Project SCS5

Hydrogen Release Behavior

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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

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.

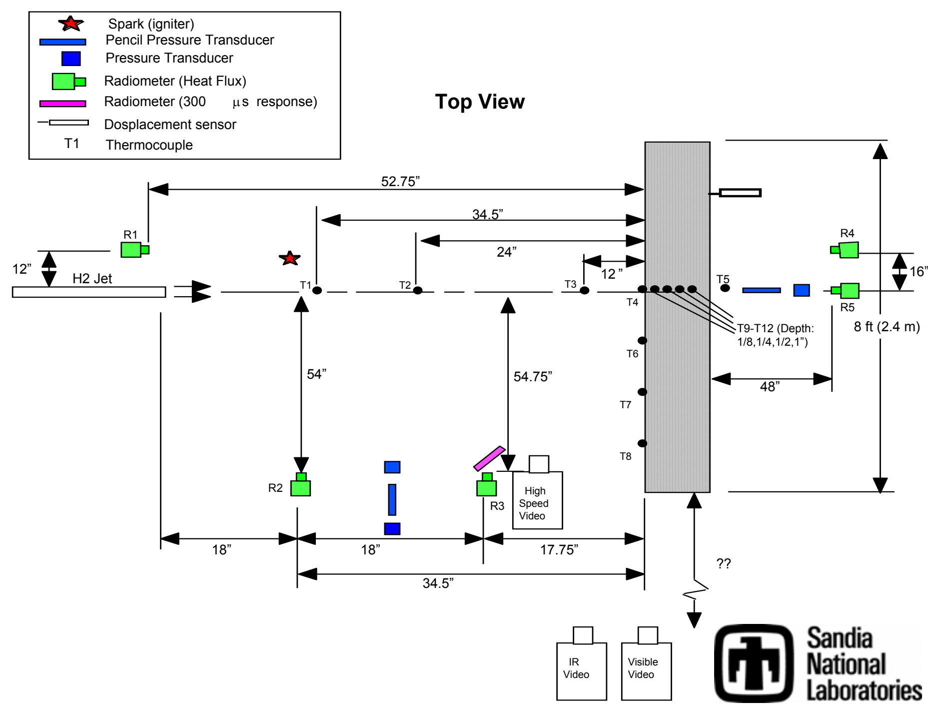
Barrier wall jet flame tests are complete

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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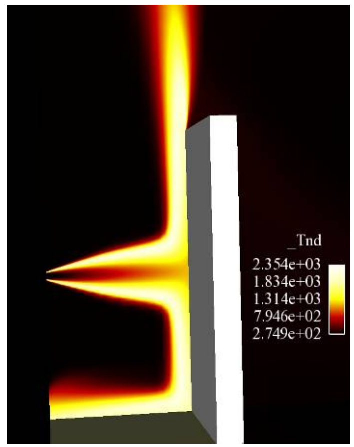
Jet flame simulations have been validated against test data

