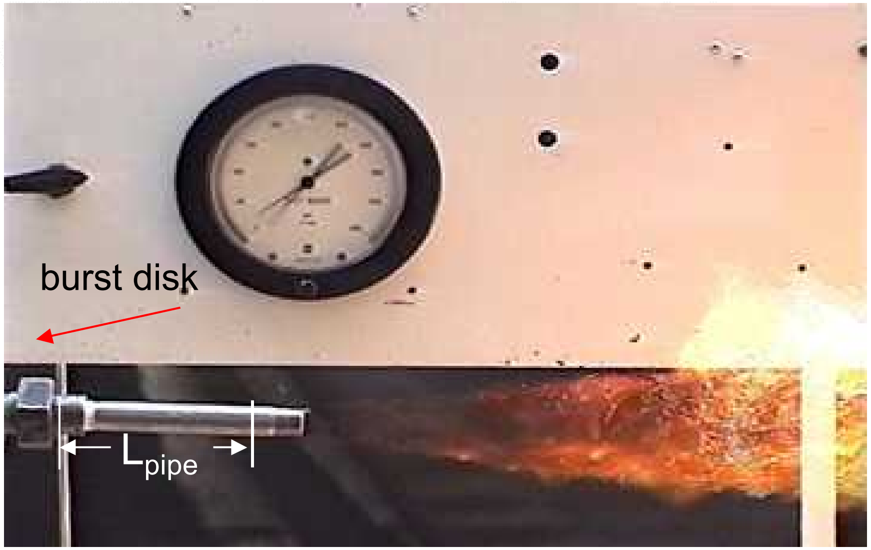
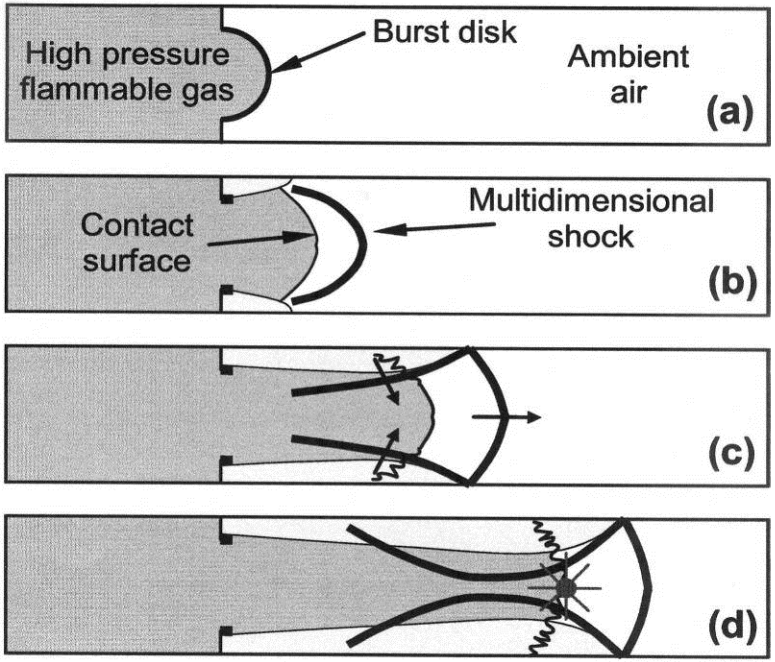
Auto-ignition experiments

Experiments at Princeton University (Prof. Fred Dryer)







- Consistent ignition occurs for release pressures above 22 atm.
- Speculated ignition due to shock heating of premixed H_2 and air.

