

VIII.6 R&D for Safety Codes and Standards: Hydrogen Release Behavior

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Project Start Date: October 1, 2003
Project End Date: Project continuation and direction determined annually by DOE

- Determine ignition and flame-up probabilities
- Quantify thermal radiation and overpressure hazards

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Safety, Codes and Standards section 3.8 of the Fuel Technologies Office Multi-Year Research, Development, and Demonstration Plan:

- (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

Contribution to Achievement of DOE Safety, Codes and Standards Milestones

This project will contribute to achievement of the following DOE milestones from the Hydrogen Safety, Codes and Standards section of the 2011 Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan:

- Milestone 2.7: Provide critical understanding of hydrogen behavior relevant to unintended releases in enclosures. (4Q, 2013)
- Milestone 2.10: Understand flame acceleration leading to transition to detonation. (4Q, 2014)
- Milestone 2.13: Develop and validate simplified predictive engineering models of hydrogen dispersion and ignition. (4Q 2015)

FY 2013 Accomplishments

- Improved confidence identifying the hazard development boundaries for circular aperture unintended releases.
- Performed experiments to examine the dispersion characteristics from non-circular releases.
- Developed layer model for concentration build-up within an enclosure, which uses the previously developed jet integral model as an input and will be the input boundary condition for a steady-state overpressure module within the quantitative risk assessment (QRA) toolkit.
- Improved radiative heat flux boundaries and associated harm prediction from hydrogen jet fires, leading to potential recommendations for reduced separation distances.

Overall Objectives

- Quantify fluid mechanics and combustion behavior of unintended hydrogen releases in support of consequence analysis for safety assessments.
- Perform relevant experiments to validate fluid mechanics and combustion behavior in both controlled laboratory and full-scale, worst-case, representative experiments.
- Support the development of regulations, codes, and standards (RCS) related to the use of hydrogen as a vehicle fuel with presentation of experimental and modeled release and combustion behavior, specific scenario analysis, and expert opinion.

Fiscal Year (FY) 2013 Objectives

- Complete validation of initial set of reduced order models to enable development of quantitative and hazard evaluation tools for high pressure hydrogen unintended releases.
- Conduct experiments to understand dominant release, ignition and combustion phenomena for unintended hydrogen releases for development and revision of RCS and best practices:
 - Support consequence analysis in the “risk informed” approach
 - Model release dynamics from relevant leak scenarios



INTRODUCTION

A principal challenge to the widespread adoption of hydrogen infrastructure is the lack of quantifiable data on its safety envelope and perception of any additional risk from hydrogen. To convince regulatory officials, local fire marshals, fuel suppliers, and the public at large that hydrogen refueling is safe for consumer use, the risk to personnel and bystanders must be quantified and minimized to an acceptable level. Such a task requires validated methods to assess the harm potential from credible failure modes and a good understanding of effective mitigation measures to control any associated hazards.

Understanding release and ignition behavior for hydrogen provides the scientific foundation necessary to perform QRAs—the use of past failures to predict the likelihood of future failures—and thereby estimate the risk of harm from an accident. The hydrogen specific QRA approach is incorporated in the development of model codes and standards to appropriately regulate the retail/commercial use of hydrogen.

Simulations and models, validated with experimental data, are the cornerstone of the hydrogen specific QRA. These simulations and models provide critical input to the overall risk evaluation. While risk is classically defined as the product of frequency and consequences, a more detailed definition, specific to hydrogen hazards, is shown in Equation 1 below. For hydrogen systems, the major hazards involve the release of hydrogen gas with subsequent ignition. Equation 1 characterizes the various factors of risk for ignition of a hydrogen release as a function of probability of a release, probability of ignition given the release type, probability of a hazard given a specific release and ignition type, and finally the probability of harm given the associated hazard. Release behavior models and experiments provide insight to factors (shown in red in Equation 1) for predicting risk.