Jet centerline aligned with center of barrier

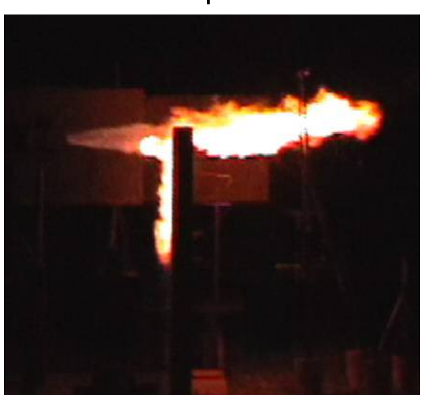
Experiment

Simulation

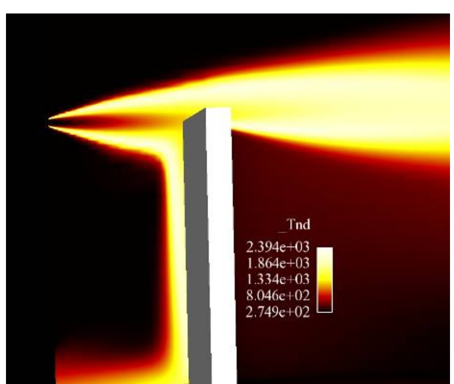


Jet centerline aligned with top of barrier

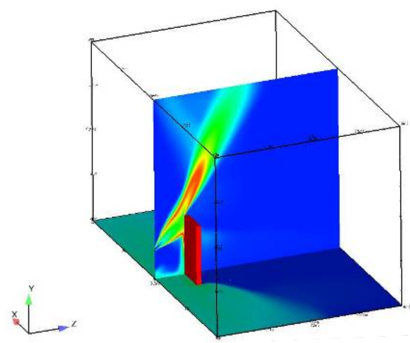
Experiment



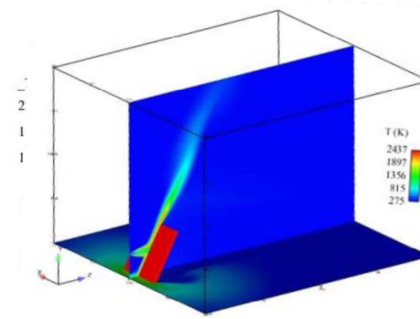
Simulation



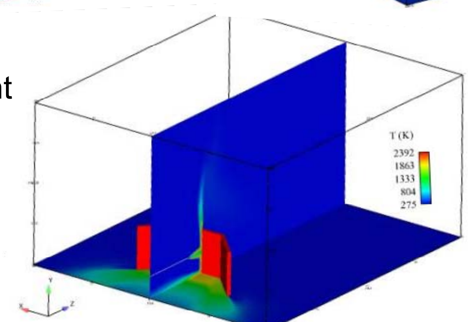
- CFD model captures qualitative trends
- no flame stabilization (hot gas recirc.) behind barrier in top of wall configuration
- flame radiation CFD model required emission model calibration to match test data (modeled emission was too high)



vertical wall
+45º impingement



60º tilted wall



3-wall configuration (135º between walls)

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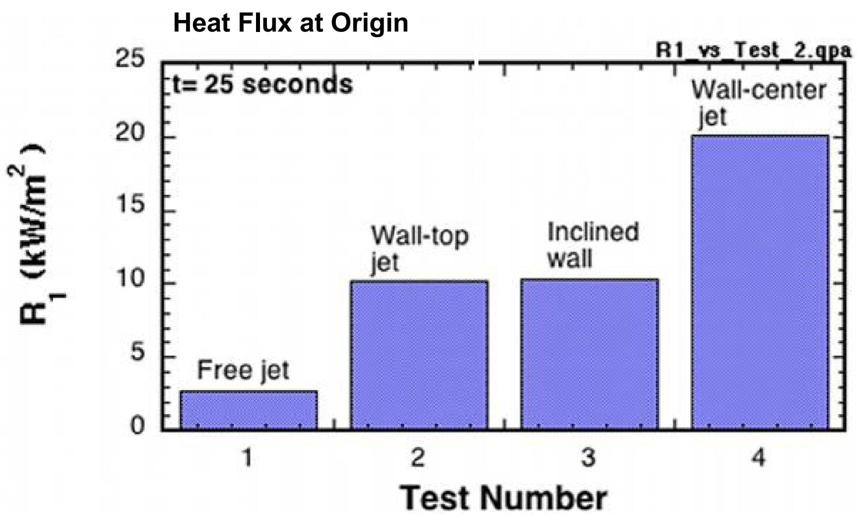
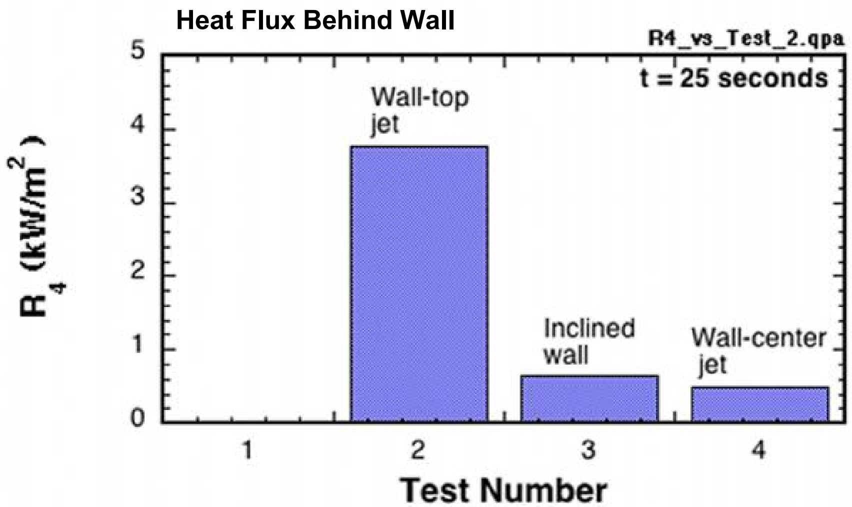
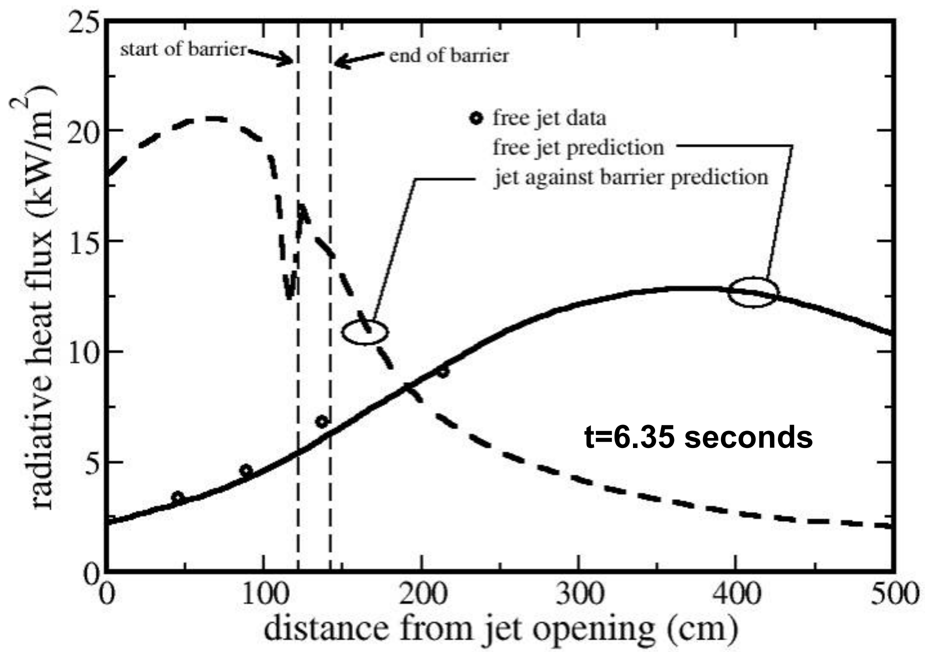
Barrier walls increase front-side thermal exposure





