Project ID # SCS010

R&D for Safety Codes and Standards: SCS Project Overview - Hydrogen Behavior

Sandia National Laboratories

Aaron Harris (Presenting)
Hydrogen SCS Project Lead

Isaac Ekoto
Principle Investigator

Team Member: Adam Ruggles

DOE Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting
May 14, 2013

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: 83%

MYRD&D 2012 Barriers

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

- Project funding DOE share: $20.4M*
- Funding received in FY12: $0.8M
- Planned funding for FY13: $0.5M

(*Project activities support project SCS#011)

Partners

- **Industry:** Air Products, Lincoln Composites, 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

reacH2

Project Approach

The Safety, Codes and Standards program coordinates 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 (SAE, GTR, IEC)
International Standards (ISO)
International Agreements (IEA, IPHE)

Objectives/Relevance

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

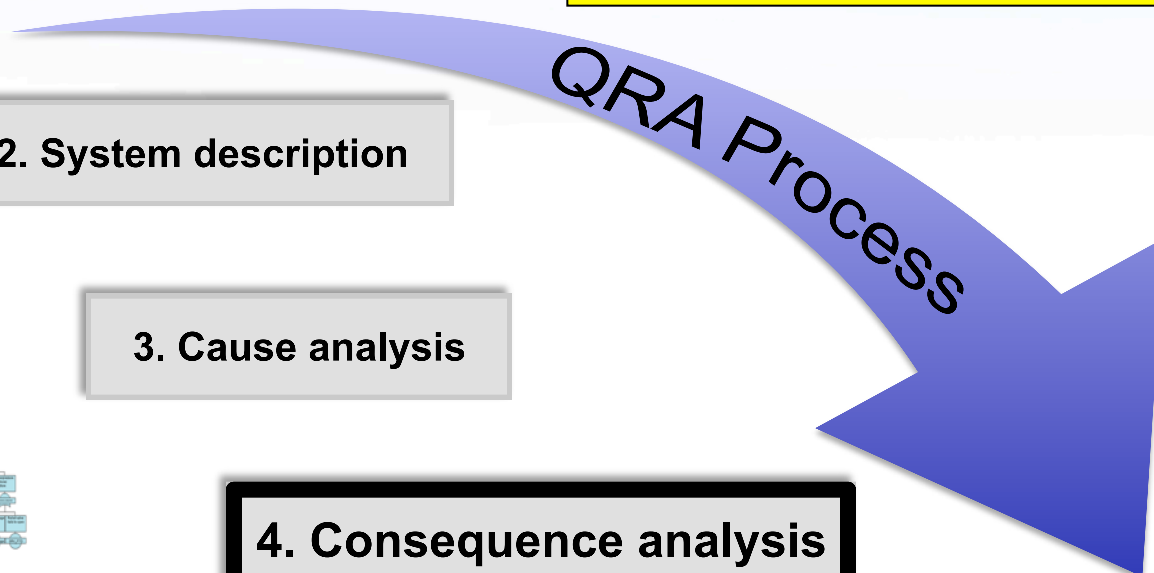
Barrier from 2013 SCS MYRDD	Project Goal
F. Enabling national and international markets requires consistent RCS	Participate as experts for IEA Task 31 along with other relevant international programs
G. Insufficient technical data to revise standards	Generate parametric hydrogen release validation data for relevant hydrogen storage, transport & delivery technology applications
L. Usage and Access Restrictions – parking structures, tunnels and other usage areas	Evaluate, model, & provide expert guidance into release consequences for identified hazard scenarios needed to develop scientifically based RCS

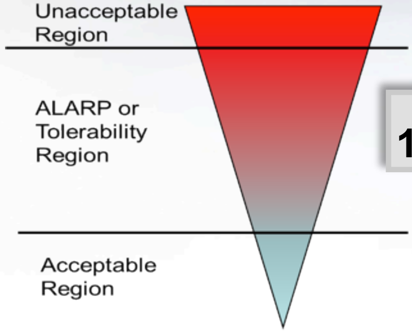
FY2013 Approach and Milestones

MYRD&D 2012 Barrier	FY13 Milestone	Status
G. Insufficient technical data to revise standards	Ignition probability experiments	Experiments complete; (article submitted: *JFM*)
	Non-circular choked release experiments	Experiments started Q2FY13
L. Usage and Access Restrictions – parking structures, tunnels and other usage areas	Enable integration of behavior tools into QRA integrated model (toolkit)	Incorporated validated dispersion, mixture accumulation, ignition probability, overpressure, & flame radiation models into QRA (SCS011)
F. Enabling national and international markets requires consistent RCS	Support IEA Task 31 Activities	IEA Task 31 Workshop in Bethesda, MD HySafe Workshop in Berlin Germany (Both in Oct 2012)

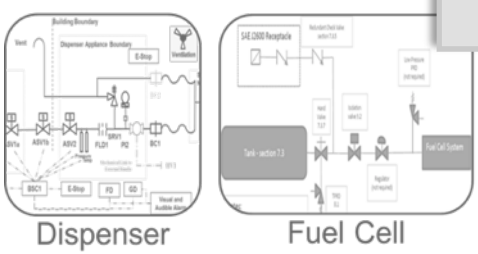
Accomplishment: Support Integrated QRA Algorithm

Reduced order consequence analysis enables creation of QRA toolkit

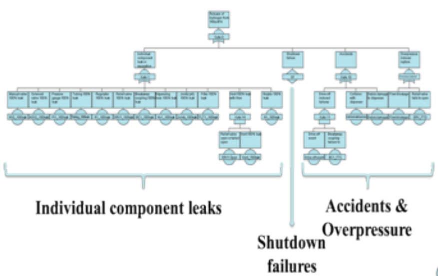




1. Set analysis goals

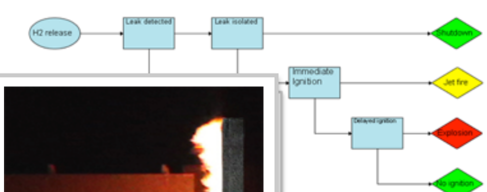


2. System description

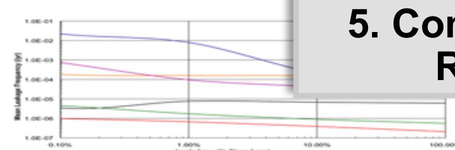


3. Cause analysis

4. Consequence analysis

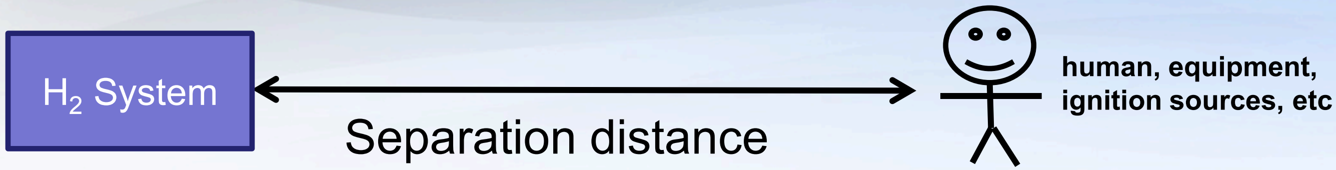


5. Communicate Results



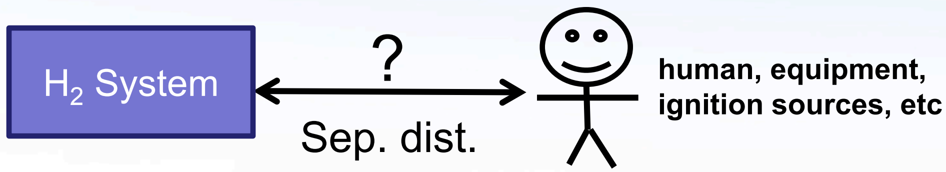
Occupation	FAR
U.S. Workforce total	1.8
Construction and extraction occupations	5.9
Industrial machinery, installation, repair, and maintenance workers	10.4
Industrial truck and tractor operators	3.0
Laborers and freight, stock, and material movers, hand	3.1
Farming, fishing, and forestry occupations	13.5

Relevance: Separation Distances



Challenge

Must reduce separation distances to accommodate H_2 in many existing gasoline forecourts



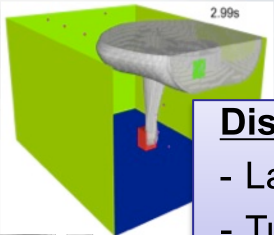
Risk informed approach provides a science-based method for subsequent code revision (SCS011 FY2010 Accomplishment)

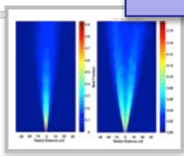
What are opportunities to reduce Separation Distances?