APPROACH

Using advanced laser-based diagnostics and imaging capabilities in the Turbulent Combustion Lab, Sandia and its partners provide quantifiable data to help accelerate the development of hydrogen fuel infrastructure.

Working with stakeholders Sandia identifies research topics to address research gaps which the science of unintended hydrogen release, ignition, and combustion might close. Research gaps are identified by multiple stakeholders,

for example the U.S. DRIVE Codes and Standards Technical Team Roadmap updated in June 2013, highlighted the need for critical data on unintended releases of liquid hydrogen and cryogenic hydrogen gas. Research topics, such as liquid hydrogen releases, are incorporated into strategic research planning activities.

Sandia developed a 5-year roadmap in 2010 with the explicit goal of addressing short-, medium-, and long-term hydrogen behavior safety research needs. The plan was based on an analysis of the current knowledge base, key SNL contributions to this knowledge base, and critical gaps that serve as barriers to the creation of future standards which can be informed by leveraging unique SNL capabilities. Research topics were divided into five main areas:

1. General release behavior (relevant release geometries, storage states, jet dynamics)
2. Ignition mechanisms (diffusion ignition, electrostatic discharge, conduction)
3. Necessary ignition conditions (minimum ignition energy, mixture ignitability)
4. Necessary flame light-up conditions (ignition characteristics, flow strain rates)
5. Light-up consequences (flame radiation, pressure, flame impingement)

To execute this plan, Sandia recreates representative hydrogen leaks using custom burners and a laser spark apparatus to pinpoint ignition at different locations within the release plume. These capabilities enable statistical characterization of the release plume and insight into phenomenological processes during ignition and transition to sustained flame light-up. Critical data generated in these experiments and the models validated with this data are not explicitly useful to the codes and standards development committees.

To ensure clear comprehension of the scientific results, Sandia works with code development organizations (National Fire Protection Association [NFPA], Canadian Standards Association, etc.) and industry partners or industry groups (such as the Compressed Gas Association). This critical communication effort uses reports, scientific journal articles or conference presentations, and may also directly participate in code development committees or provide presentations to industry partners or industry groups.

The overarching goal of behavior science is the determination of consequences from unintended hydrogen releases. Accurately predicting the consequences of

$$Risk \propto \sum_{i,j,k} P(\text{Release}_i) P(\text{Ignition}_j | \text{Release}_i) P(\text{Hazard}_k | \text{Ignition}_j \cap \text{Release}_i) P(\text{Harm} | \text{Hazard}_k)$$

EQUATION 1. Risk as a function of probability of a release, probability of ignition given a release, probability of a hazard given a release and ignition, and finally the probability of harm given the hazard.

unintended hydrogen release is critical to the development of a comprehensive QRA toolkit that aggregates arbitrary system failure mode analysis with quantifiable consequence modeling. Ultimately this toolkit would be used to improve existing codes and standards as well as provide flexibility in the application of the codes, thus accelerating development of hydrogen fuel infrastructure.

RESULTS

Improved Accuracy of Ignition Conditions

Current analysis techniques used to develop regulations, codes and standards traditionally use the 1% mean concentration boundary, which corresponds to $\frac{1}{4}$ of the hydrogen lower flammability limit, to determine separation distances for electrical equipment, sensor placement, and other ignition sources. The ignition probability boundary, or the boundary where ignition is possible, has been reliably determined based on our recent work and highlighted in Figure 1. This metric is a more suitable approach to be used to by the codes and standards community to define

separation distances based on concerns about proximity to ignition sources. This work has highlighted boundaries based on mean concentration envelopes are overly conservative since the potential for ignition is prohibitively low in a large portion of this boundary. Further measurements of the jet light-up boundary, defined as the region where incipient ignition kernels can transition into sustained flames with true hazard, have revealed additional potential to reduce separation distances further. Analytic determination of this separation boundary remains an ongoing area of research. Understanding the physical behavior in this context provides critical data to the RCS developers and allows them to understand to what degree the regulations are conservative.