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



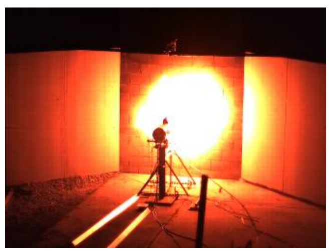
Barrier wall over-pressure mitigation

Frame 1 (t = 137 msec)
Spark ignition

Frame 5 (t = 145 msec)

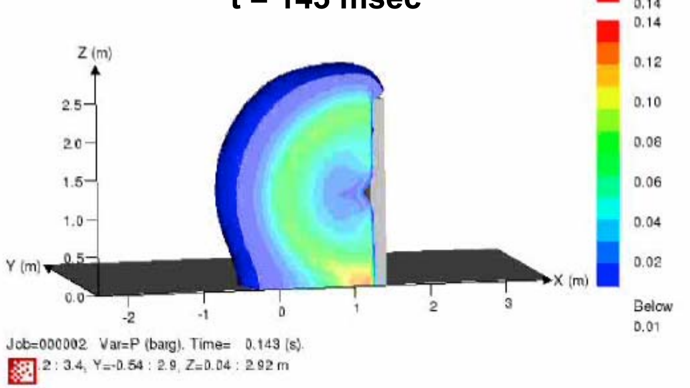
Frame 10 (t = 155 msec)

Frame 15 (t = 165 msec)

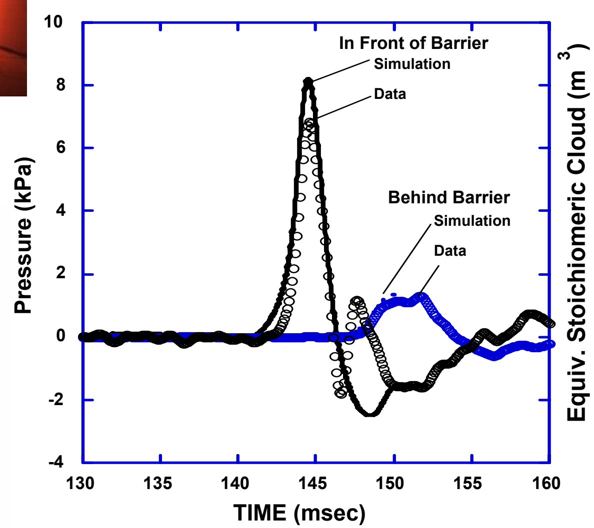


- Barrier wall test parameters:
  - over-pressure on front and back of barrier
  - barrier wall configuration geometry
  - time of release before ignition
  - point of ignition
- Simulations are guiding next set of large-scale experiments (Spring 2008)

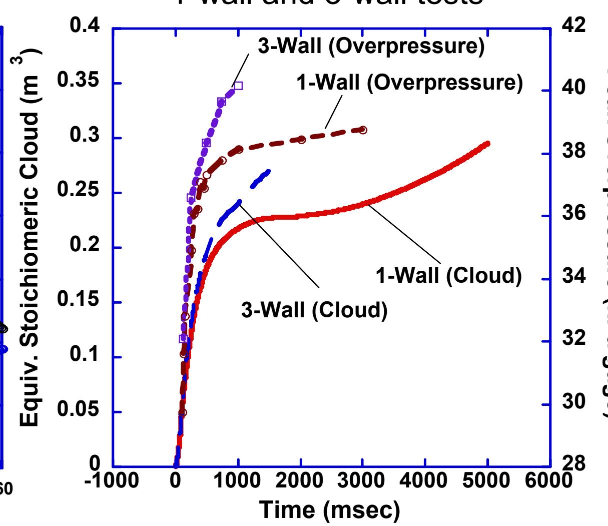
Single Wall Test
Simulation - Overpressure (barg)
t = 143 msec