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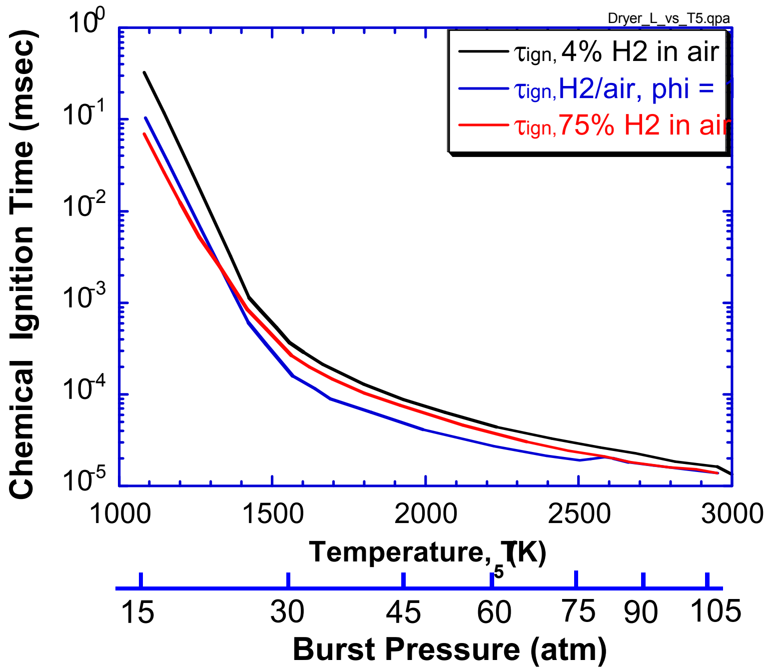
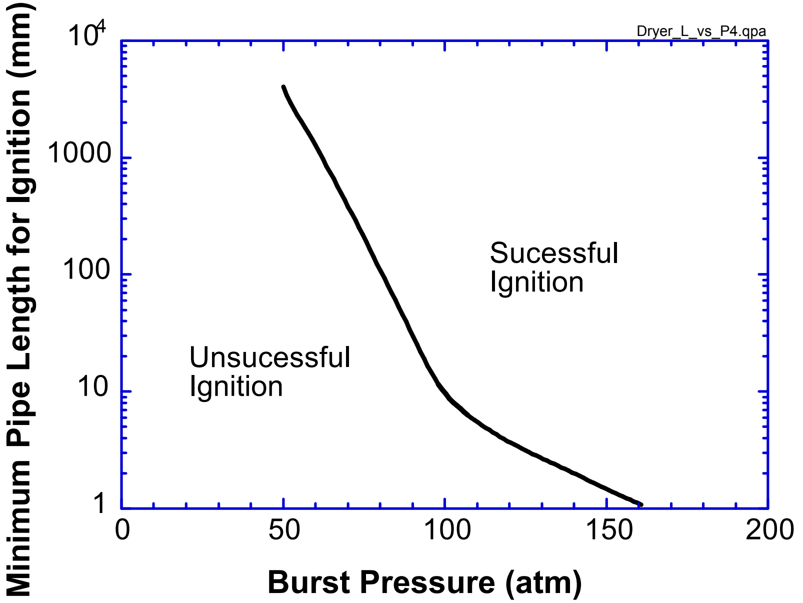
Auto-ignition trends (numerical)

Chemical ignition calculations show exponential decrease in ignition delay with burst pressure.



1-D, unsteady, compressible reacting flow simulation predicts critical ignition lengths decrease rapidly as burst pressure increases.



- If gases mix and reach a critical temperature in sufficient time, ignition will occur; this is a strong function of burst pressure.
- Numerical simulations are being used to design experiments to characterize spontaneous Ignition:
  1) small-scale laboratory experiments amenable to advanced diagnostics to elucidate the critical mechanisms involved.
  2) large-scale testing to further identify and characterize various ignition scenarios and develop mitigation strategies (with SRI).

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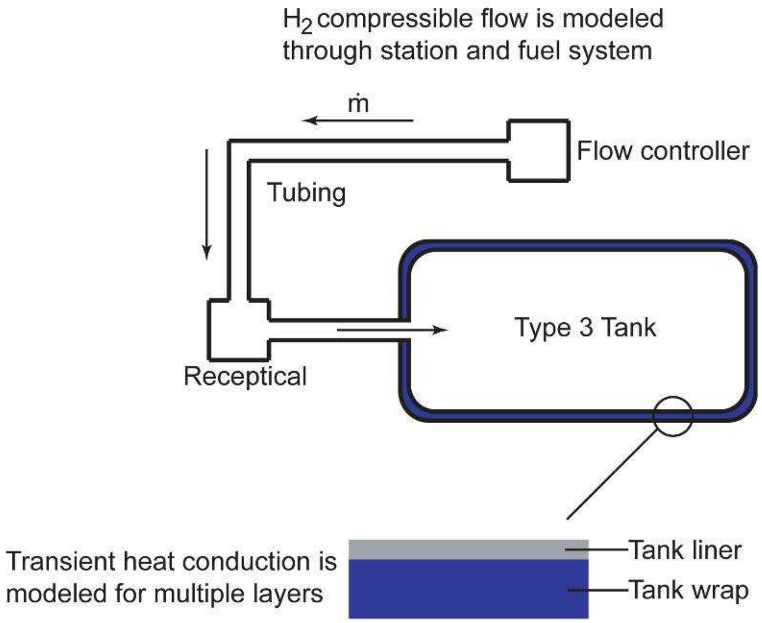
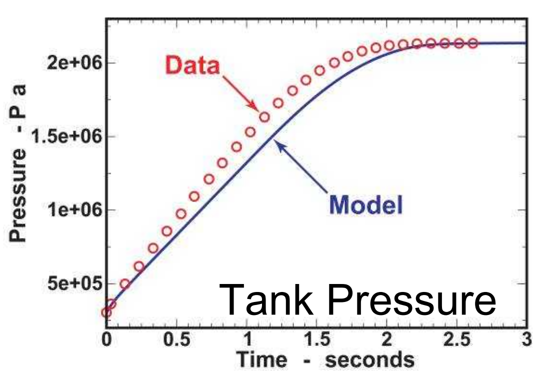
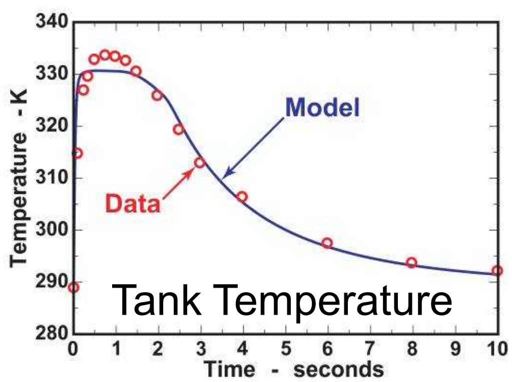
Model-development for the multi-client 70 MPa fast-fill study