Evaluation of Unintended Releases from Non-circular Openings

Most experimental investigations of underexpanded hydrogen jets have been limited to circular nozzles in an attempt to better understand the fundamental jet-exit flow physics and model this behavior with pseudo source models. However, many realistic compressed storage leak exit geometries, such as those from component housing cracks

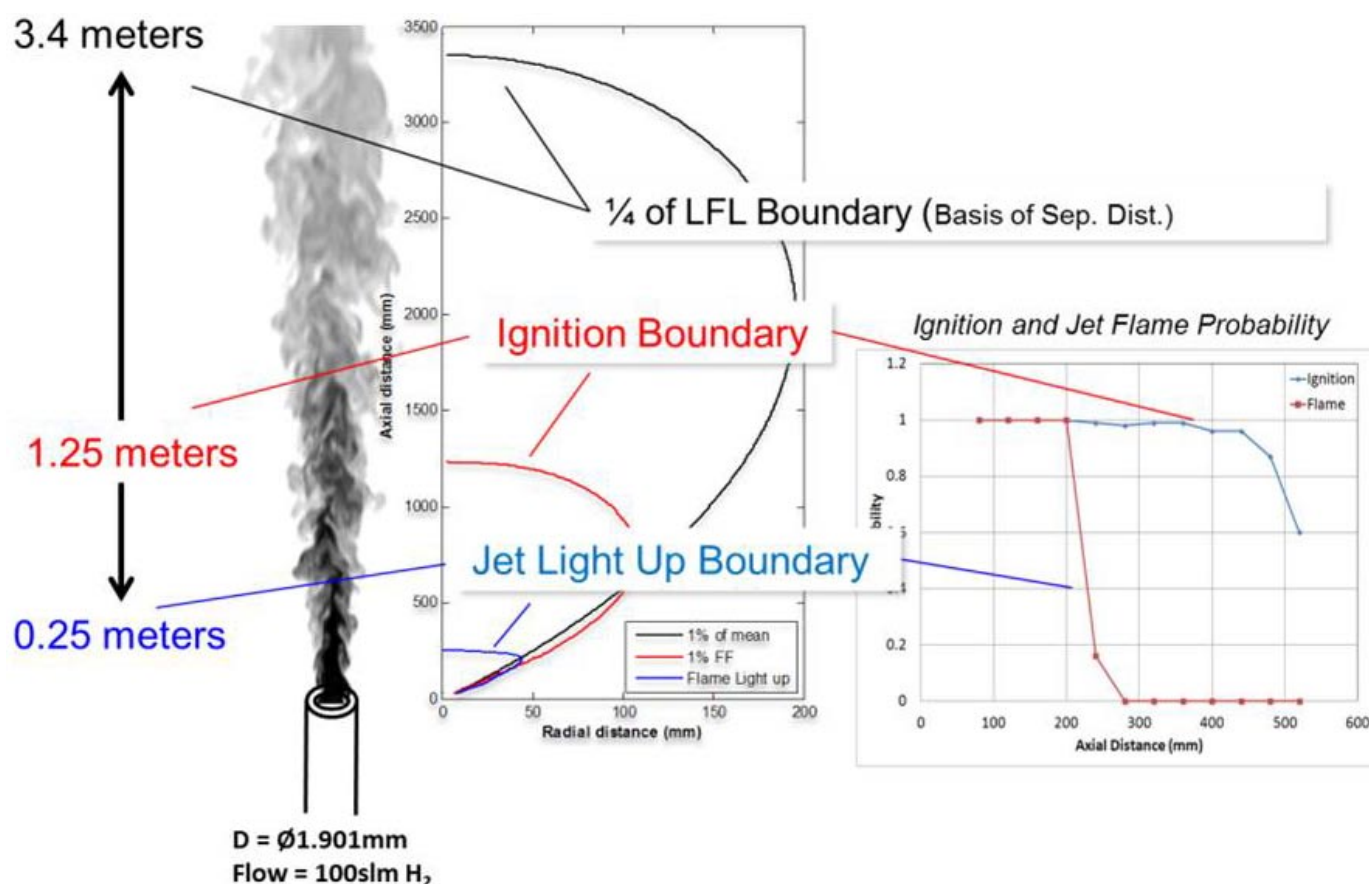


FIGURE 1. Schematic of the measured safety boundaries for a given low pressure release (1.9 mm release diameter, 100 slm flow rate) (1) Traditional Exclusion Zone Boundary: $\frac{1}{4}$ of the lower flammability limit, (2) Ignition Boundary: the envelope where ignition is possible (3) Jet Light-Up Boundary: the envelope where flame sustenance is possible.

or leaky fittings, are not expected to be circular. This past year, jet dispersion characteristics from choked rectangular slot nozzles with aspect ratios from 2 to 8 were investigated and compared with an equivalent circular nozzle. Schlieren imaging was used to observe the jet-exit shock structure

while quantitative planar laser Rayleigh scattering was used to measure downstream dispersion characteristics. The top image of Figure 2 is a Schlieren image of the shock structure from a circular nozzle along with corresponding images from major and minor axes views of a slot nozzle. The