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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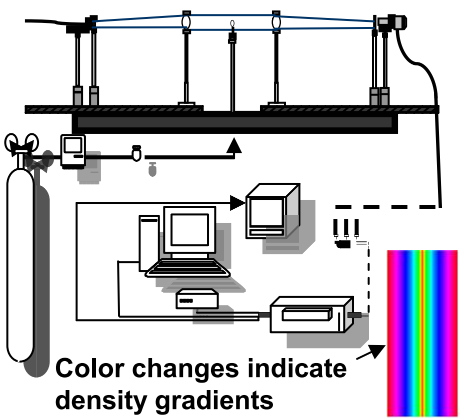
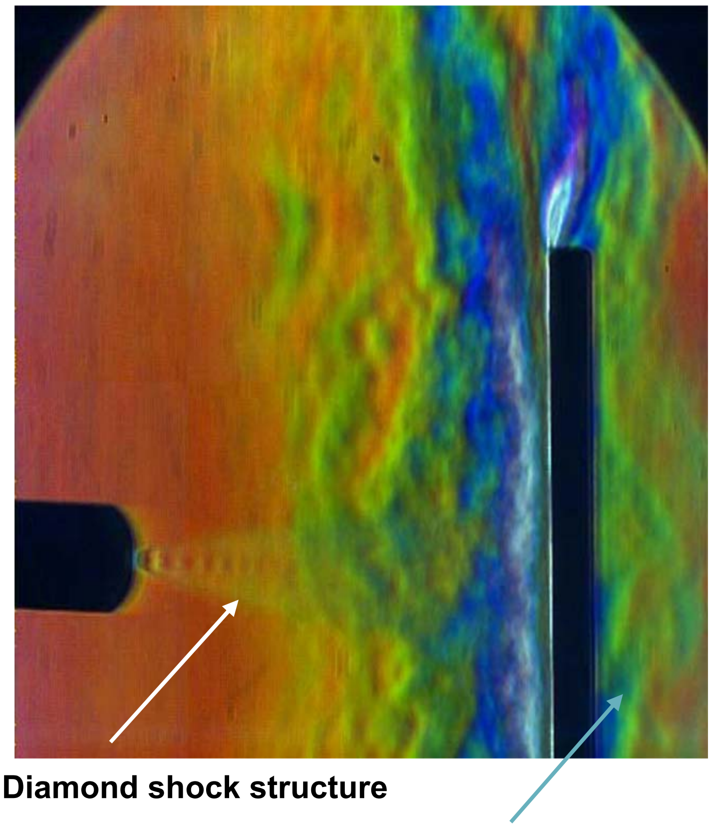
Near-wall concentrations are needed to understand ignition timing

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



Supersonic Helium Jet



- 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

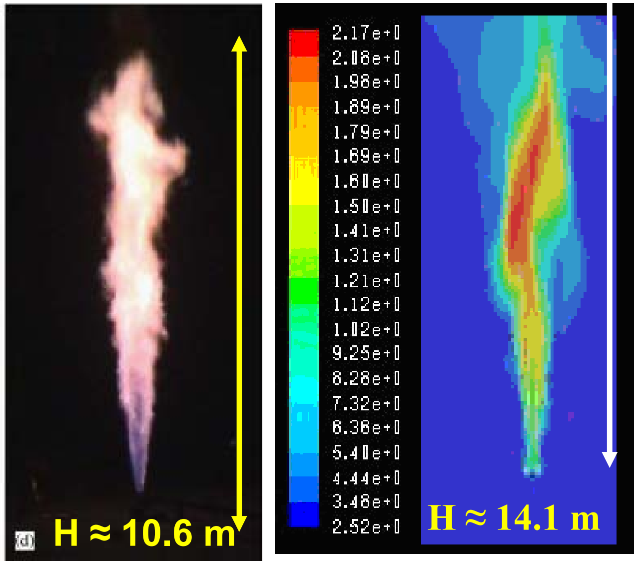
HYPER Project - EU project to create permitting guidance for stationary fuel cells