- Reduce Uncertainty in QRA
  - Improve access and accuracy of existing experiential datasets
  - **Improve understanding of underlying physical behavior of unintended releases – dispersion, ignition, light-up, radiation and overpressure**
- Use QRA to benchmark novel mitigation strategies
  - Leak detection and mitigation,
  - Low cost overhead and underground storage
  - Reduced leak occurrence through improved methods and best practices

reacH2

Approach: Consequence Model Input to QRA



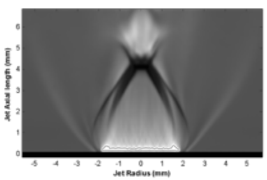


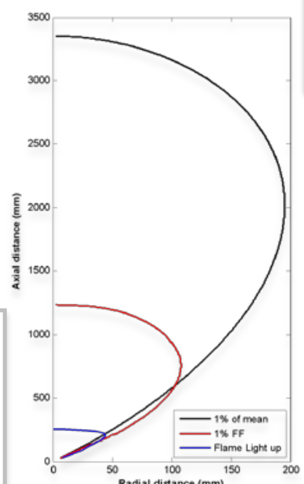
Challenge
QRA toolkit accuracy limited by consequence model accuracy but cannot easily integrate CFD

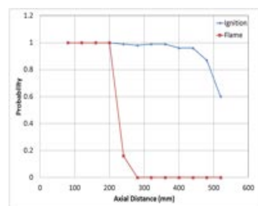
Dispersion Characteristics
- Laminar Flow
- Turbulent jet
- Volumetric rupture
- Enclosure Accumulation

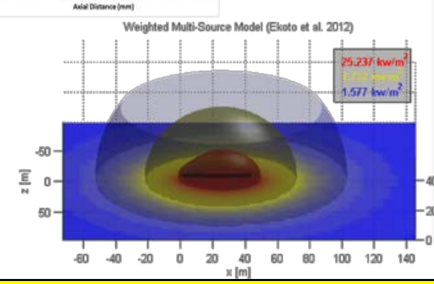
Ignition Probability
- Ignition mechanism
- Mixture ignitability
- Ignition delay/location
- Sustained light-up

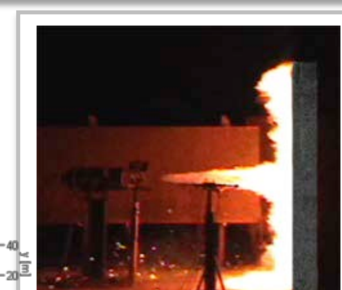
Hazard Characteristics
- Flame radiation
- Overpressure (deflagration/detonation)
- O_2 dilution/depletion











Approach: Consequence modules capable of integration into QRA algorithm

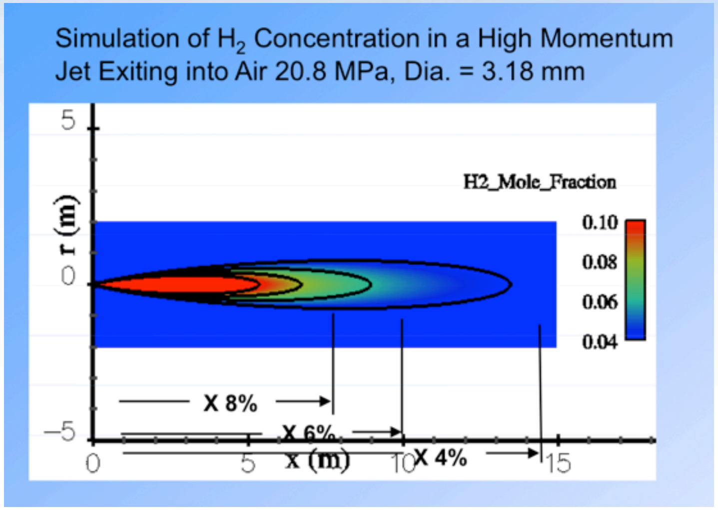
Co-Benefit: Stand-alone consequence tools for investigation of release behavior

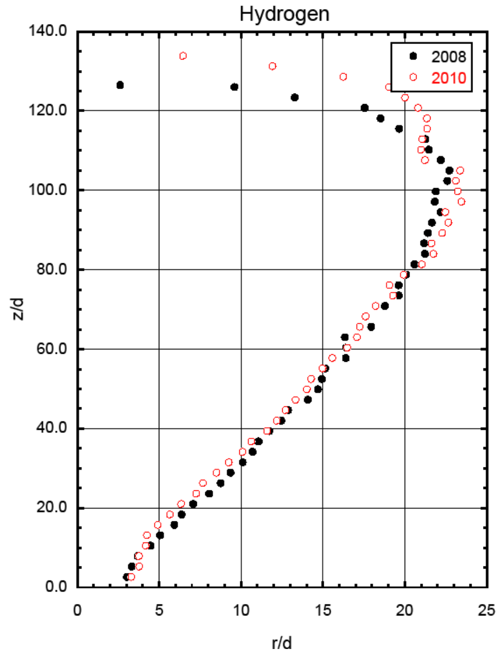
Previous Accomplishments

<u>2010</u>

Mole Fraction Prediction for Jet Release

(current QRA approach used 1% **mean concentration** or ¼ of the LFL to predict jet fires and deflagrations)



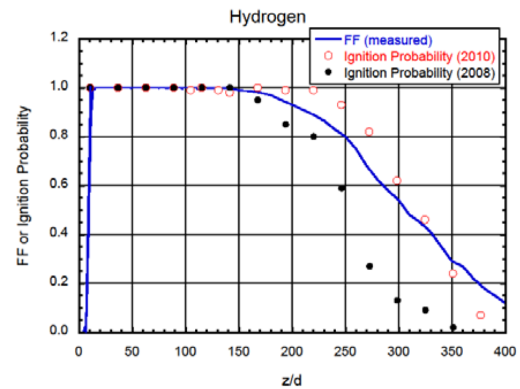


Turbulent H_2 jets light up boundaries from 2008 and 2010 measurements

<u>2011 & 2012</u>

←Identify Flame Light up Boundary

Improved Flammability Factor prediction for probability of Ignition →



Centerline FF profiles and the 2008 and 2010 ignition probability measurements

LFL is ***an insufficient metric for*** a Jet Flame Hazard

FY13 Accomplishment

reacH2

Obtained high confidence in identifying the boundaries of the jet flame hazard for all ***circular*** unintended releases…