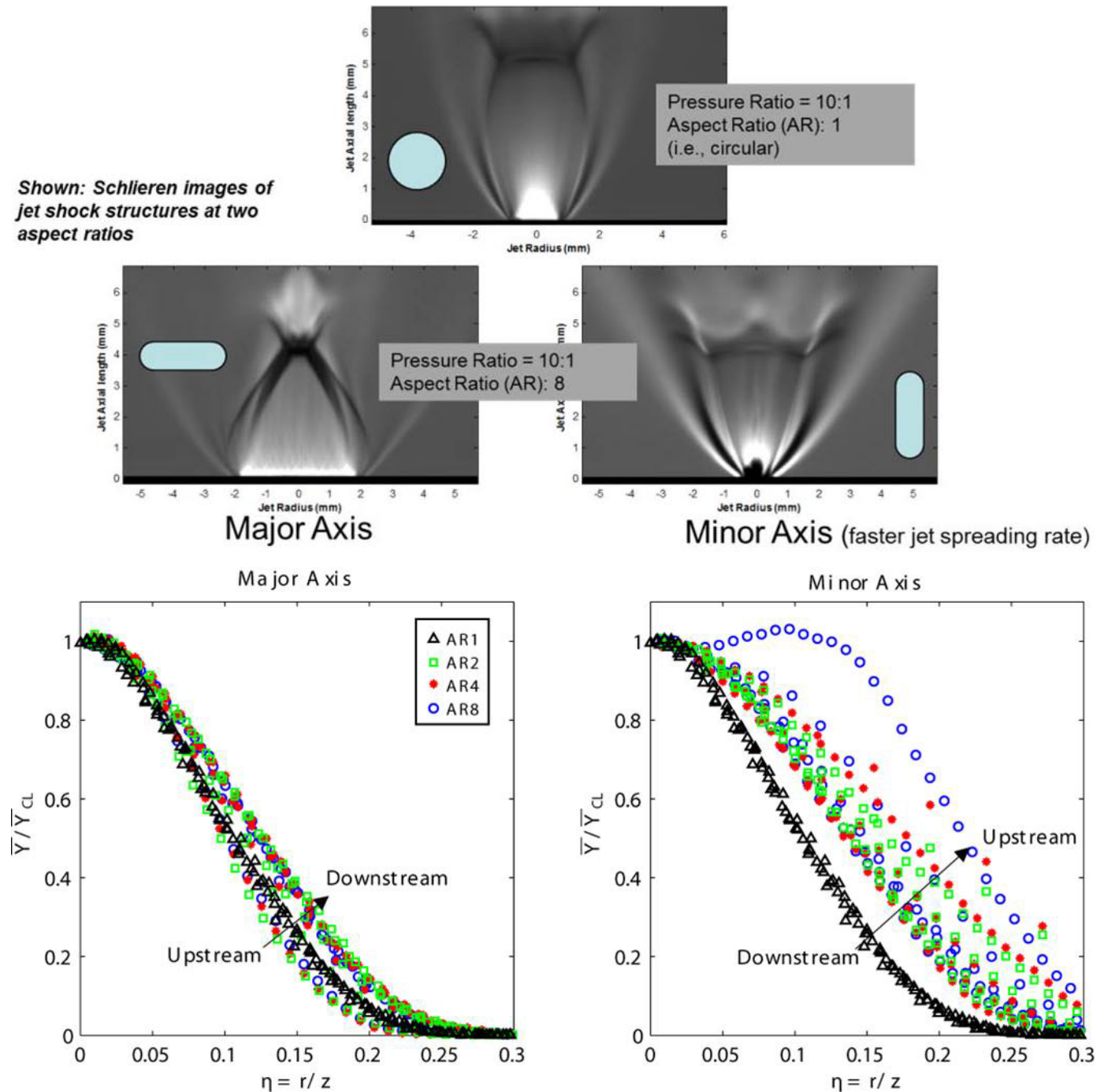


FIGURE 2. Top: Schlieren images of releases with different aspect ratios, with the planar nozzle view indicated by the light blue shape. The top image is of a symmetric circular release, while the bottom two images are of the major and minor axes of a slot nozzle with an aspect ratio of 1:8. These images highlight the asymmetric nature of the shock structure at the release exit for slot nozzles. Bottom: Radial mean mass fraction profiles in the major (left) and minor (right) axes planes for the circular nozzle and three slot jets with respective aspect ratios of 2, 4, and 8 that were extracted at discrete downstream radial locations and were plotted against the non-dimensional radial coordinate, η .

bottom image shows the influence of downstream dispersion characteristics relative to the characteristic circular nozzle. The current QRA method does not account for these differences, which can result in unrealistic predictions for modeled failure modes. These results provide physical insight and much needed model validation data for model development.

Developed Layer Model for Accumulation of Hydrogen from an Unintended Releases

Overpressure hazards can result from two different mechanisms. The first involves the rapid blowdown from a high pressure reservoir within a sufficiently confined volume—ignition is not necessary since a substantial pressure rise is possible from the rapidly expanding gas into the ambient. The second mechanism results from delayed ignition and subsequent development of a deflagration/detonation wave from accumulated flammable gas layers, typically due to slower leaks into larger confined volumes. Prediction of the hazard require accurate modeling of all phenomena related to the hazard, which includes the initial release blowdown and dispersion, the development of an accumulation layer at the ceiling, and (if required) the combustion of this flammable layer. Both hazards take advantage of Sandia developed network flow models, source models, and integral dispersion models. This past year an additional model that predicts the accumulation of gas and

buildup of pressure within a confined space that accounts for passive ventilation (such as a warehouse or repair facility) was developed. At the moment, the developed layer model is only accurate for steady state prediction, but will be improved to accommodate unsteady releases in FY 2014. Furthermore, the layer model output is being used as an input boundary condition for a lean flame deflagration model for hazards that involve ignition of flammable mixture, necessary requirements for developed QRA toolkits.