Model features

- Real gas compressible flow is modeled for hydrogen delivery system and fuel system.
- Heat transfer from tank gas to tank wall is modeled using convective heat transfer correlation.
- Heat conduction is modeled for multiple layers in tank wall.
- Model is easily adapted to alternate fuel delivery configurations.





Model reproduces tank gas pressure and mass averaged temperature during fill. Data is from Sandia helium gas transfer experiment.

Consortium testing status

- Chrysler testing completed
- Nissan testing completed
- GM testing completed
- Ford testing to be completed by 5/2008
- Toyota testing to be completed by 6/2008

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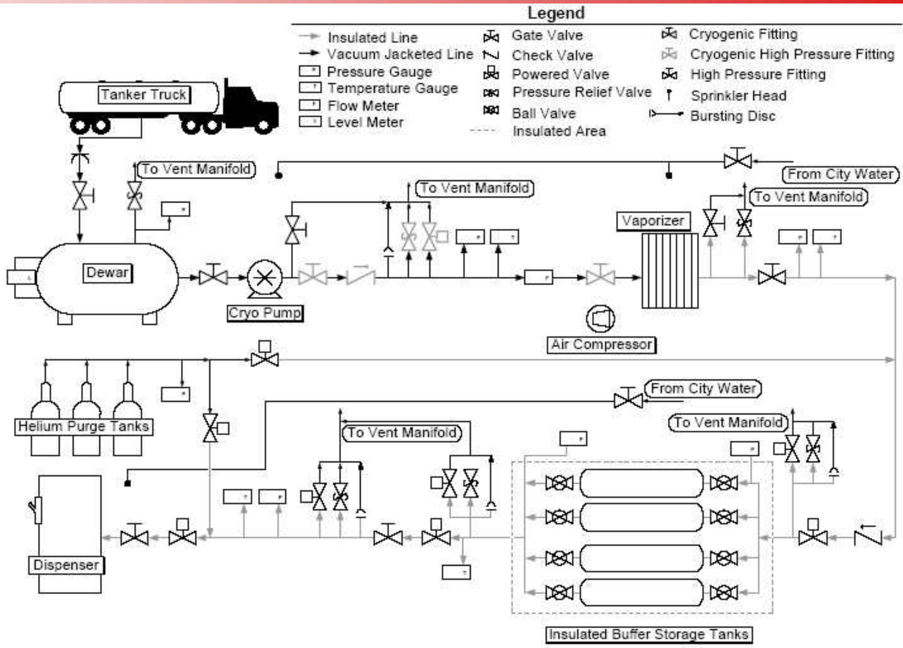
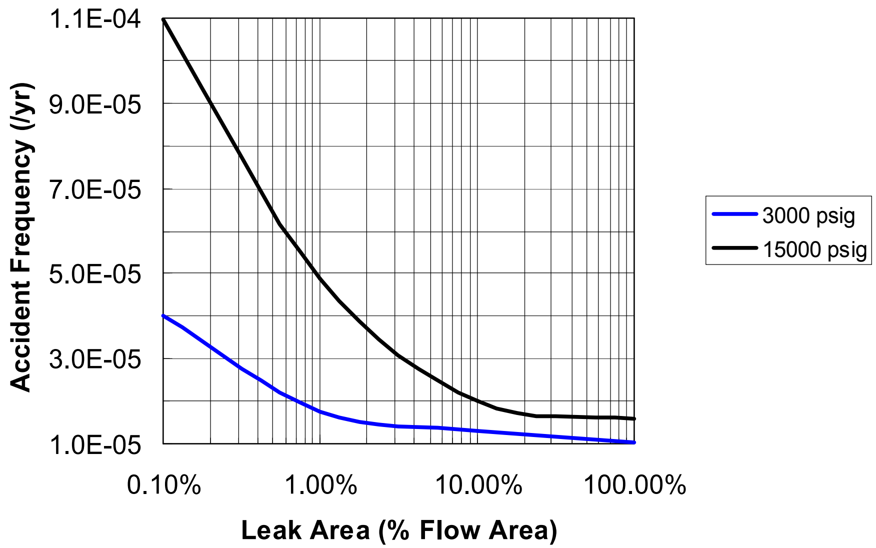
Risk-based fueling station evaluation