3.4 meters

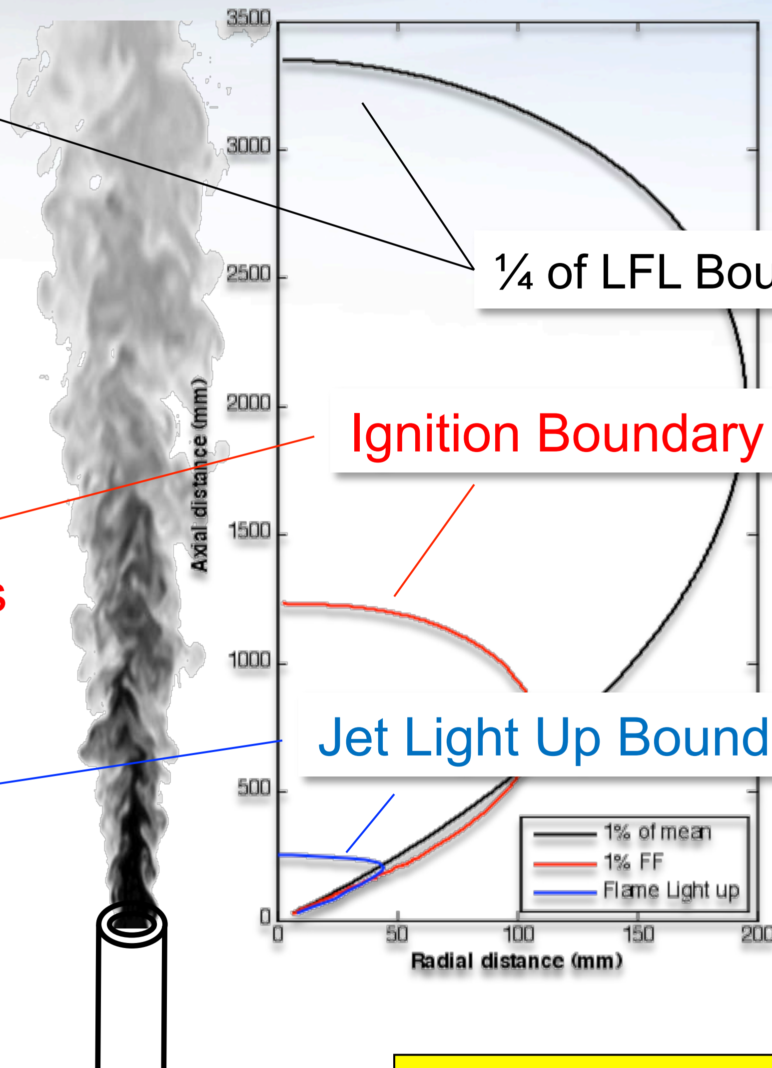
1.25 meters

0.25 meters

¼ of LFL Boundary (Basis of Sep. Dist.)

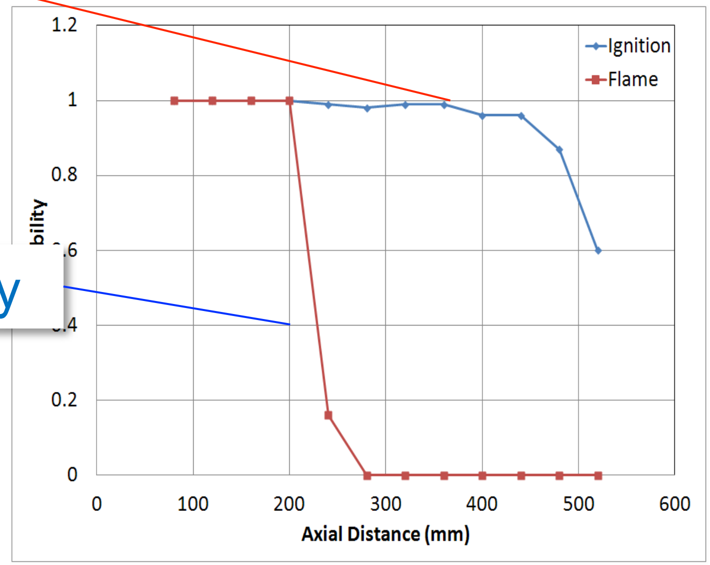
Ignition Boundary

Jet Light Up Boundary



D = Ø1.901mm
Flow = 100slm H_2

Ignition and Jet Flame Probability

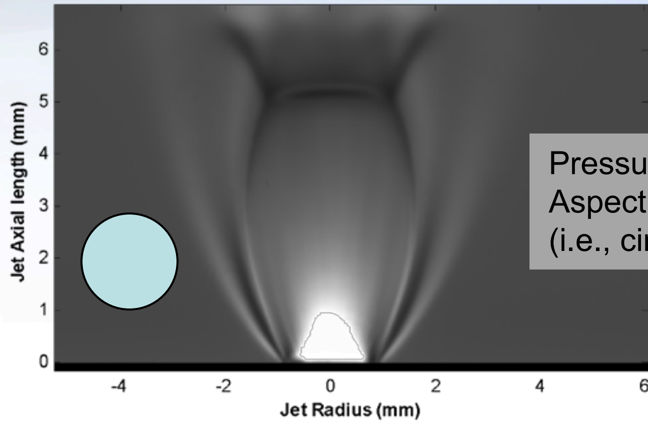


… this provides a pathway for reduced separation distances through integrated QRA process

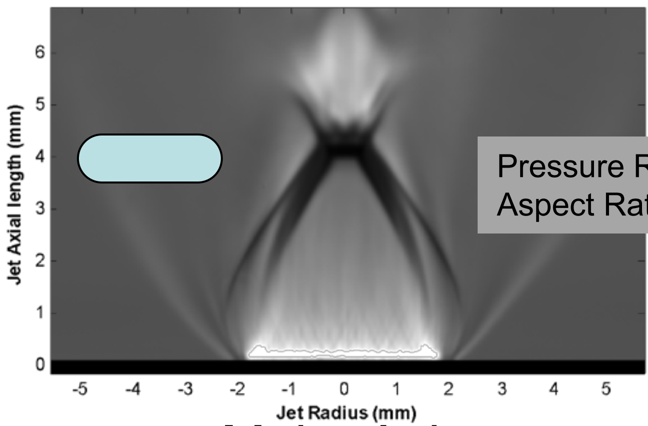
FY13 Accomplishment

Conducted experiments using non-circular openings

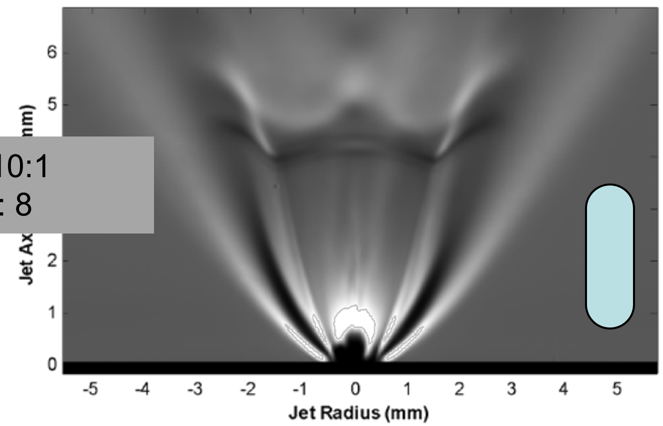
Shown: Schlieren images of jet shock structures at two aspect ratios



Pressure Ratio = 10:1
Aspect Ratio (AR): 1
(i.e., circular)



Pressure Ratio = 10:1
Aspect Ratio (AR): 8



Major Axis

Minor Axis (faster jet spreading rate)

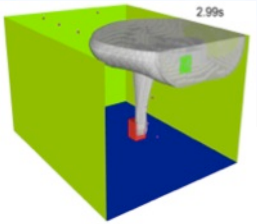
Discussion: Containment vessel or component housing cracks, leaky fittings, etc. (high aspect ratio releases) are likely to have different dispersion characteristics current QRA modules do not account for these differences – Reduced accuracy must be considered error thus reducing the accuracy of the QRA result

