

R&D Needs for Reduced Order H₂ Release/Ignition Behavior Models – The SNL Perspective

Isaac Ekoto Principle Investigator Daniel Dedrick Hydrogen Program Manager

Bill Houf (retired), Terry Johnson, Adam Ruggles, Aaron Harris Sandia National Laboratories

> Antonio Ruiz Program Manager: DOE FCT Codes and Standards Program Element October 17, 2012

This presentation does not contain any proprietary, confidential, or otherwise restricted information

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







How best can risk management approaches incorporate H₂ behavior models?

One first needs to decide the appropriate risk approach: Prescriptive vs.



Example: Pipe rupture potential from internal pressure

- Reference extreme pressure selected (e.g., MAWP)
- Validated method used to compute hoop stresses
- Safety Factor (SF) used to account for QAQC issues and uncertainty in calculation methods









Operation Space: Working Pressure

 $^{\dagger}P(A|B)$ conditional probability that event A occurs for a given event B

How best can risk management approaches incorporate H₂ behavior models? Prescriptive vs. QRA

Both approaches work best for mature technologies with **well-established**, **data driven**, threat envelopes; however,

For limited data constraints QRA probabilities can be reduced to fundamental processes and evaluated with deterministic models.

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















Centerline constants agree well with literature reported values.

COMBUSTION RESEARCH FACILITY

Self-similarity in established flow zone require **TRE** centerline values/trajectories to describe plume. S ¦ V_{CL}exp(-r²/B² Established Flow Zone g Integral plume model Zone 3 **S**₃ $\frac{\partial}{\partial S} \int_0^{2\pi} \int_0^\infty \rho u r dr d\phi = \rho_\infty E$ Flow Establishment Х Zone $\frac{\partial}{\partial S} \int_0^{2\pi} \int_0^{\infty} \rho u^2 \cos \theta \, r dr d\phi = 0$ Zone 2 $\frac{\partial}{\partial S} \int_{0}^{2\pi} \int_{0}^{\infty} \rho u^{2} \sin \theta \, r dr d\phi = \frac{\partial}{\partial S} \int_{0}^{2\pi} \int_{0}^{\infty} (\rho_{\infty} - \rho) g r dr d\phi$ **S**₂ Zone 1 Initial Entrainment $\frac{\partial}{\partial S} \int_{0}^{2\pi} \int_{0}^{\infty} (Y_{\infty} - Y) r dr d\phi = 0$ **S**₁ Houf & Schefer, Int J H₂ Energy, 2008 S₀

Buoyant and momentum driven flows examined to determine appropriate entrainment rates.

COMBUSTION RESEARCH FACILITY

Higher order statistics determined from self-similarity.

$$ar{Y} = f(ar{Y}_{CL}, \eta); Y' = g(ar{Y}_{CL}, \eta)$$

Where,
 $\eta = rac{r^*}{(r-z_{0j})};$ normalized radial
 $z_{0j}:$ momentum virtual origin
Richards and Pitts, J Fluid Mech 1993





Non-linear correlation between intermittency and ratio of 1st & 2nd order statistical moments.

- Linear relationship often assumed
- Results impact PDF prediction

A more suitable intermittency correlating parameter is needed





2 parameter Beta: Skewness/Kurtosis ($\eta < 0.15$), deviates from measured values.

4 parameter Beta: better matches data, but more variables needed to specify PDF bounds

No existence of H₂ jet superlayer observed



2D high resolution imaging enables turbulent length scale measurements.



Similar integral time scales can be determined from frequency based measurements – more discussion of the relevance later.

COMBUSTION RESEARCH FACILITY

Initial & flow establishment zones require extra modeling for different flows: choked, LH2, etc. RE



Notional Nozzle Models

Madal	Со	nservatio	Critical			
Woder	Mass Momentum		Energy	Entropy	Assumptions	
Birch et al. (1984) Ruggles & Ekoto (2012)†	X		X		$T_2 = T_0$ $V_2 = \text{sonic}$	
Ewan & Moodie (1986) Ruggles & Ekoto (2012)†	X		X		$T_2 = T_1$ $V_2 = sonic$	
Molkov (2008)	x		x		V_2 = sonic S ₁ (Abel Noble) S ₂ (Ideal gas) T ₂ ≈ T ₁	
Birch et al. (1987) Schefer et al. (2007)†	x	X	x		$T_2=T_0$	
Yüceil & Ötügen (2002) Ruggles & Ekoto (2012)†	X	X	X		V ₂ supersonic (no Mach disk)	
Harstad & Bellan (2006) Winters & Houf (2008) [†]	X	X	X	X	All fluid passes through Mach disk	

[†] Updated with Abel-Noble state modeling:

$$p = Z\rho RH_2T; Z = (1 - b\rho)^{-1}$$

Limited validation data available to compare model performance.



Validates notional nozzle concept and provides *d*^{*} values to assess notional nozzle model performance.

