R&D for Safety Codes and Standards: Hydrogen Behavior

Sandia National Laboratories

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DOE EERE FCT Annual Merit Review
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Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000
Overview

Timeline
- Project start date: Oct. 2003
- Project end date: Sept. 2015
- Percent complete: 80%

Barriers (2012 MYRD&D)
- 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
- Total project funding (to date)
  - DOE share: $15.4M ($13.6M)*
- FY11 Funding: $1.3M ($1.2M*)
- Planned Funding in FY12: $0.8M ($0.7M*)

*(R&D core, no IEA contracts)

Partners
Industry: Air Products, Lincoln Composites, HIPOC, FCHEA, CTFCA, SRI
Govt: NREL, CSTT, NIST, PNNL
SDO/CDO: NFPA, ICC, ISO, CSA, SAE, ASME
International: IEA, Longitude 122 West, HYPER, HySAFE, IPHE, I2CNER
Coordinate 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, GTR)
- International Standards (eg. ISO)
- International Agreements (IEA, IPHE)

Metrics for Success
- Number of codes, standards, regulations impacted
- Degree of harmonization
Risk conventionally defined as: **Frequency × Consequences**

A more detailed definition relates **harm probability** to **accident occurrence** as:

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

- Large potential permutations that strongly depend on release scenarios
- Assignment solely from incident statistics is prohibitive

Terms currently approximated through the use of lookup tables, e.g.,

**Hydrogen Ignition Probabilities**

<table>
<thead>
<tr>
<th>Tchouelev</th>
<th>HYSAFE</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Hydrogen Release Rate [kg/s]</strong></td>
<td><strong>Immediate Ignition Probability</strong></td>
</tr>
<tr>
<td>&lt;0.125</td>
<td>0.008</td>
</tr>
<tr>
<td>0.125-6.25</td>
<td>0.053</td>
</tr>
<tr>
<td>&gt;6.25</td>
<td>0.23</td>
</tr>
<tr>
<td>&gt;10</td>
<td></td>
</tr>
</tbody>
</table>

**However:**
- Other factors control ignition probability (e.g., flow velocity, ignition mechanisms, mixing)
- Ignition does not have uniform hazard criteria
- No insight into risk reduction strategies possible

**Deterministic modeling enhances probability quantification & provides physical insight for focused risk reduction strategies.**

\[ P(A|B \cap C) \] is the conditional probability that event A occurs for given events B and C.
Objectives:

SNL R&D for H₂ Safety, Codes & Standards (SCS)

Develop Science Basis for H₂ SCS
- Risk-Informed R&D
- Hydrogen Effects in Structural Materials
- Hydrogen Behavior
  - Fast fill experiments/modeling
    - Validation experiments for SAEJ2601 fill protocols
  - Release & ignition experiments/modeling
    - Choked flow dispersion model development
    - Qualitative high-speed flame ignition imaging
    - Flame light-up engineering model development
  - Validated consequence modeling
    - Large-scale jet flame radiation analysis

Harmonize H₂ SCS Development
- Consequence & Risk:
  - Participation in: HIPOC, ISO, NFPA, ICC
- International Engagement:
  - Participation in: ISO, IEA, SAE, IPHE, GTR, H2CAN

Standards advocacy ensures transfer of science-based H₂ SCS knowledge to code development committees.
Fast Fill Modeling

Terry Johnson (PI)
SNL
Experiments

Jianjun Ye
Zhejiang University, PRC
CFD Modeling

Partners and Collaborators:
Lincoln Composites and Zhejiang University, PRC
We seek to develop validation databases through H₂ fast-fill experiments at specified and relevant pressure ramp rates with measurements of:

- Transient gas tank pressure and mass-averaged tank temperature
- Total hydrogen gas enthalpy and mass flow rate entering the tank
- Final uniform tank temperature/pressure after the fill

- Tank and gas temperatures measured at discrete locations
  - 4 tank wall measurements, each at 4 depths
  - 5 gas temperature measurements
- Inlet & closed end pressure measurement
- Infrared tank exterior temperature imaging
Accomplishments:
- Initial fill and release data collected for model validation