FY13 Accomplishment

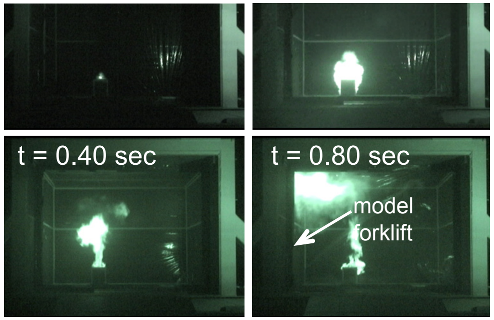
Reminder: Overpressure is the result of accumulation and delayed ignition

Developed layer model and coupled with jet dispersion model to produce a steady state overpressure module for use in QRA toolkit…

Accomplishment Details:



- Evaluate Existing Models for accuracy (FY13)
  - Integral model for jet dispersion (FY08 Accomplishment)
- Develop Accumulation Model
  - **Layer model for accumulation of H2 at the ceiling/ balanced by ventilation (FY13)**
    - **Note: available for steady condition but need to create layer model for unsteady condition**
- **Use dispersion and accumulation model to determine the overpressure based on ignition for steady condition (FY13)**
- **- Validate using experimental data (FY11)**

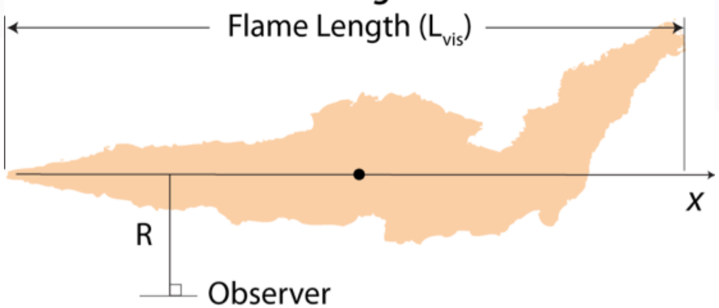


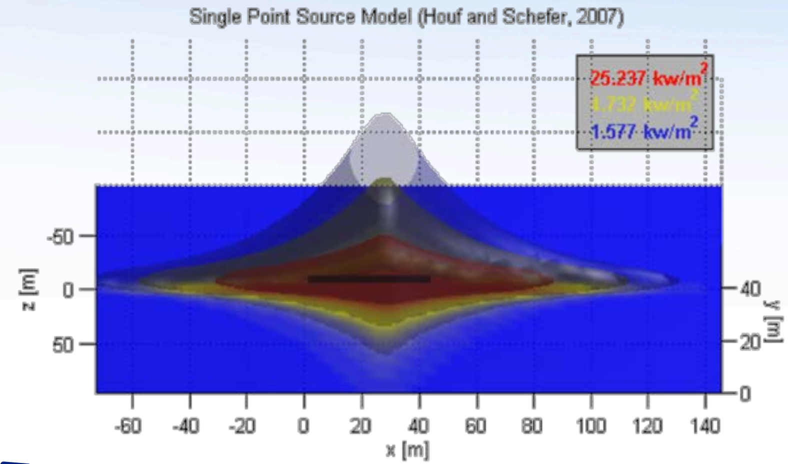
…this overpressure module fills the last gap in consequence analysis for version 1.0 of QRA toolkit

FY2013 Accomplishment

d_j [mm]	[kg/s]	L_{vis} [m]	p_0 [barg]	T_0 [K]	T_{amb} [K]	p_{amb} [bar]
50.8	7.4	48.5	62.1	288	280	1.01

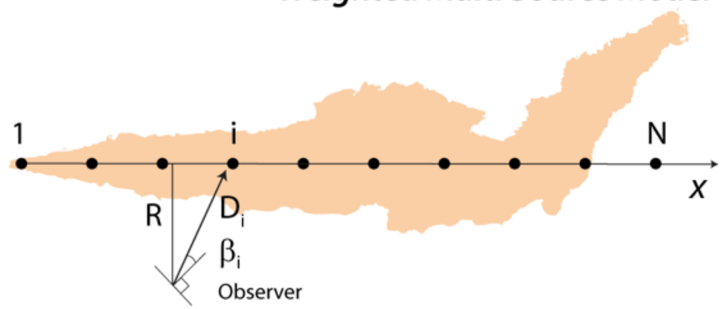
Single Point Source Model

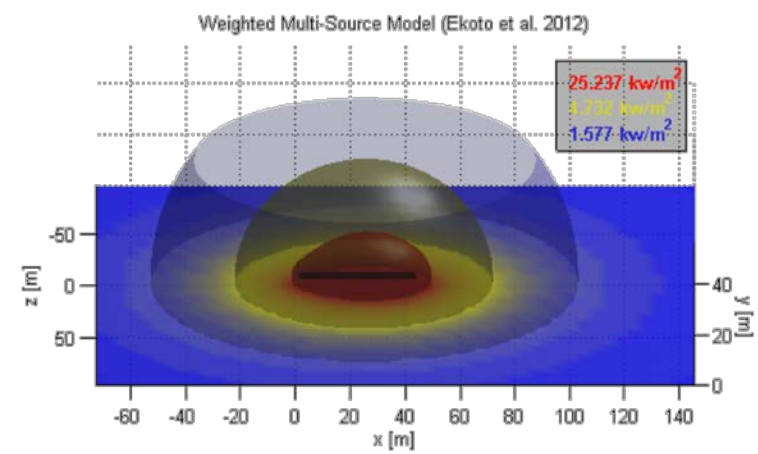




Old model used to inform NFPA 2/55

Weighted Multi Source Model





Improved radiative heat flux boundaries, improves accuracy of harm prediction for radiation from ignited releases, leading to potential recommendations for reduced separation distances

Collaborations

Key Investigators/Major Participants

- **Air Liquide –** France; Sidonie Ruban
- **Air Products and Chemicals Inc. –** Allentown, PA; Jimmy Li (PI), Leonard Creitz, & Dave Farese
- **Commissariat à l'Energie Atomique (CEA) –** France; Sergey Kudriakov & Alexey Velikorodny
- **Health and Safety Laboratory –** Great Britain; Deborah Willoughby, Phil Hooker
- **Joint Research Centre –** Netherlands, Daniele Baraldi (PI)
- **Karlsruhe Institute of Technology –** Germany; Thomas Jordan (PI) & Alexei Kotchourko
- **SRI International –** Menlo Park, CA; Mark Groethe (PI), Erik Merilo
- **Université du Québec à Trois-Rivières –** Canada; Pierre Benard (PI), Andre Tchouvelev & Boris Chernyavsky
- **University of Ulster –** Ireland; Vladimir Molkov

Additional Collaborations

- **Zhejiang University –** China; Jianjun Ye
- **Tsinghua University –** China; David Christopher
- **Kingston University –** Great Britain; Jennifer Wen

Proposed Future Work

FY13

- Support SCS011 QRA toolkit development with respect to incorporating consequence analysis modules
- Update jet dispersion models with non-circular (high aspect ratio) results

FY14

- Investigate the effect of gas temperature, particularly lower temperatures on release behavior (flammability and dispersion)– eventually leading to liquid hydrogen dispersion reduced order models
- Develop overpressure reduced order model for unsteady condition (dynamic flow conditions)
- Continue investigation of sustained flame and efforts to produce accurate prediction of conditions that lead to jet light up