Representational Sandia National Laboratories



Weighted pseudo sources that account for both: (1) subsonic Mach disk & (2) supersonic slip

COMBUSTION RESEARCH FACILITY

Many leaks are non-circular: e.g., cracks, leaky fittings, ruptures



Elevated jet area ratios for high AR leaks result in faster concentration decay rates

High-fidelity validation data from H_2 jets needed to make empirical corrections is unavailable.



Integral model updated with NIST state modeling & CRE energy conservation for LH2 plumes.





Winters & Houf, Int J H₂ Energy, 2011.

Saturated Vapor Leak ¹							
Pipe ID (mm)	Leak Diameter⁴ (mm)	Distance⁵ (m)					
6.35 mm (1/4 in)	1.100	4.431					
12.7 mm (1/2 in)	2.200	8.861					
19.05 mm (3/4 in)	3.299	13.29					
25.4 mm (1 in)	4.399	17.71					
31.75 mm (1.25 in)	5.499	22.13					
38.10 mm (1.5 in)	6.599	26.55					
44.45 mm (1.75 in)	7.699	30.96					
50.80 mm (2 in)	8.799	35.36					

Saturated Liquid Leak ²							
Pipe ID (mm)	Leak Diameter⁴ (mm)	Distance⁵ (m)					
6.35 mm (1/4 in)	1.100	5.659					
12.7 mm (1/2 in)	2.200	11.26					
19.05 mm (3/4 in)	3.299	16.75					
25.4 mm (1 in)	4.399	22.11					
31.75 mm (1.25 in)	5.499	27.31					
38.10 mm (1.5 in)	6.599	32.37					
44.45 mm (1.75 in)	7.699	37.29					
50.80 mm (2 in)	8.799	42.06					

Subcooled Liquid Leak ³							
Pipe ID (mm)	Leak Diameter⁴ (mm)	Distance⁵ (m)					
6.35 mm (1/4 in)	1.100	9.611					
12.7 mm (1/2 in)	2.200	15.9					
19.05 mm (3/4 in)	3.299	21.94					
25.4 mm (1 in)	4.399	27.64					
31.75 mm (1.25 in)	5.499	33.09					
38.10 mm (1.5 in)	6.599	38.34					
44.45 mm (1.75 in)	7.699	43.46					
50.80 mm (2 in)	8.799	48.4					

Distance to 4% H₂ Mole Fraction from a 3% leak (Model validation limited to 80 K jet release data from KIT)

Additional validation data needed at more relevant temperatures.



Electrostatic discharge (ESD) from entrained charged particles.

Low H_2 minimum ignition energy (~0.02 mJ)

CRE

Sample B Iron (III) Oxide Fe₂O₃

Repeatable ignitions from spark discharges between isolated conductors.





200x



Merillo et al., Proc ICHS, 2011



Modeling ESD requires particle information (size, number, type) along with modeled spark discharge behavior.

COMBUSTION RESEARCH FACILITY

Flammability Factor maps from concentration statistics *RF*agree well with laser-spark ignition probabilities.



Prediction of FF depends only on prediction of PDF.

Several methods have been developed to model the transition of incipient ignition to sustained light-up. Blow Out Stability: Fuel Mixture [v/v]-Blow Out Sta



COMBUSTION RESEARCH FACILITY



COMBUSTION RESEARCH FACILITY





New acetone seeded LIF diagnostic enables turbulent mixing measurements

Turbulent diffusion primarily controls mixing in non-reacting jets

For non-reacting H₂/air mixtures:

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

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

Coupled velocity/concentration statistics



Measurements to be coupled with OH LIF and used to conditionally sample velocity/scalar fields around developing ignition kernels.









RE Rediant fractions derived from radiative heat flux measurements from strategically placed radiometers.



 y_s : Stoichiometric mass fraction



Non-dimensional radiant power determined using <u>RE</u> single source model with an exponential shape factor.





Sivathanu & Gore, Combust Flame, 1993

Large spread in single-point source computed radiant fractions from measured heat fluxes.



Measured radiant fraction values were ~80% higher than predictions based on flame residence time correlations.

COMBUSTION RESEARCH FACILITY

Smaller spread in radiant fraction data & better RE agreement with residence time correlations.

Jet	<i>d_j</i> [mm]	<i>ṁ</i> [kg/s]	<i>L_f</i> [m]	p₀ [barg]	T₀ [K]	RH [%]	T _{amb} [K]	p _{amb} [mbar]	U _{wind} [m/s]	Wind dir [°]
1	20.9	1.0	17.4	59.8	308.7	94.3	280	1022	2.84	68.5
2	52.5	7.4	48.5	62.1	287.8	94.5	280	1011	0.83	34.0

Weighted Multi Source Model



Hankinson & Lowesmith, Combust Flame, 2012

- D_i : Distance from observer to source point *i*
- β_i : Angle between observer normal and vector $\mathbf{D_i}$
- w_i : Weight factor for source point i





Nonetheless, measured radiant fraction values were still ~40% higher than predictions based on flame residence time correlations.