Experimental Results

<table>
<thead>
<tr>
<th>Test #</th>
<th>Initial pressure (psi)</th>
<th>Final pressure (psi)</th>
<th>Fill time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20</td>
<td>1500</td>
<td>60</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>1500</td>
<td>90</td>
</tr>
<tr>
<td>3</td>
<td>20</td>
<td>1500</td>
<td>150</td>
</tr>
<tr>
<td>4</td>
<td>20</td>
<td>1500</td>
<td>300</td>
</tr>
<tr>
<td>5</td>
<td>20</td>
<td>1000</td>
<td>90</td>
</tr>
<tr>
<td>6</td>
<td>20</td>
<td>2000</td>
<td>90</td>
</tr>
<tr>
<td>7</td>
<td>145</td>
<td>2000</td>
<td>90</td>
</tr>
<tr>
<td>8</td>
<td>290</td>
<td>2000</td>
<td>90</td>
</tr>
<tr>
<td>9</td>
<td>725</td>
<td>2000</td>
<td>90</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Test #</th>
<th>Initial pressure (psi)</th>
<th>Final pressure (psi)</th>
<th>Release rate (g/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1300</td>
<td>20</td>
<td>1.5</td>
</tr>
<tr>
<td>2</td>
<td>1300</td>
<td>20</td>
<td>0.75</td>
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<td>3</td>
<td>1300</td>
<td>20</td>
<td>1.0</td>
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<td>4</td>
<td>1300</td>
<td>20</td>
<td>1.9</td>
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<td>5</td>
<td>1700</td>
<td>20</td>
<td>0.4</td>
</tr>
<tr>
<td>6</td>
<td>1700</td>
<td>20</td>
<td>1.5</td>
</tr>
<tr>
<td>7</td>
<td>1700</td>
<td>20</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Model Results:
- Model completed, currently in validation
- Goal: results available for SAE Interface Group (J2601) discussion; Sept 2012
- Goal: Comparison with other research and industrial datasets in support of 2015 vehicle deployment
Broad Approach to Risk Reduction

Risk, as defined in the objectives, is quantified by coupling validated physical modeling with stochastic scenario frequencies.

Dispersion
- Permeation
- Buoyant creeping flow
- **Turbulent jet**
- Volumetric rupture

Ignition
- Ignition mechanism
- **Mixture ignitability**
- Ignition delay/location
- Sustained light-up

Hazard
- **Flame radiation**
- Overpressure (deflagration/detonation)
- $O_2$ dilution/depletion

Harm
- Burns
- Lung damage
- Shrapnel wounds
- Building collapse

FY12 Research Activities
Stochastic scenario frequencies: incident data, environmental/human factors, system design/mitigation

SNL H₂ SCS R&D

Risk

SNL National Laboratories
Fundamental Hydrogen Release Behavior

Isaac Ekoto (PI)
*SNL*
Experiments

Adam Ruggles
*SNL*
Experiments

**Partners and Collaborators:**
Université du Québec à Trois-Rivières (CAN)
Scalar field of a momentum driven, turbulent $\text{H}_2$ jet was examined via high-resolution Planar Rayleigh Scatter Imaging (PLRS).

**PIXIS 400B low noise CCD Camera**
- 2 x 2 binning for 3.94 pix/mm resolution
- ~400:1 signal-to-noise
- 5 interrogation regions (37 x 125 mm$^2$)
- 400 images per interrogation region

$r_0 = 0.95 \text{ mm}$
$L_{\text{pipe}} = 250 \text{ mm}$
$Q = 100 \text{ lit/min}$
$Fr_{\text{den}} = 1170$

Air co-flow & barriers to minimize impact of room currents

High power injection seeded ND: Yag laser (1 J/pulse, 532 nm)

Additional diagnostics include Particle Image velocimetry (PIV), Laser Doppler Velocimetry (LDV) and OH Laser Induced Fluorescence (LIF).
Radial statistics collapse when plotted against normalized radial coordinates.

\[ \bar{Y} = f(\bar{Y}_{CL}, \eta); Y' = g(\bar{Y}_{CL}, \eta) \]

Where,

\[ \eta = \frac{r^*}{(r-z_{0j})}; \text{ normalized radial coordinate} \]
\[ z_{0j}: \text{ momentum virtual origin} \]

Richards and Pitts, 1993

- Collapsed statistics slightly deviate from traditional models, which impact ignitability predictions embedded in QRA models

Non-linear correlation observed between intermittency and the ratio of the 1\textsuperscript{st} and 2\textsuperscript{nd} statistical moments.
- Contradicts linear relationship often assumed in CFD modeling approaches
- Results impact PDF distribution prediction