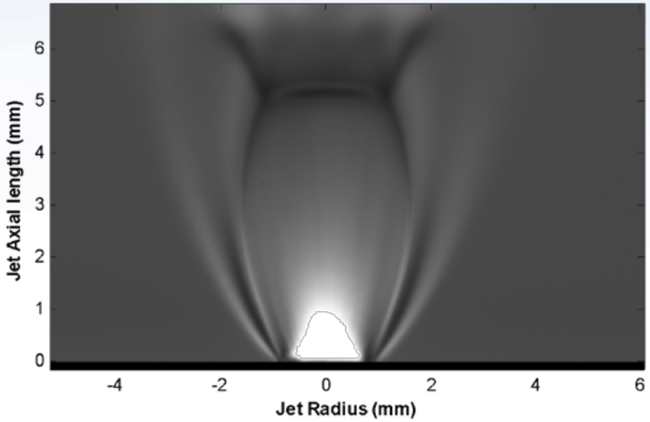
Summary

- **Relevance**: Address lack of safety data, technical information relevant to development of Codes & Standards.
- **Approach**: *Improve dispersion, ignition and hazard prediction through reduced order models as stand alone tools or as integrated components of QRA toolkit*
- **Technical Accomplishments**:
  - Increased confidence of ignition prediction and jet light up boundary for circular releases
  - Began investigation of non-circular (high aspect ratio) releases
  - Developed reduced order overpressure model
  - Improved jet flame radiative heat flux boundaries
- **Future Work**:
  - Assist with integration of reduced order models into integrated QRA toolkit
  - Incorporate results of non-circular releases experiments in jet dispersion models

Technical Back-Up Slides

Dispersion Characteristics from non-circular releases investigated

Schlieren images of jet shock structure



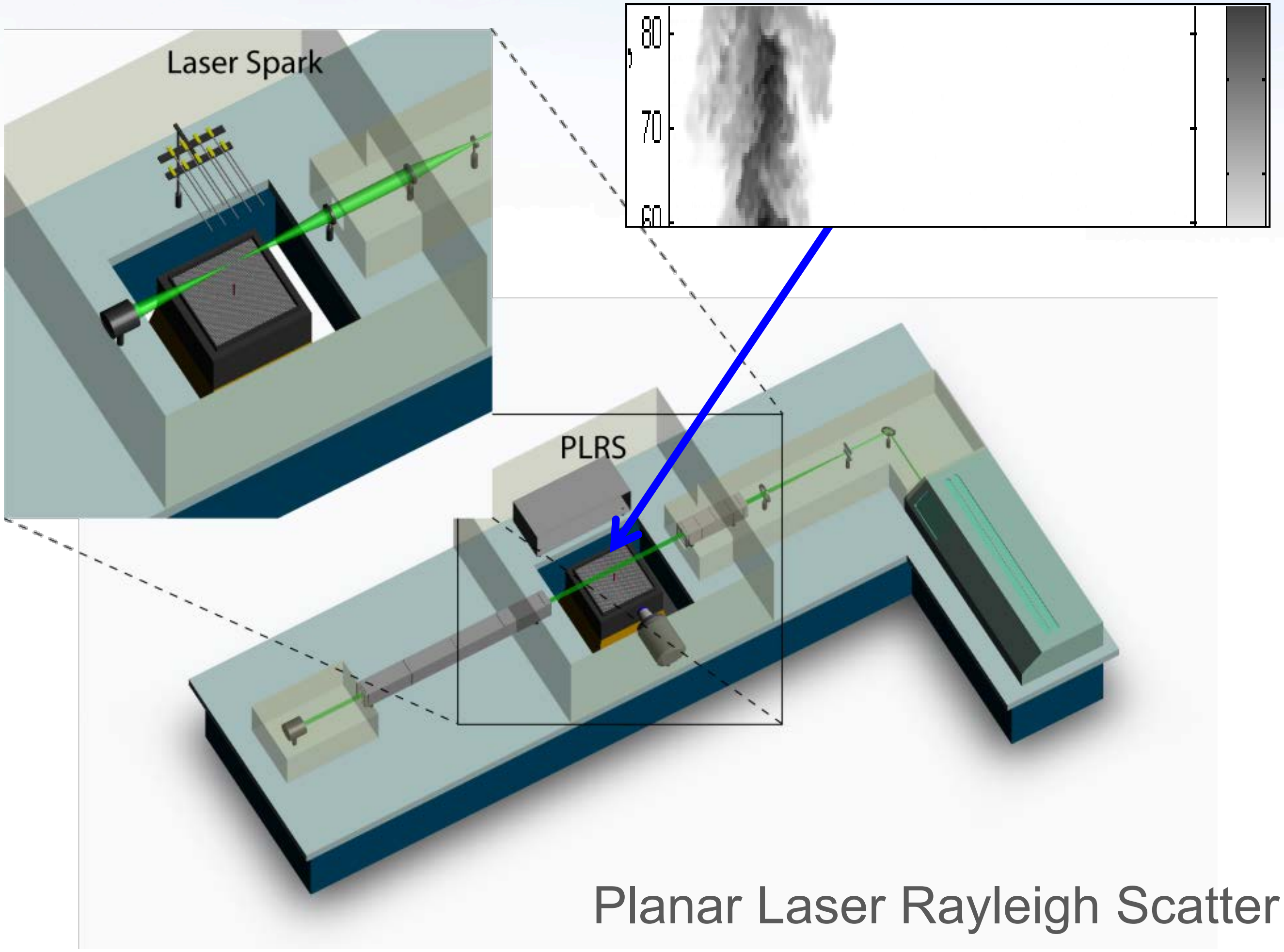
Pressure Ratio = 10:1

Aspect Ratio (AR): 1 (i.e., circular)

Can be modeled with pseudo source models (Ruggles & Ekoto 2012)

High aspect ratio releases (e.g., cracks, leaky fittings) are likely to have different dispersion characteristics but no modeling method currently exists.

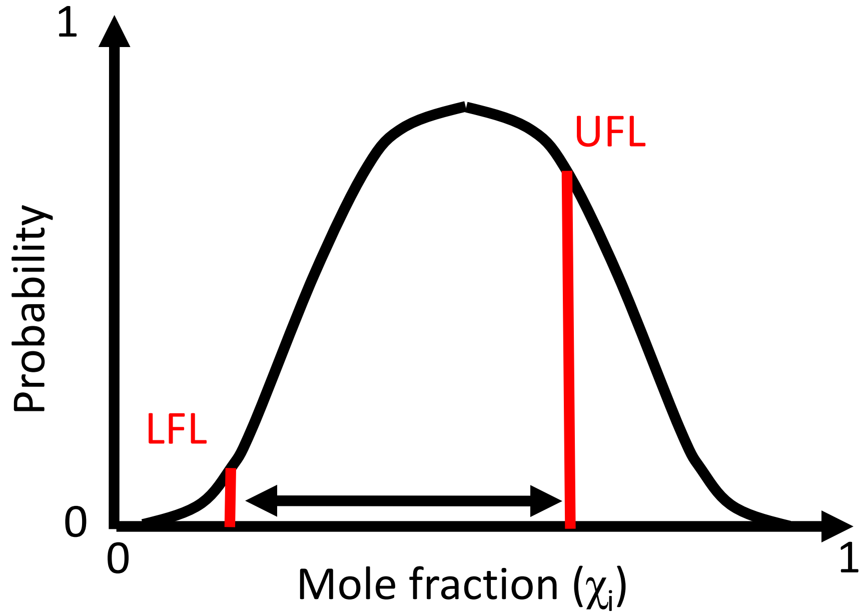
High Resolution Planar Scalar Data Used to Investigate Ignition Probability



Planar Laser Rayleigh Scatter Imaging

Ignition Probability: Flammability Factor (FF)

$$FF = \int_{LFL}^{UFL} PDF \; d\chi_i$$



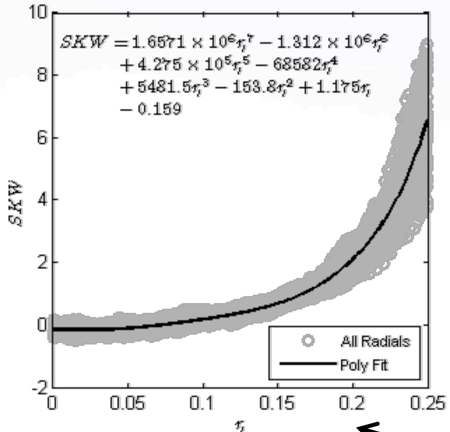
Highly Dependent on <u>Probability Density Function</u> (PDF)