<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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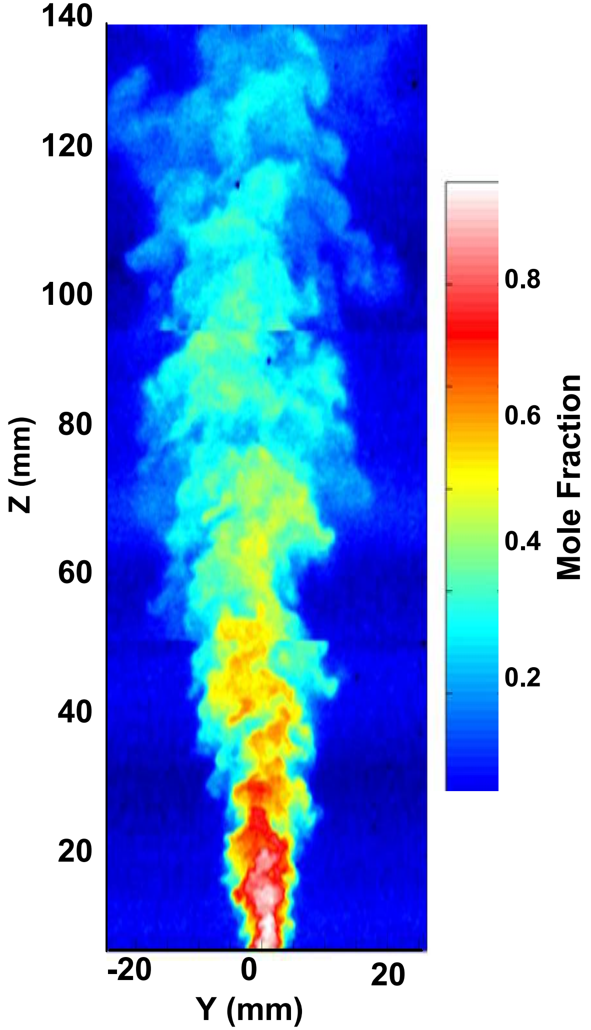
Ignition phenomena



- 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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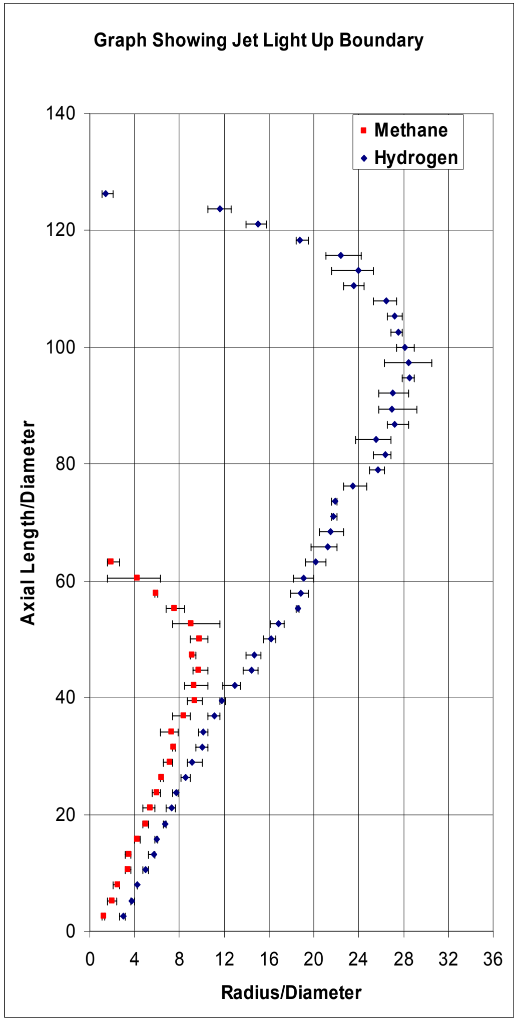
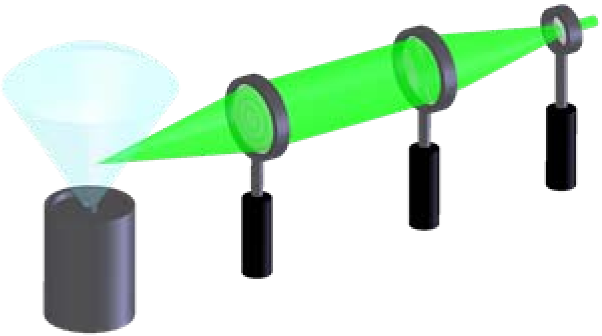
Jet ignition probability measurements