- A more suitable intermittency correlating parameter is based on the ratio of conditioned and non-conditioned mean statistics
- Intermittency likewise influences ignitability predictions in QRA models
Mixture Ignitability

- Mixture ignitability is a function of the mass fraction distribution (PDF) and jet intermittency.
- PDF is commonly reconstructed from Beta function distributions.

$$P_C(Y_{H2}) = \frac{Y_{H2}^{\alpha-1}(1-Y_{H2})^{\beta-1}}{B(\alpha, \beta)}, \text{ where } \bar{Y} = \frac{\alpha}{\alpha+\beta}, \text{ and } \bar{Y}'\bar{Y}' = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$$

Conditioned probability that neglects $\gamma = 0$ values

- Skewness & Kurtosis are measures of the goodness of measured to modeled PDFs
- Beta fit often worse than a Gaussian fit

Created benchmark data to evaluate optimum distribution functions, that are used to model mixture ignitability
High-Source Pressure Hydrogen Release Behavior

Isaac Ekoto (PI)  Adam Ruggles
SNL  SNL
Experiments  Experiments

Partners and Collaborators:
Commissariat à l’Energie Atomique (FR)
Joint Research Centre (NL)
Choked Flow Releases

- Notional nozzle models represent complex underexpanded jet shock structure with an equivalent jet exit diameter.

### Notional Nozzle Models

<table>
<thead>
<tr>
<th>Model</th>
<th>Conservation Equations</th>
<th>Critical Assumptions</th>
</tr>
</thead>
</table>
| Birch et al. (1984) Ruggles & Ekoto (2012)† | X | T₂ = T₀  
| Ewan & Moodie (1986) Ruggles & Ekoto (2012)† | X | T₂ = T₁  
| Molkov (2008) | X | V₂ = sonic  
| Birch et al. (1987) Schefer et al. (2007)† | X | T₂ = T₀  

† Original model updated with Abel-Noble hydrogen equation of state:

\[ p = ZρRH₂T; \quad Z = (1 - bρ)^{-1} \]

s₀: stagnation conditions

Validation datasets are still needed
Accomplishment:

Notional Nozzle Concept Validated

\[
\frac{p_0}{p} = 10; \\
d_{\text{jet}} = 1.5 \text{ mm}
\]

Constant centerline decay, jet spreading, and unmixedness observed.

Mass weighted effective diameter 
\[
d^* = d_{\text{eff}} \sqrt{\frac{\rho_{\text{eff}}}{\rho_{\text{air}}}}
\]
fit to the data so that mass fraction decay rates matched incompressible values.

Radial statistics collapsed when measured \(d^*\) was used to normalize radial coordinates.

- Acquired benchmark \(d^*\) values for validation of current notional nozzle models and facilitate development future model
- Notional Nozzle models are integral to dispersion predictions from QRA models that inform NFPA 2 code development
Sustained Light-Up Probability

Isaac Ekoto (PI)  
*SNL*  
Experiments

Adam Ruggles  
*SNL*  
Experiments

Partners and Collaborators:
Flame light-up: Mixture ignitability is a necessary but insufficient criterion

Two possible pathways from ignition kernel development:

- Laser Spark
- Kernel Growth
- Light-up
- Extinction

Test Case:
1.91 mm tube (unchoked)
100 lit/min flow rate

Determined flame light-up boundaries from localized ignition sources e.g., ESD ignition

Schefer et al., 2011

Ignitability Probability
Light-up Probability
High-speed flame ignition imaging elucidates sustained light-up mechanisms. Imaging observations indicate sustained flame light-up correlates with 1D flame front propagation speeds.

Rapid volumetric ignition kernel growth
Kernel forms into turbulent flame front
Flame front broadens
Front **overcomes** flow convection

Ignition w/ light-up

Ignition w/o light-up

Slower kernel growth
Thinner, less turbulent flame front
Front **overcome** by convection
Flame Radiation

Isaac Ekoto (PI)  
SNL  
Experiments

Adam Ruggles  
SNL  
Experiments

Partners and Collaborators:  
Air Products and Chemicals Inc.
H₂ Flame radiation significantly lower than corresponding HC flames.

\[
X_{rad} = \frac{S_{rad}}{m_{fuel} \Delta H_c} \times \frac{W_f^2 L_f y_s}{m_{fuel}}
\]