- Risk assessment of different refueling station configurations are being performed to identify dominant risk contributors and to evaluate the effectiveness of preventative and mitigation feature
    - deterministic assessments (Failure Modes and Effects Analysis)
    - quantitative assessments (QRAs)
- Developed models will be incorporated into NREL web-based tool for permitting hydrogen refueling stations





Separation distances based on leak areas between 1% and 10% of the system flow area result in risk values close to the risk guideline selected by NFPA-2

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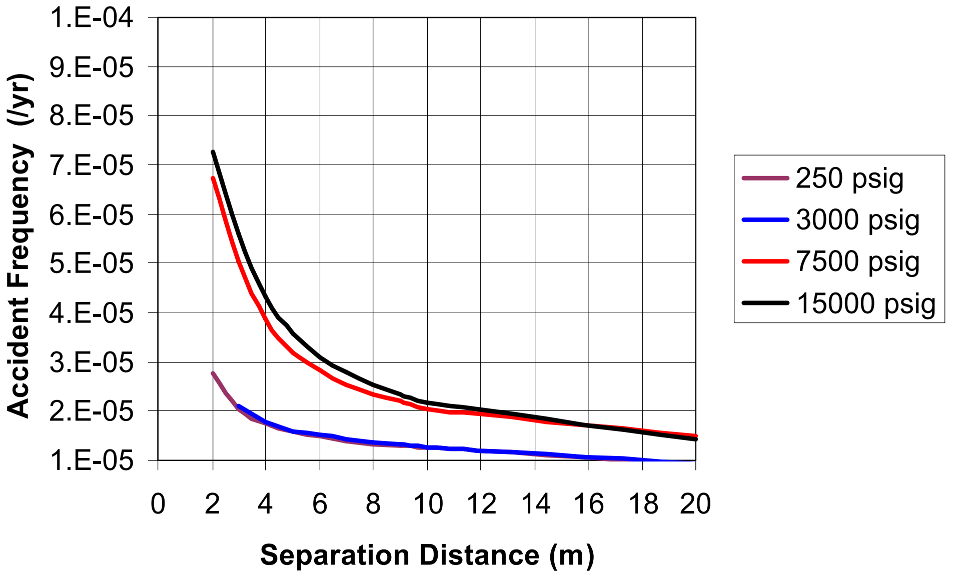
Separation distance technical basis

- Sandia introduced quantitative risk assessment (QRA) techniques to incorporate applied research on unintended releases into a risk-informed decision-making process for separation distances
  - technical support provided by Sandia staff, Jeff LaChance and William Houf, to NFPA 2 Task Group 6
  - Sandia performed QRA of a NFPA 2 specified hydrogen facility
  - hydrogen component leakage data analysis performed and incorporated into QRA

- Code developers utilized information from QRA and leakage data analysis to establish basis for selecting leak diameter used to determine separation distances

- Sandia deterministic models were then used to develop new separation distance for selected leak diameters



- The newly created separation distance guidelines will be proposed in the next cycle of NFPA 55 - proposals submitted Feb. 2008

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Future work

Remainder of FY08

- Finish barrier wall effectiveness work and publish
- Develop scientific theory for ignition criteria for turbulent hydrogen leaks
- Finish heat transfer model calibration for 70 MPa fueling process
- Develop gap analysis and project plan for liquid hydrogen releases
- Screen odorant chemicals for stability and fuel cell compatibility (Enersol / Penn St)
- Risk-informed permitting tool

FY09

- Develop scientific theory for ignition criteria for turbulent hydrogen leaks
- Confined releases: fuel storage cabinets, parking structures, tunnels
- Liquid hydrogen releases
- Risk-informed hazard mitigation strategies