COMBUSTION RESEARCH FACILITY

A surface reflection model with an *assumed* reflectance *RE* of 0.5 used to correct for surface irradiance effects:





A surface reflection model with an assumed reflectance **CRE** of 0.5 used to correct for surface irradiance effects:



WMS point emitters replaced by spheres:



Jet

1

2

Surface Reflectance 33 Clipped view area A_{clip} : Total view area w/ infinite reflector A_{inf}:



Ekoto et al., Proc Int Pipeline Conf, 2012

Measured radiant fractions now within ~20% of predictions.

COMBUSTION RESEARCH FACILITY

An integral model is needed to handle wind & CRF buoyancy effects

Jet	<i>d_j</i> [mm]	<i>ṁ</i> [kg/s]	<i>L</i> _f [m]	p₀ [barg]	T₀ [K]	RH [%]	T _{amb} [K]	p _{amb} [mbar]	U _{wind} [m/s]	Wind dir [[°]]
1	20.9	1.0	17.4	59.8	308.7	94.3	280	1022	2.84	68.5
2	52.5	7.4	48.5	62.1	287.8	94.5	280	1011	0.83	34.0

Jet 1 (3/4" diameter)



Jet 2 (2" diameter)







Experimental scenario analysis and CFD modeling were used to evaluate indoor refueling hazards.

CFD used to evaluate optimal sensor placement



Flame front propagation imaged (3 sec ignition delay)



Large-scale experiments



Mitigation measures such as active/passive ventilation and blowout panels examined



COMBUSTION RESEARCH FACILITY



Summary of Correlation Gaps

General H₂ Release Behavior Gaps:

- Intermittency model needs refinement along with new PDF prediction methods
- PDFs for spatial and temporal integral scales needed
- Data needed to analyze aspect ratios impact for different leak geometries

Ignition Mechanism Gaps:

- Particle laden flow models need to be incorporated w/ existing plume dispersion models
- Charge generation and spark discharge mechanisms need to be investigated.

Flame Light-up Gaps:

 Greater understanding about ignition transition point and/or more data on blowout stability limits is needed.

Hazard Analysis Gaps:

- Integral model needed for large-scale flame radiation modeling
 - Greater consideration of reflective radiation?
- Heterogeneous confined/delayed ignition models are needed
 - Can integral dispersion models be used to form initial conditions?

A significant need exists to consolidate existing models and correlations into some sort of QRA framework







- Controls located outdoors with storage
- Dispenser appliance and number of components indoors reduced
- May not contain gas detector
- Retains required isolation and controls aspects

Indoor Non-Public Fast Fill* Dispenser P&ID

Alt. Case 1



- Remove fire alarm system
- Remove ventilation system
 - e.g., cold storage with limited ventilation & recirculation
- Remove gas detection

Indoor Non-Public Fast Fill* Dispenser P&ID

Alt. Case 2

Without QRA, many of these alternate dispenser layouts would not be possible.

COMBUSTION RESEARCH FACILITY

Representation Sandia National Laboratories

Validated CFD approach used to evaluate full-scale scenarios and inform indoor refueling requirements.

Forklift tank and release parameters:

35 MPa storage pressure, 0.8 kg H_2 , 6.35 mm orifice dia.

Warehouse:

7.62 m ceiling, 3 room volumes

Analysis performed in support of NFPA 2/55

Overpressure vs. Warehouse Volume



Can dispersion be predicted from integral plume & ceiling layer models? How do we account for obstacles?

Are reduced order overpressure models using flammable volumes viable?



Additional diagnostics include Particle Image Velocimetry (PIV), Laser Doppler Velocimetry (LDV) and OH Laser Induced Fluorescence (LIF).

COMBUSTION RESEARCH FACILITY

Representational Sandia National Laboratories

Self-similarity in the established flow zone requires only centerline values/trajectories to describe plume.





Schefer, Houf, Williams, Int J H₂ Energy, 2008

Zones 1 and 2 generally neglected for small (unchoked) gas leaks from circular orifices.

Representation Sandia National Laboratories







Centerline constants agree very well with literature reported values.

How best can risk management approaches incorporate H₂ behavior models?

Advantages:

- Straightforward implementation
- Uniform & easily verifiable acceptance criteria
- Works well for clearly defined applications

Disadvantages:

- Unable to weight for harm potential
- Difficult to account for cascade events & complex systems
- Suboptimal resource allocation



COMBUSTION RESEARCH FACILITY

Prescriptive

Representational Laboratories





How best can risk management approaches incorporate H₂ behavior models?

Advantages:



- Risk weighted according to harm potential resources allocated where needed
- Non-obvious systemic risk can be identified
- · Additional risk contributors (i.e., human factors) can be included
- Quantifiable insight into risk mitigation strategies

Disadvantages:



Accurate probabilities require expansive datasets

Operating Range: P(A)

Failure Potential: *P*(B)

 $Risk: P(A|B)^{\dagger}$

Operation Space

 $^{\dagger}P(A|B)$ conditional probability that event A occurs for a given event B

Probability