Where:
- \(X_{rad}\) = radiant fraction
- \(S_{rad}\) = surface emissive power
- \(\Delta H_c\) = heat of combustion
- \(m_{fuel}\) = fuel mass flow rate
- \(W_f\) = flame width/length
- \(L_f\) = flame residence time
- \(y_s\) = stoichiometric mixture fraction

Turns & Myhr, (1991)

Previously Accomplished:
- Radiation Experiments

H₂ lab
H₂ T#1
H₂ T#2
H₂ T#3
CH₄ Turns & Myhr
CH₄ lab
CO/H₂ Turns & Myhr

Universal correlation developed for small & mid-sized flames, regardless of fuel gas type, where:

\[
S_{rad} \propto a_p T_f^4 \tau_f
\]

- \(a_p\) = plank-mean absorption
- \(T_f\) = adiabatic flame temperature

Molina et. al, (2007)

Does developed correlation hold for larger scale hydrogen jet flames?

Does not account for absorption differences!
Accomplishment:

✓ Worked with industrial partner to apply SNL flame radiation models to understand large-scale flame radiation behavior

<table>
<thead>
<tr>
<th>Jet</th>
<th>$d_j$ [mm]</th>
<th>$L_j$ [m]</th>
<th>$p_0$ [barg]</th>
<th>$T_0$ [K]</th>
<th>RH [%]</th>
<th>$T_{amb}$ [K]</th>
<th>$p_{amb}$ [mbar]</th>
<th>$U_{wind}$ [m/s]</th>
<th>$\theta$ [°]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20.9</td>
<td>17.4</td>
<td>59.8</td>
<td>308.7</td>
<td>94.3</td>
<td>280</td>
<td>1022</td>
<td>2.84</td>
<td>68.5</td>
</tr>
<tr>
<td>2</td>
<td>52.5</td>
<td>48.5</td>
<td>62.1</td>
<td>287.8</td>
<td>94.5</td>
<td>280</td>
<td>1011</td>
<td>0.83</td>
<td>34.0</td>
</tr>
</tbody>
</table>

Measurements performed by Advantica (2008)

Measured heat fluxes ~40% higher than predicted values
Collaborations:

International and Industry R&D Collaborations

General release, ignition, and light-up phenomena for non-buoyant $\text{H}_2$ leaks

Pierre Benard & Boris Chernyavsky, Université du Québec à Trois-Rivières, Canada
- Detailed Large Eddy Simulations (LES) used to elucidate fundamental release behavior and relevant ignition and light-up mechanisms. (IEA, IPHE, ISO and NFPA)

Characterization of near-nozzle shockwave behavior and compressible shear layer growth from compressed $\text{H}_2$ releases

Sergey Kudriakov & Alexey Velikorodny, Commissariat à l’Energie Atomique (CEA), France
- Detailed LES to model the interplay between complex shockwave and flow phenomena (e.g., Görtler vortices in the barrel shock) from high source pressure releases. (IEA, IPHE, ISO and NFPA)

Reduced order modeling of complex $\text{H}_2$ release phenomena

Daniele Baraldi, Joint Research Centre (JRC), Netherlands
- Reduced order simulations (i.e., 2-equation Reynolds Averaged Navier-Stokes turbulence modeling) of compressed $\text{H}_2$ leaks that rely on validated notional nozzle models for jet-exit boundary conditions. (IEA, IPHE, ISO, NFPA and Industry Hazard Analysis)

Large-scale flame radiation measurements and modeling

Jimmy Li & Leonard Creitz, Air Products and Chemicals Inc., Allentown PA
- Evaluation and improvement of current radiative heat flux predictive methodologies for large-scale hydrogen jet flames. (ISO, NFPA and Industry Hazard Analysis)

Multidimensional modeling of Type IV fast-fill

Jianjun Ye, Institute of Process Equipment, Zhejiang University, P. R. China
- Multidimensional modeling of SNL fast fill experiments to validate fill model protocol development (GTR, ISO TC 197, SAE J2601, and CSA HGV 4.3).
H2CAN/Sandia collaboration on Hydrogen Safety

- Sandia hosted hydrogen safety workshop - April 11-12
- Workshop Goal: Coordinate hydrogen safety efforts between H2CAN and US Programs

- Strong alignment of efforts identified at ICHS hosted by Sandia in Sept 2011
- Further reinforced by IEA Task 31 meeting in Jan 2012
  - Identified several near-term risk and behavior collaborative topics
  - Research roadmap presented during IEA Task 31 meeting – April 2012
Future Work