Developed by Birch et al, 1979, 1981, 1984
Demonstrated for H2 by Schefer et al, 2011

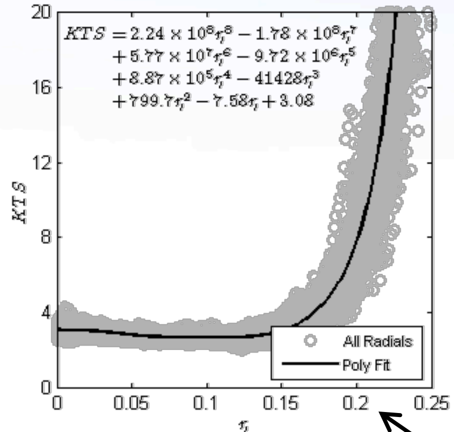
Ignition Probability: Flammability Factor (FF)

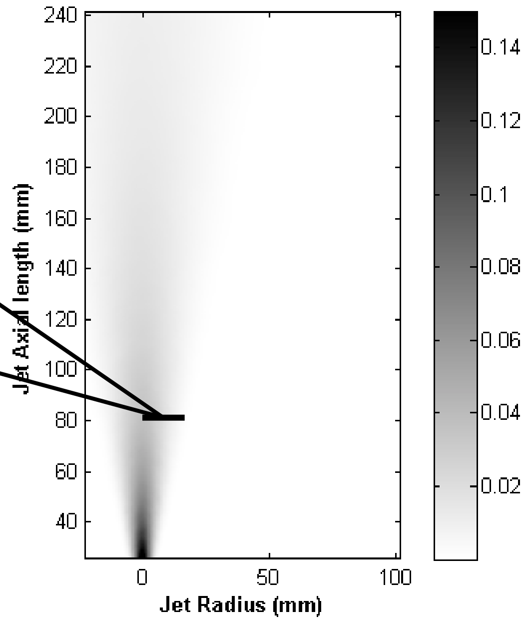
$$FF = \int_{LFL}^{UFL} PDF \; d\chi_i$$

Skewness: PDF skew



Kurtosis: PDF flatness





Skewness and Kurtosis were self-similar in established flow region

reacH₂

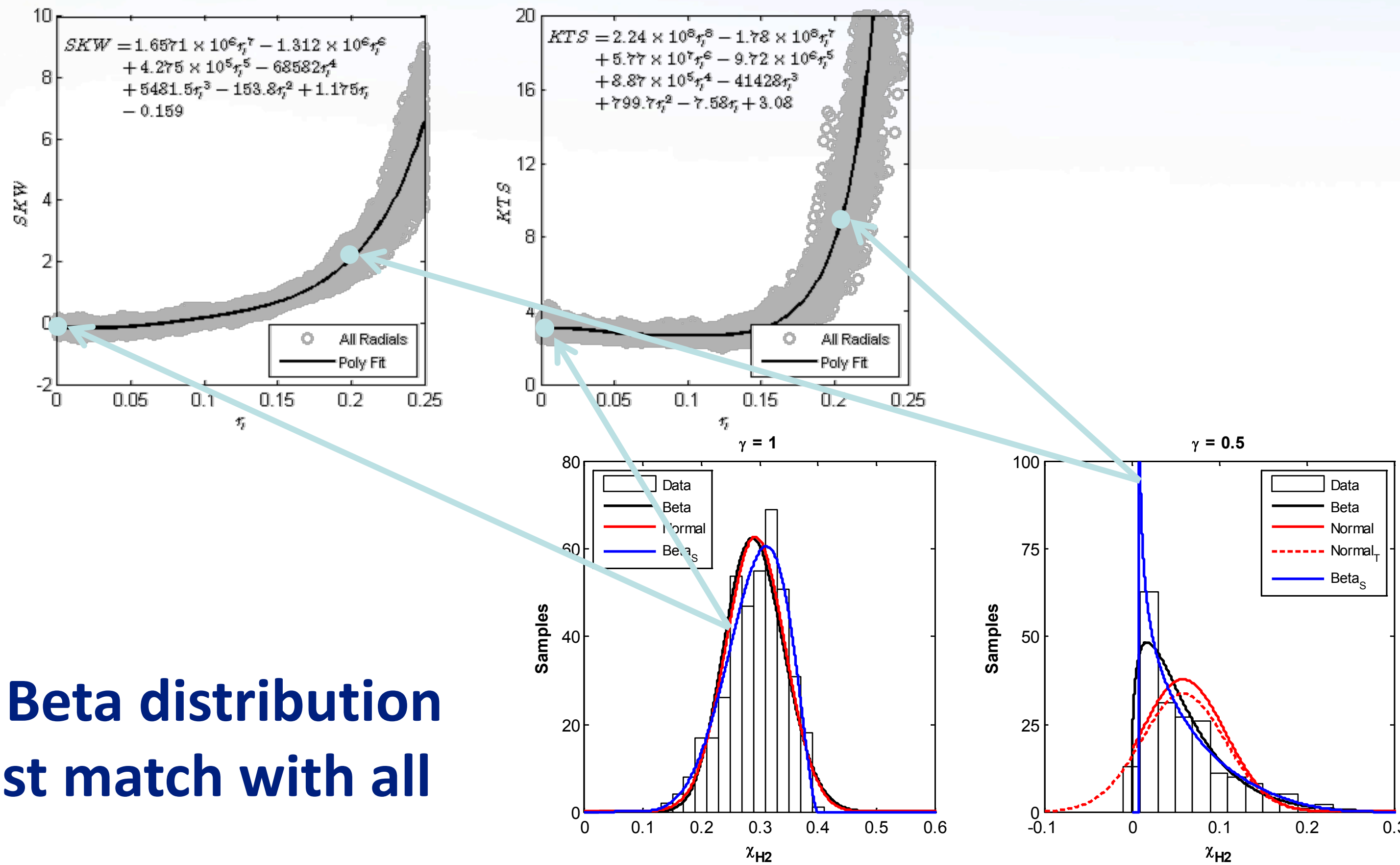
Ignition Probability: Flammability Factor (FF)

$$FF = \int_{LFL}^{UFL} PDF \; d\chi_i$$

Outer regions PDFs were highly non-Gaussian

Skewness: PDF skew

Kurtosis: PDF flatness



Jet Center

Jet Edge

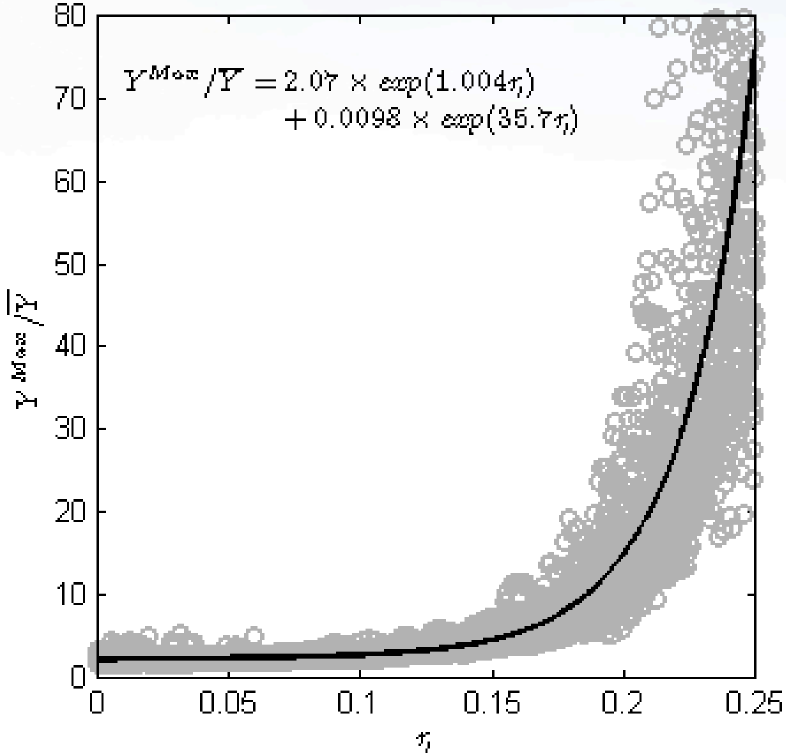
Scaled Beta distribution had best match with all data