Summary

- SNL staff supported the application of our risk-informed approach to help the NFPA 2 Task Group 6 establish a technical basis for separation distances
- Developing a risk-informed permitting tool (with NREL)
- Barrier walls are being characterized as a jet mitigation strategy for set back reduction
  - jet flame model validation is complete
  - performing over-pressure tests
  - sharing data and learning with international partners (HYPER)
- Developing mechanisms for hydrogen ignition
  - lean limit mechanism in flowing systems
  - auto-ignition mechanism
  - influence fire code set backs and detection standards

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Additional Slides

Responses to Previous Year Reviewers' Comments

This project was not reviewed in 2007.

Publications & Presentations

1. Schefer, R. W. and Houf, W, G., “Investigation of Small-Scale Unintended Releases of Hydrogen: Momentum-Dominated Regime”, accepted in *IJHE*, 2008.

2. Schefer, R. W. and Houf, W, G., “Investigation of Small-Scale Unintended Releases of Hydrogen: Buoyancy Effects”, accepted in *IJHE*, 2007.

3. Houf, W. G., Evans, G., and Schefer, R. W., “Analysis of Jet Flames and Unignited Jets from Unintended Releases of Hydrogen”, 2nd International Conference on Hydrogen Safety, San Sebastian, Spain, September 11-13, 2007.

4. Houf, W. G. and Schefer, R. W., “Analytical and Experimental Investigation of Small-Scale Unintended Releases of Hydrogen,” *IJHE*, Vol. 33, No. 4, pp. 1435-1444, February, 2008.

5. Schefer, R. W., Groethe, M., Houf, W. G., and Keller, J. O., “Experimental Evaluation of Barrier Walls for Risk Reduction of Unintended Hydrogen Releases”, 17th World Hydrogen Energy Conference, Brisbane, Australia, June 15-19, 2008.

6. Houf, W. G., Schefer, R. W., Evans, G., and Groethe, M., “Barriers for Mitigation of Unintended Releases of Hydrogen”, 17th World Hydrogen Energy Conference, Brisbane, Australia, June 15-19, 2008.

Publications & Presentations

7. Houf, W. G., Schefer, R. W., Evans, G., “Analysis of Barriers for Unintended Releases of Hydrogen,” National Hydrogen Association Meeting, Sacramento, CA, March 30 - April 3, 2008.

8. Houf, W. G. and Schefer, R. W., “ Investigation of Small-Scale Unintended Releases of Hydrogen,” SAE 2007 Transactions, Journal of Materials & Manufacturing, March, 2008.

9. LaChance, J. L., “Risk-Informed Separation Distances for Hydrogen Refueling Stations,” 2nd International Conference on Hydrogen Safety, San Sebastian, Spain, September 11-13, 2007.

10. LaChance, J. L., Tchouvelev, A. V., and Ohi, J., “Risk-Informed Process and Tools for Permitting Hydrogen Fueling Stations,” 2nd International Conference on Hydrogen Safety, San Sebastian, Spain, September 11-13, 2007.

11. LaChance, J. L., Brown, J., Middleton, B., and Robinson, D., “Data for the Use in Quantitative Risk Analysis of Hydrogen Refueling Stations,” National Hydrogen Association Meeting, Sacramento, CA, March 30 - April 3, 2008.

Publications & Presentations

12. LaChance, J. L. and Houf, W. G., “Risk-Informed Separation Distances for Use in NFPA Hydrogen Codes and Standards,” 17th World Hydrogen Energy Conference, Brisbane, Australia, June 15-19, 2008.

13. Tchouvelev, A. V., LaChance, J. L., and Engebo, A., “IEA Task 19 Hydrogen Safety Effort in Developing Uniform Risk Acceptance Criteria for the Hydrogen Infrastructure,” National Hydrogen Association Meeting, Sacramento, CA, March 30 - April 3, 2008.

14. HYPER Work Package 4 Interim Modelling Report, October 30, 2007

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Critical assumptions and issues

- Issue: Safety, Codes and Standards program element is moving to Office of Vehicle Technologies in FY09. We are concerned about losing hydrogen focus within the new program office and the additional layer of coordination burden placed on HFCIT staff.

- Issue: we continue to manage "conflict of interest" as both researchers and participants in codes and standards development. We participate in the development process to the extent of assisting other developers understand and apply the DOE-funded research. We avoid participating in code writing and decision-making that could that could be perceived as promoting a particular research agenda. Research directions are derived from code development needs provided by organizations such as HIPOC and NFPA Research Foundations.