• FY12
  – Acquire fundamental turbulent diffusivity measurements for **unreacting** flow fields to support flame light up model development
  – Work with NFPA 2 to finalize indoor refueling requirements
  – Enhance current notional nozzle model approaches using acquired data as validation benchmark
  – Help incorporate mitigation credit table into NFPA, ISO codes
  – With collaborators, validate burst pressure ratio performance test
  – With collaborators, analyze large-scale jet flame data
  – Participate in IPHE round robin fast-fill test and model validation activities

• FY13
  – Acquire fundamental turbulent diffusivity measurements for **reacting** flow fields for light-up model development
  – Develop fundamental light-up model framework based on turbulent flamelet concepts
  – Update radiative heat flux model for large-scale jet flames
  – Develop characteristic heat flux predictive model for pipeline ruptures
Summary

• Sandia R&D program develops the scientific basis for national and international codes and standards development
  – Enables deployment of hydrogen systems and infrastructure
• Fast-fill hydrogen fueling of Type IV tanks were experimentally examined in support of SAEJ2601, GTR and other RCS.
• Characteristics of predictive choked flow dispersion models were examined against Sandia generated validation datasets.
  – Deficiencies identified & updated models are under development
• Qualitative high-speed ignition imaging elucidated potential sustained flame light-up mechanisms.
  – Light-up boundaries for choked flow releases were experimentally mapped
  – Flamelet models can be used to predict light-up boundaries—experimental apparatus needed to measure relevant flow and combustion variables was constructed
• Measured radiative heat fluxes from large-scale H₂ flames were compared against model predictions.
  – Deficiencies identified and model improvements are ongoing
• Engaged international & industry collaborators to address complex R&D and RCS issues
Technical Back-Up Slides
Excellent agreement observed between computed & measured mole fraction statistics if measured $d^*$ was used.

Poor $d^*$ prediction

<table>
<thead>
<tr>
<th>Source Model</th>
<th>$d^*$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Birch et al. (1984)</td>
<td>0.947</td>
</tr>
<tr>
<td>Ewan &amp; Moodie (1986)</td>
<td>0.993</td>
</tr>
<tr>
<td>Birch et al. (1987)</td>
<td>0.790</td>
</tr>
<tr>
<td>Yuceil &amp; Örungen (2002)</td>
<td>0.790</td>
</tr>
<tr>
<td>Harstad &amp; Bellan (2006)</td>
<td>1.440</td>
</tr>
<tr>
<td>Molkov (2008)</td>
<td>0.993</td>
</tr>
<tr>
<td>SNL Data (2011)</td>
<td>0.867</td>
</tr>
</tbody>
</table>

*All models use Able-Noble EOS

Mixing in the slip region?

Abel-Noble EOS
- Works well at ambient $T$
- Cryogenic states poorly predicted
  (present in barrel shock; $T < 70$ K)

What is the best way to incorporate these refinements?
Is something else missing?
Fundamental Hydrogen Release Behavior

Isaac Ekoto (PI)  
*SNL*  
Experiments

Adam Ruggles  
*SNL*  
Experiments

**Partners and Collaborators:**  
Université du Québec à Trois-Rivières (CAN)
Raw signal intensity corrections used to create a quantitative concentration image

\[ R = p_F \cdot O_R \cdot (I \cdot S_t + S_B) + E_B + B_G \]

Mole Fraction \( (\chi_{H2}) \propto I \)

Mass Fraction \( (Y_{H2}) \propto \chi_{H2} \)
Incompressible free-jets:

\[
\frac{1}{\bar{Y}_{CL}} = K_c \frac{z-z_{0Y}}{r^*} \rightarrow r^* = K_c \frac{z-z_{0Y}}{\bar{Y}_{CL}}
\]

Where:
- \(\bar{Y}_{CL}\): centerline mass fraction
- \(r^* \equiv r_0 \sqrt{\frac{\rho_{jet}}{\rho_{air}}}\): mass weighted effective radius
- \(K_c\): centerline decay rate constant
- \(z\): axial coordinate
- \(z_{0Y}\): mass fraction virtual origin

Seamless reconstruction of mass fraction statistics from stitched together interrogation regions

- Constant centerline decay (\(= 0.105\)) and jet spreading rates (\(0.113\))
- Constant unmixedness (\(\equiv Y'_{CL}/\bar{Y}_{CL} = 0.22\))