Improved Flame Radiation Evaluation

Radiative heat fluxes from small to medium-scale hydrogen jet flames (<10 m) compare favorably to theoretical predictions provided the product species thermal emittance and optical flame thickness are corrected for. However, recent heat flux measurements from two large-scale horizontally orientated hydrogen flames (17.4 and 45.9 m) revealed that current methods underpredicted the flame radiant fraction, defined as the radiative energy escaping relative to chemical energy released, by 40% or more. Newly developed weighted source flame radiation models have demonstrated substantial improvement in the heat flux predictions, particularly in the near-field, and allow for a sensible way to correct potential ground surface reflective irradiance. Results depicted in Figure 3 show that inaccuracies in the experimental measurement were partially explained when the model type is changed from a single-point source model (simplified

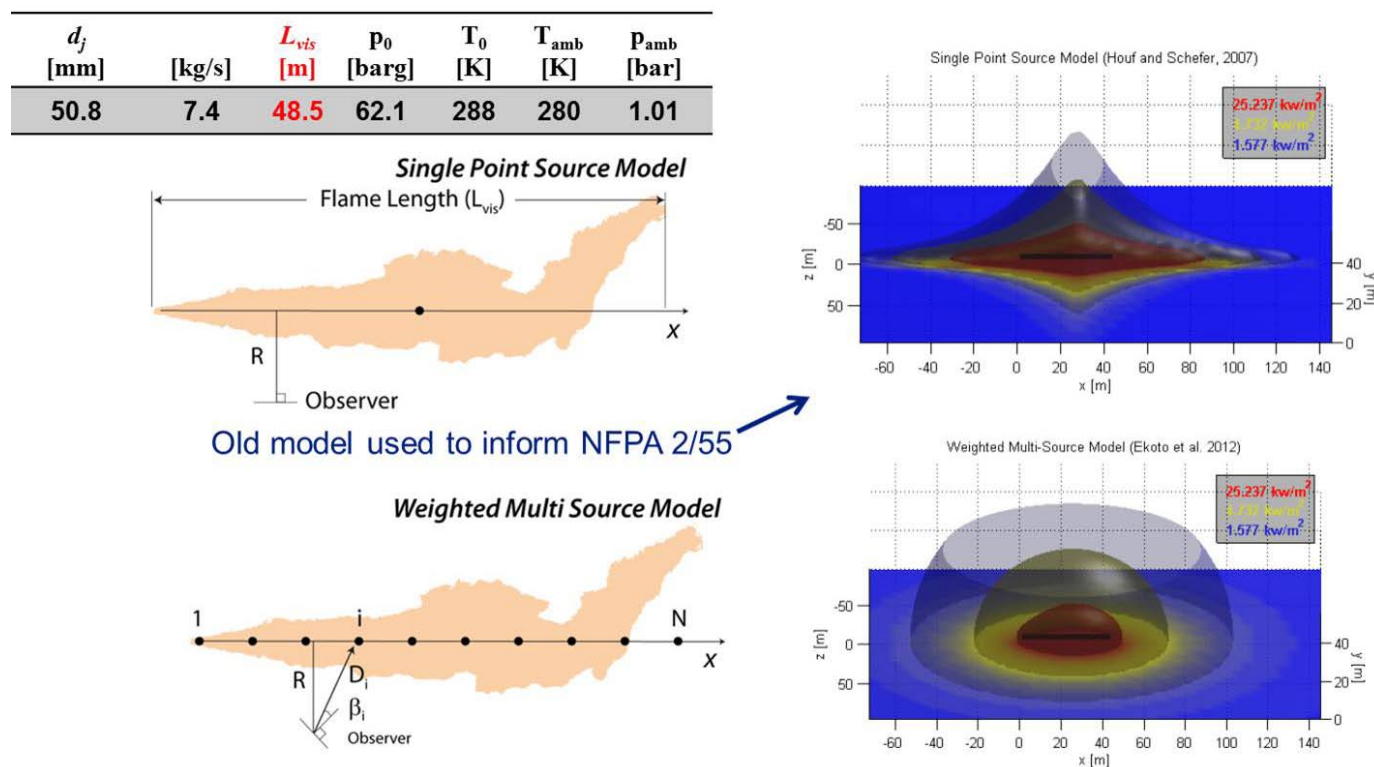


FIGURE 3. Summary of the results for prediction of radiation surface using two model techniques: single-point source model and weighted multi-source model.