- 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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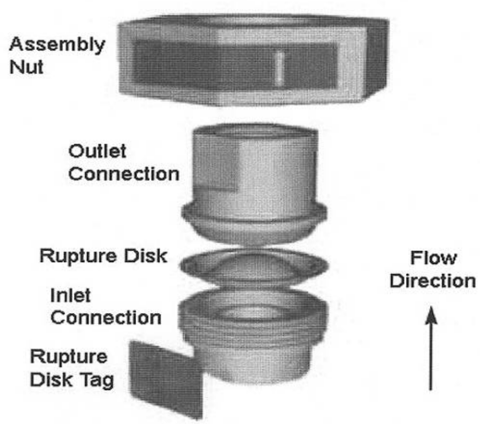
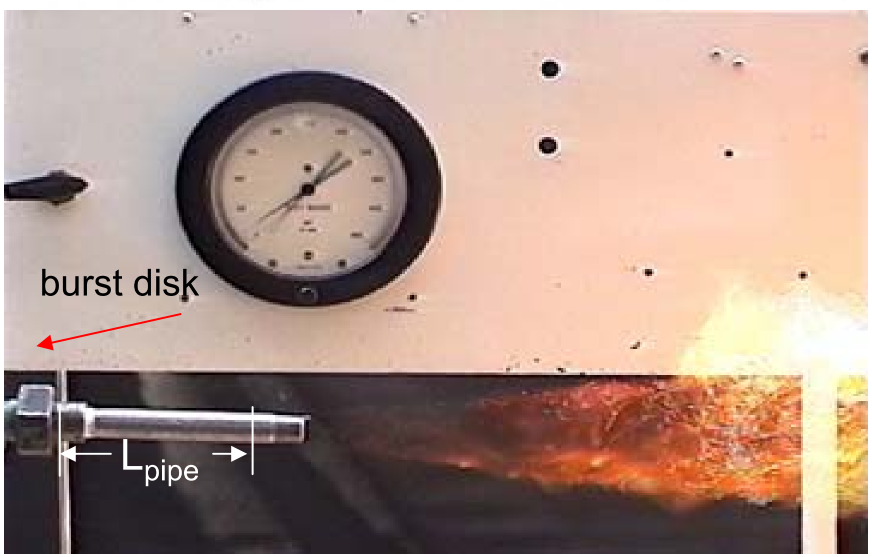
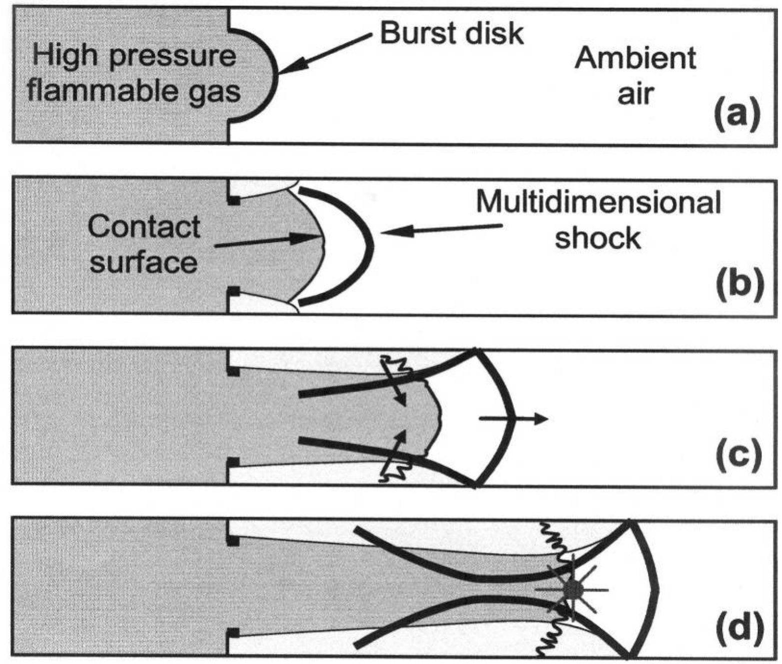
Auto-ignition experiments

Experiments at Princeton University (Prof. Fred Dryer)