Sandia National Laboratories

CRF

Ignition Probability: Flammability Factor (FF)

$$FF = \int_{LFL}^{UFL} PDF \; d\chi_i$$



Scaled Beta Distribution

$$P_\beta(Y) = \frac{(Y-a)^{\alpha-1}(b-Y)^{\beta-1}}{\mathrm{B}(\alpha,\beta)(b-a)^{\alpha+\beta-1}}$$

$$\mathrm{B}(\alpha,\beta) = \int_0^1 t^{\alpha-1}(1-t)^{\beta-1}\,dt$$

Where:

$$\alpha = \overline{Y}\left[\frac{\overline{Y}(1-\overline{Y})}{\overline{Y'^2}} - 1\right]$$

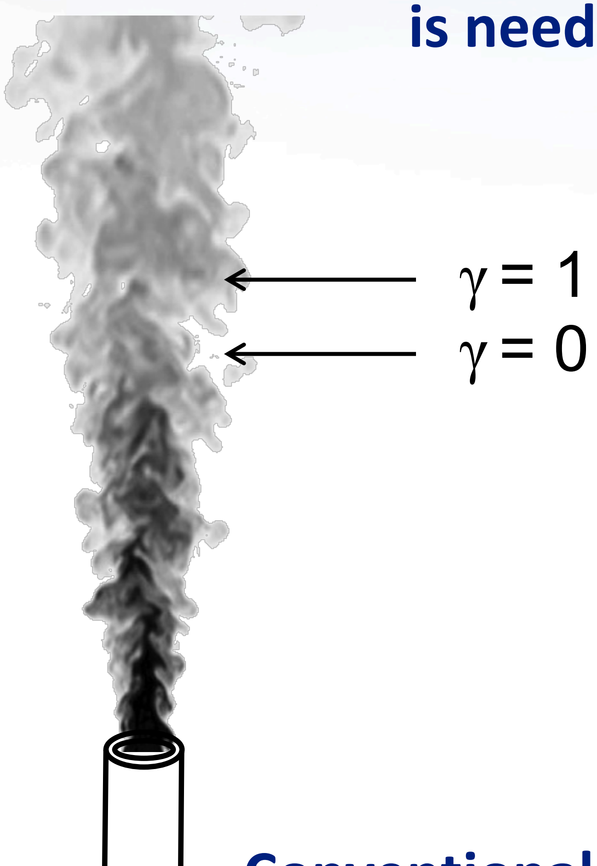
$$\beta = (1-\overline{Y})\left[\frac{\overline{Y}(1-\overline{Y})}{\overline{Y'^2}} - 1\right]$$

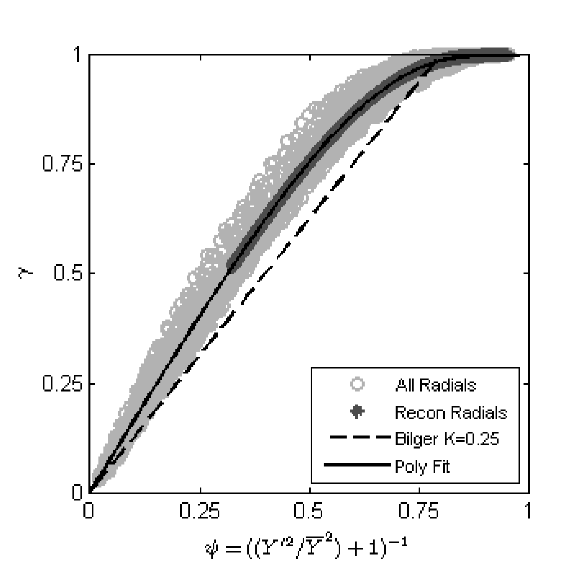
Lower limit (a) = 0 at all locations

Upper limit (b) collapsed to common curve

Ignition Probability: Flammability Factor (FF)

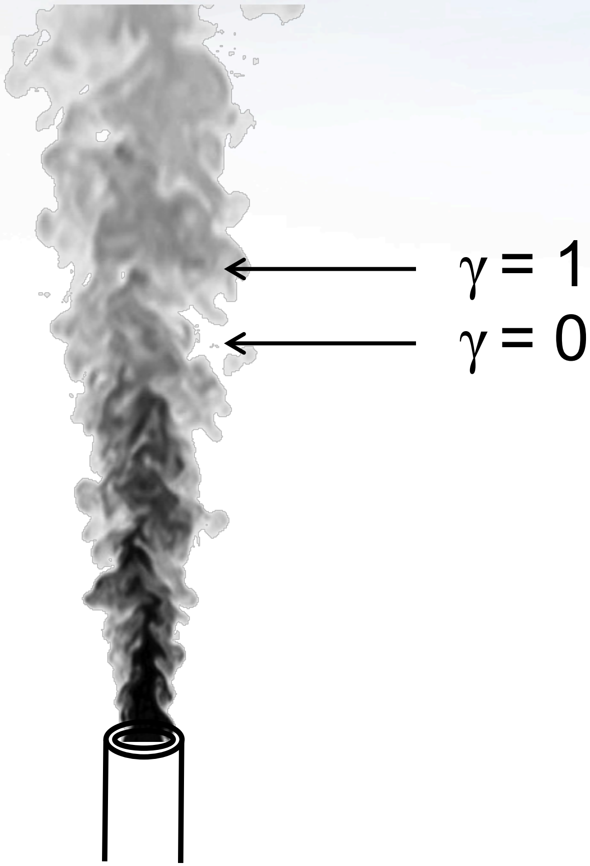
Intermittency (probability of H2 at a given region) is needed to scale PDF

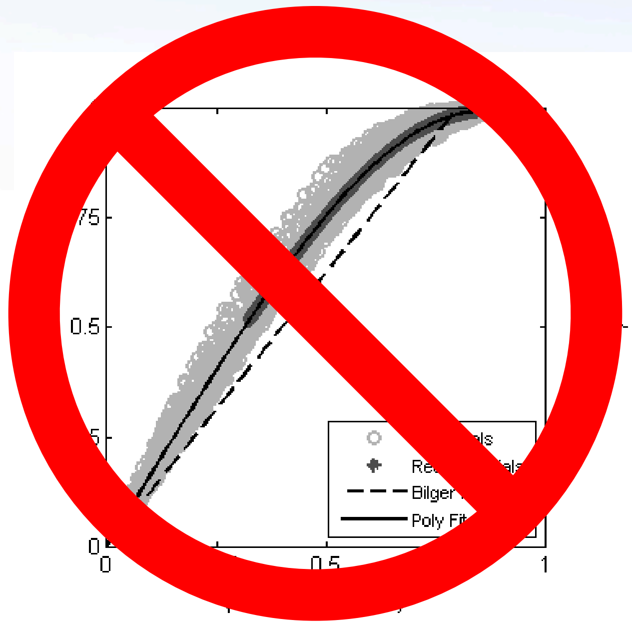


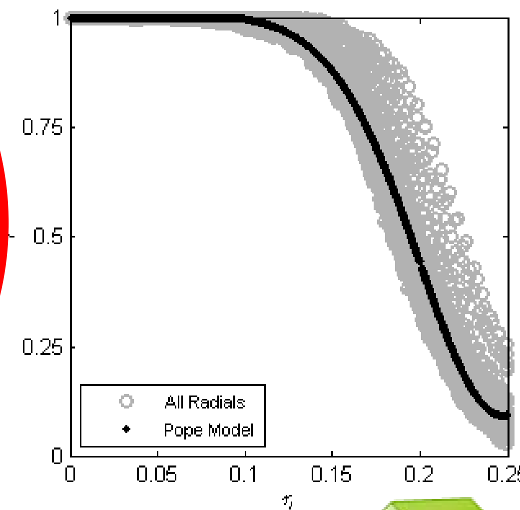


Conventional definition by Kent & Bilger (1977) failed

Ignition Probability: Flammability Factor (FF)