radiation model) to a weighted multi-source model. In particular, near-field radiative heat flux predictions (within $\frac{1}{2}$ of the visible flame length) where hazards are greatest had substantially better agreement with the measurements. Additional radiative addition corrections from partially reflective surfaces were developed and found to be potentially large contributors to the overall heat flux budget. Further model improvements are possible if the impact of flame trajectory from wind/buoyancy considerations are incorporated and are under development in FY 2014. Since the single-point source model was previously used to generate scientific justification for fire codes (i.e., NFPA 2) the improved accuracy of the weighted multi-source model can further address commercial barriers within safety, codes, and standards such as separation distances. The next step for this work is interaction with fire code development committees to ensure that they are provided the current scientific understanding of the hazards of hydrogen releases.

CONCLUSIONS AND FUTURE DIRECTIONS

- Conclusion: The jet light-up boundary is finite, predictable and provides a much more accurate prediction of light-up probability than either the lower flammability limit or the ignition boundary.
 - Future work: Fully define the jet light-up boundary and incorporate into prediction tools for QRA.
- Conclusion: Circular nozzles are not sufficient to cover the range of possible realistic release scenarios and it is important to be able to model the downstream characteristics of slot nozzles.
 - Future Work: Fully characterize the effect of higher aspect ratios and determine an appropriate distribution for release shapes to more accurately predict dispersion, ignition and subsequent hazards within QRA.
- Conclusion: Overpressures from hazards within enclosure can be accurately modeled using Sandia developed release, dispersion, accumulation, and deflagration models.
 - Future Work: Continue development on the deflagration combustion model and update the modeling framework to accept non-steady releases. A substantial validation campaign is needed to test the model accuracy and improve where needed.
- Conclusion: The single-point source model is insufficient in prediction of radiation from large flames. A weighted multi-source model shows better prediction capabilities in the near-field where hazards are greatest.
 - Future Work: Provide a brief report on the results of the experiment to NFPA 2 working groups for consideration in the current code revision cycle.

FY 2013 PUBLICATIONS/PRESENTATIONS

1. Ekoto IW, Ruggles AJ, Creitz LW, Li JX, Updated Jet Flame Radiation Modeling with Corrections for Buoyancy, ICHS, (accepted).
2. Ruggles AJ, Ekoto IW, Experimental investigation of nozzle aspect ratio effects on underexpanded hydrogen jet release characteristics, ICHS, (accepted).
3. Ruggles AJ, Ekoto IW, Radial probability density function characterization for self-similar turbulent hydrogen jets, J Fluid Mech, (submitted).
4. Houf WG, Evans GH, Ekoto IW, Merilo EG, Groethe MA, Hydrogen fuel-cell forklift vehicle releases in enclosed spaces. Int J Hydrogen Energy, 2013;39:8179-89.
5. Ekoto IW, Houf WG, Evans GH, Merilo EG, Groethe MA, Experimental investigation of hydrogen release and ignition from fuel cell powered forklifts in enclosed spaces. Int J Hydrogen Energy, 2012;37:17446-56.
6. Ruggles AJ, Ekoto IW, Ignitability and mixing of underexpanded hydrogen jets. Int J Hydrogen Energy, 2012;37:17549-60.
7. Ekoto, IW, R&D Needs for Reduced Order H2 Release/Ignition Behavior Models - The Sandia Perspective, HySafe Research Priorities Workshop , BAM, Berlin, Oct 16, 17, 2012.
8. Ekoto, IW, Large Scale Flame Radiation Modeling, IEA Experts Meeting, BAM, Berlin, Oct 4, 5, 2012.
9. Ekoto IW, Houf WG, Ruggles AJ, Creitz LW, Li JX, Large-Scale Hydrogen Jet Flame Radiant Fraction Measurements and Modeling. Proc International Pipeline Conference, Calgary, Canada, Sept 24-28, 2012.