In-line Screw Type Burst Disk



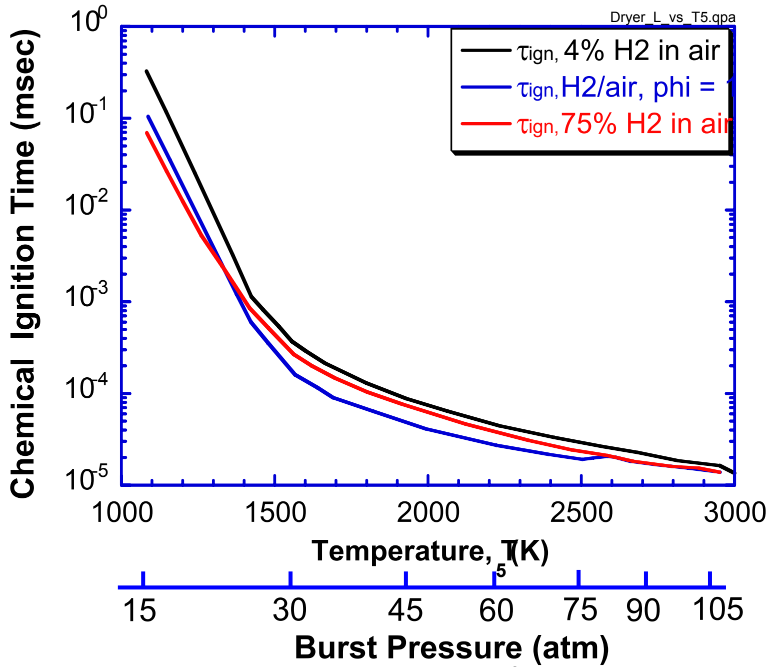




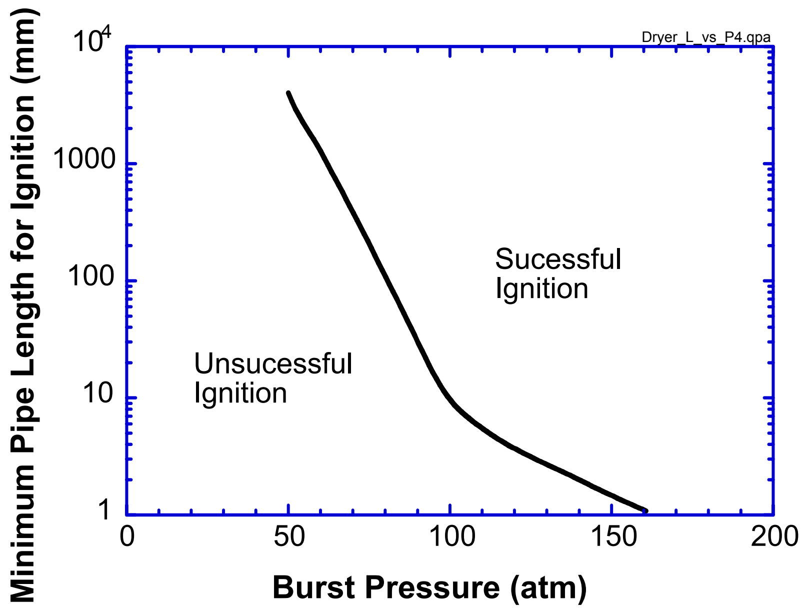
- Consistent ignition occurs for release pressures above 22 atm.
- Speculated ignition due to shock heating of premixed H_2 and air.

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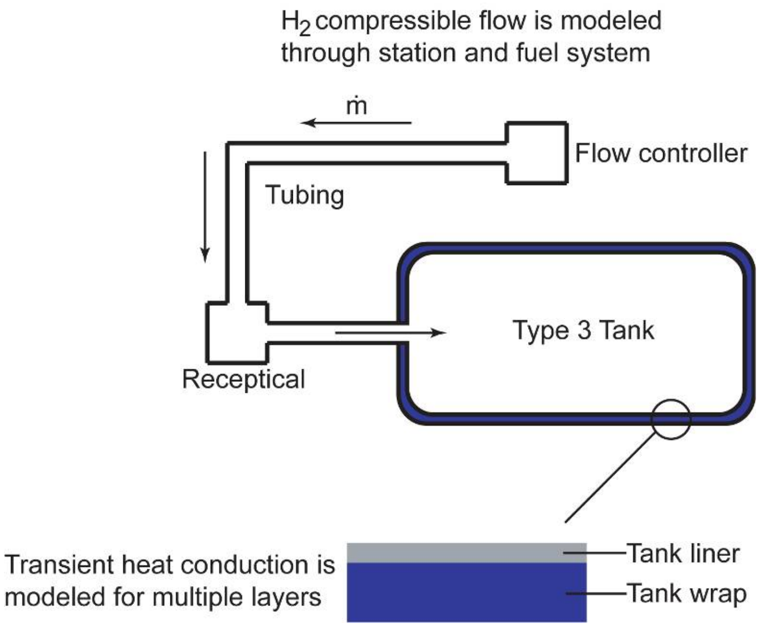
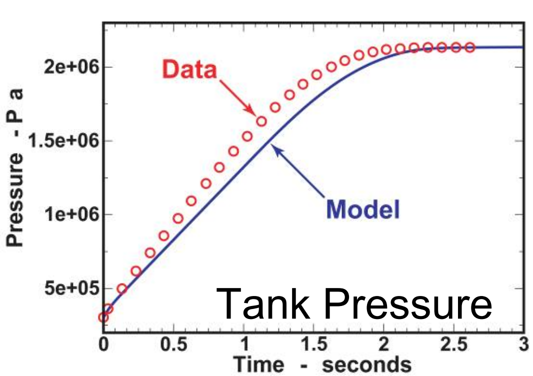
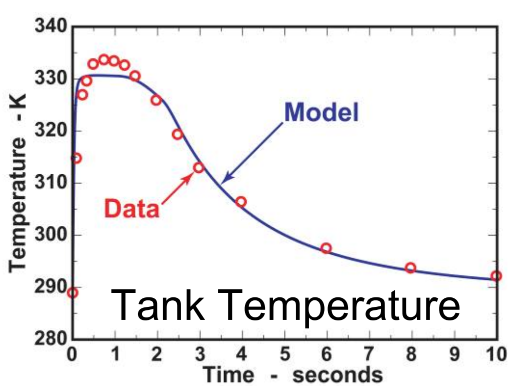
Model-development for the multi-client 70 MPa fast-fill study







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

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.