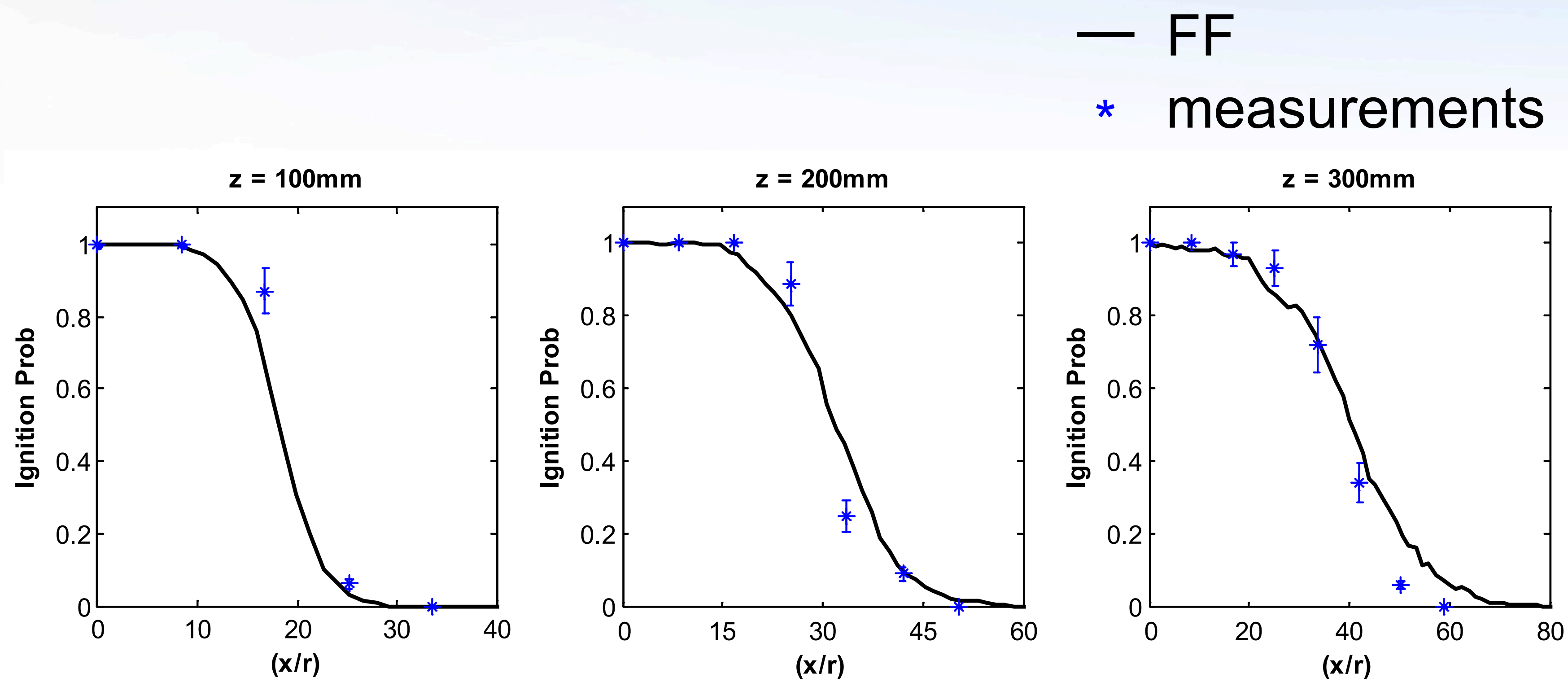




Intermittency found to be self-similar and collapsed to uniform curve

Ignition Probability: Flammability Factor (FF)

$$FF = \int_{LFL}^{UFL} PDF \; d\chi_i$$



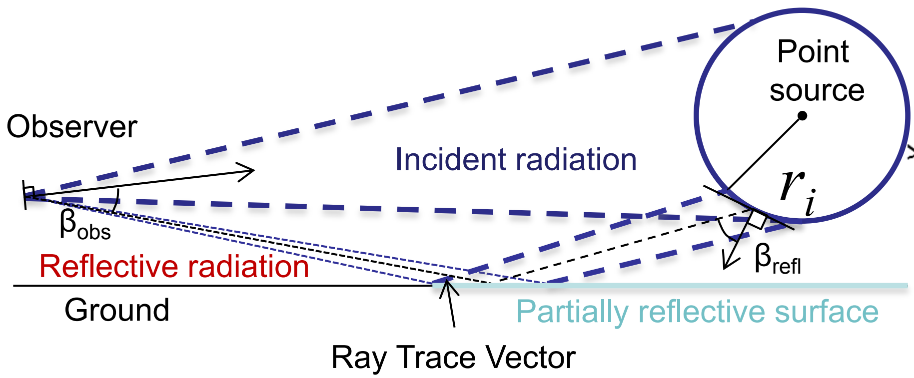
Ignition probability predictions (FF) in good agreement with measurements & improved over those by Schefer et al. 2011

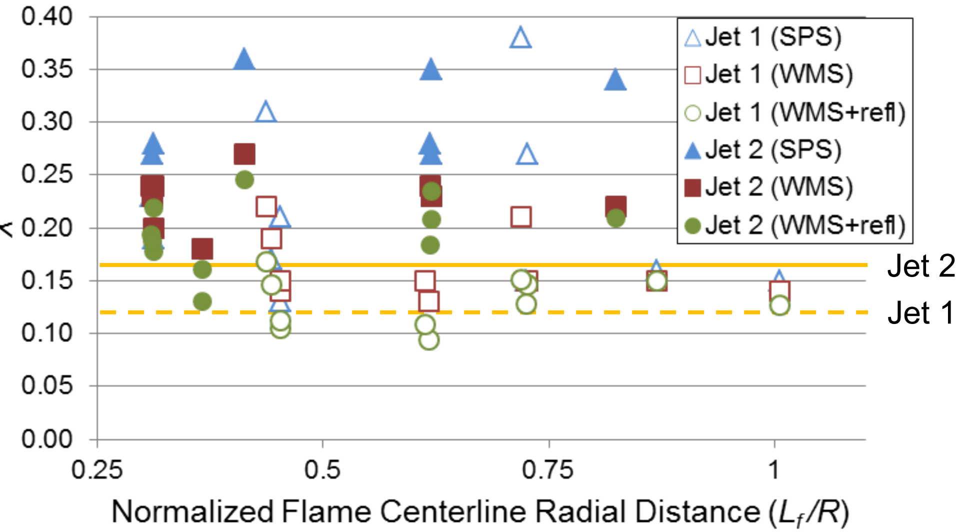
Submitted to JFM (Mar 2013)

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

Jet	d_j [mm]	[kg/s]	L_f [m]	p_0 [barg]	T_0 [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

WMS point emitters replaced by spheres:





Ekoto et al., Proc Int Pipeline Conf, 2012

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

Measured radiant fractions now within ***~20% of*** predictions.