Centerline constants agree very well with literature reported values.
Measured PDFs were compared to Beta function distribution produced from measured 1st and 2nd order statistical moments.

\[ P_C(Y_{H2}) = \frac{Y_{H2}^{\alpha-1}(1-YH_2)^{\beta-1}}{B(\alpha, \beta)}, \text{ where } \bar{Y} = \frac{\alpha}{\alpha+\beta}, \text{ and } \bar{Y}' \bar{Y}' = \frac{\alpha \beta}{(\alpha+\beta)^2(\alpha+\beta+1)} \]

Conditioned probability that neglects \( \gamma = 0 \) values

Skewness & Kurtosis values for \( \eta < 0.15 \), deviate from measured values.
- Beta fit often worse than a Gaussian fit

What is a more suitable distribution function? Is a 3rd PDF needed to account for a superlayer?
Along with conventional statistics (mean/rms, PDFs, intermittency), 2D high-res. imaging enables **turbulent length scale** measurements.

\[ \Lambda = \int_0^\infty \frac{Y_{H2}(x)'Y_{H2}(x + dx)'}{Y_{H2}'Y_{H2}'} \, dx \]

\[ \frac{1}{\lambda^2} = -\frac{1}{2} \frac{\partial^2}{\partial x^2} \left( \frac{Y_{H2}(x)'Y_{H2}(x + dx)'}{Y_{H2}'Y_{H2}'} \right) \]

Are non-reacting flow integral length-scales suitable for turbulent flame speed determination in light-up models? Can energy density spectra be reproduced from the integral length scale, or is an integral time scale needed instead?
New diagnostic capability that enables direct turbulent diffusion measurements was designed & constructed in FY12.

Along with molecular diffusion, $D$, turbulent diffusion, $D_{turb}$, controls mixing.

For unreacting H$_2$/air mixtures mixture density is:

$$\rho = Y_{H_2}\rho_{H_2} + (1 - Y_{H_2})\rho_{air}$$

and,

$$D_{turb} \equiv \frac{1}{\nabla Y_{H_2}} \left[ \frac{\overline{u'Y_{H_2}'} + \frac{\overline{u}}{\rho} \rho'Y'_{H_2} + \frac{Y_{H_2}}{\rho} \rho'u'}{1} \right]$$

Direct measurements possible only through coupled velocity and concentration statistics

System construction complete; 1$^{st}$ measurements in Q4FY12.

How will these measurements compare to detailed LES?

$u$: Particle Image Velocimetry
$Y_{H_2}$: Acetone laser fluorescence
- PIV seed particles interfere w/ Rayleigh scatter
Sustained Light-Up Probability

Isaac Ekoto (PI)  
*SNL*  
Experiments

Adam Ruggles  
*SNL*  
Experiments

Partners and Collaborators:
Flamelet models can be used to predict these turbulent flame front propagation speeds.

H₂ preferentially diffuses toward reaction front (differential diffusion)
- Increased flame front distortion
  Driscoll, 2007

\[
S_{Turb} = f(\Sigma, u', \Lambda, S_{Lam}, \alpha_{H_2}, D_{H_2}, D_{diff}, D_{turb}, q, c)
\]

- \(\Sigma\): flame surface density
- \(u'\): fluctuating turbulent velocity
- \(\Lambda\): integral length scale
- \(S_{Lam}\): laminar flame speed
- \(\alpha_{H_2}\): thermal diffusivity
- \(D_{H_2}\): molecular diffusivity
- \(D_{diff}\): differential diffusion
- \(D_{turb}\): turbulent diffusivity
- \(q\): heat release
- \(c\): reaction progress variable
Fast Fill Modeling

Terry Johnson (PI)
SNL
Experiments

Jianjun Ye
Zhejiang University, PRC
CFD Modeling

Partners and Collaborators:
Lincoln Composites and Zhejiang University, PRC
Tank CFD model under development to compare against validation datasets.

- Ansys Fluent V14.0
- 3D to capture buoyancy effects
- Structured grid for the tank
- Unstructured flow grid
- NIST real gas state modeling
- Coupled fluid dynamics & heat transfer

Future Work
- Broaden test matrix to include different tank geometries & types
- Upgrade test facility to accommodate 70 MPa fast filling experiments
- Create generalized from validation data as a comparative standard for developing refueling protocols