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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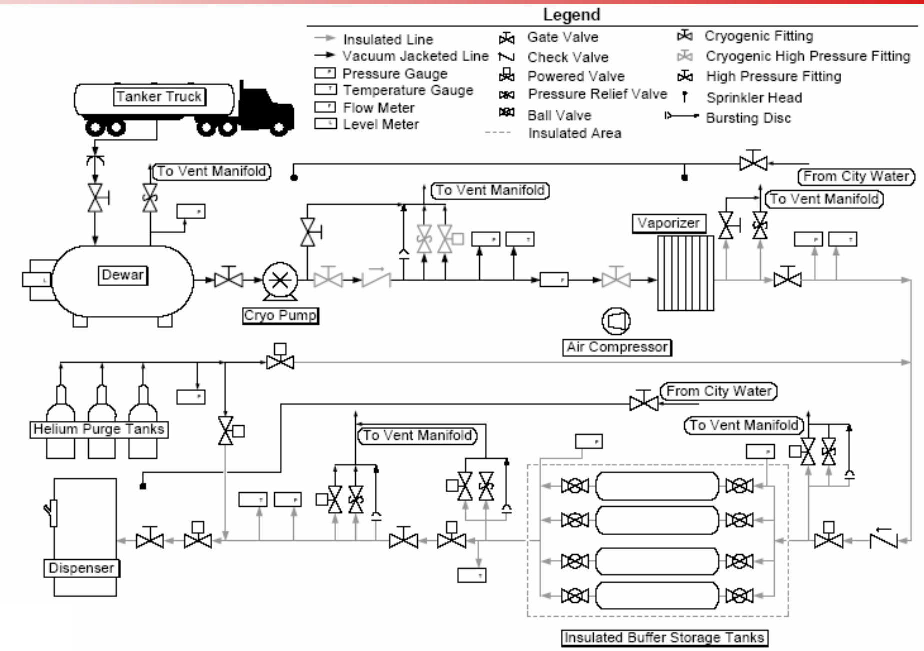
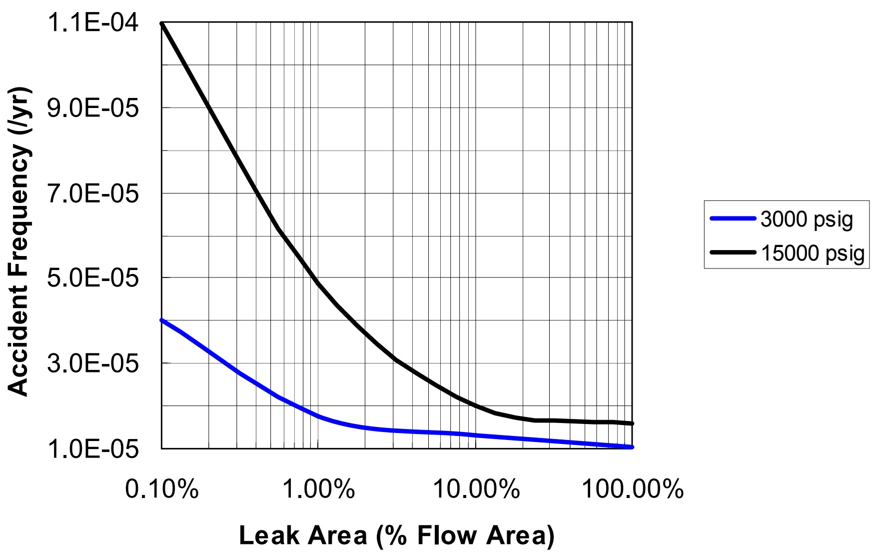
Risk-based fueling station evaluation

- 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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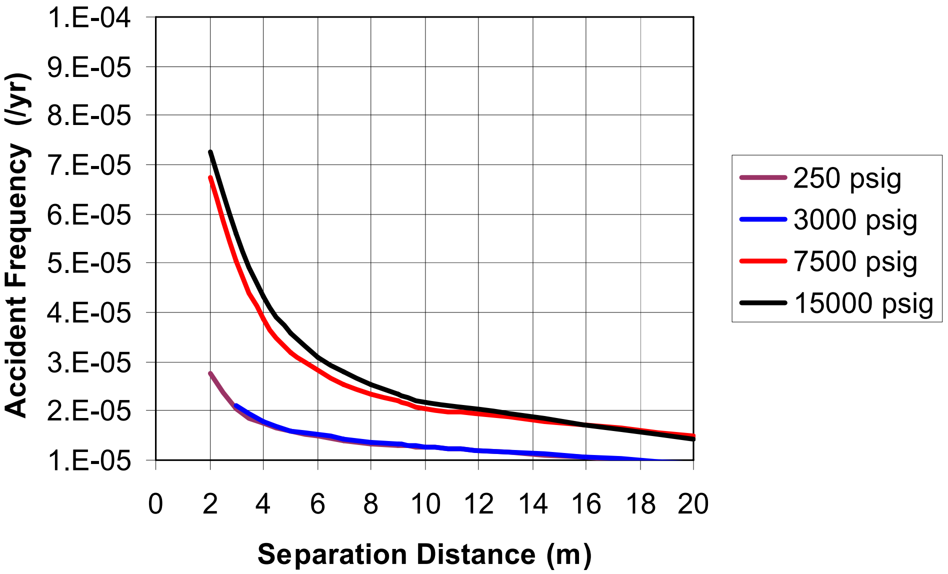
Separation distance technical basis

- 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