Hydrogen Jet Ignition Experiments and Modeling

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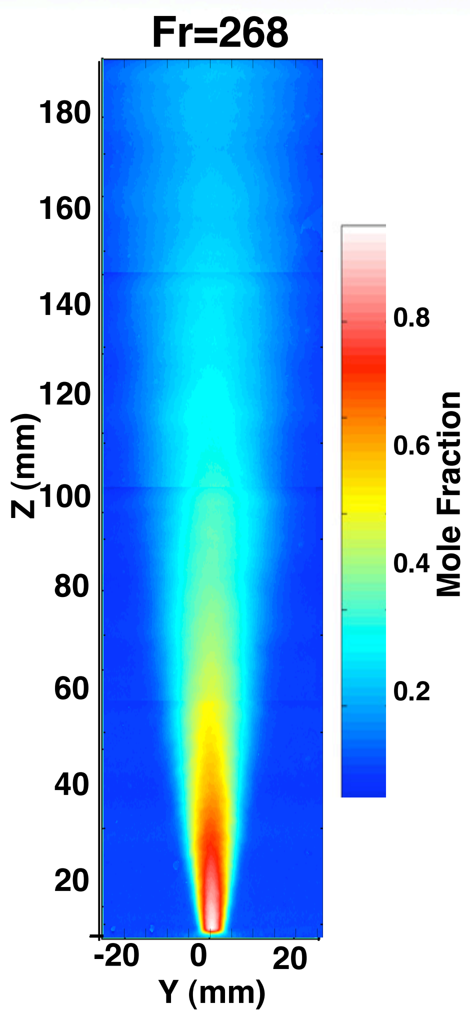
Flame Ignition Limits: Ignitable Gas Envelope Considerations

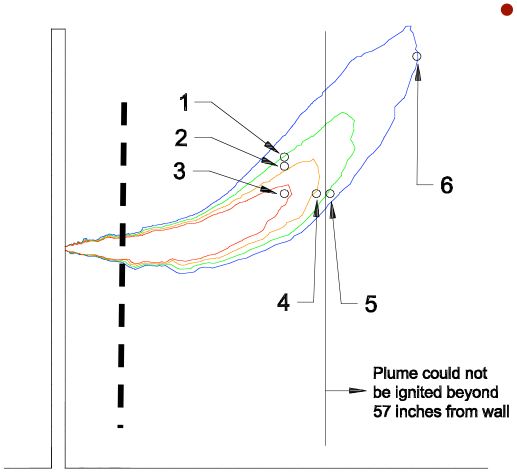
- Vertical H_2 Jet (d_j=1.9 mm)



- **The ignitable gas envelope is important to establishing separation distances for unintended releases of hydrogen.**
- **The extent of the ignitable gas envelope can be based on several criteria. Which is best for Codes & Standards development?**
- **For example:**
  - **Time-averaged H_2 concentration field reveals extent of cloud within traditional flammability limits (4% LFL to 75% RFL).**
  - **Do traditional (static) flammability limits provide a suitable measure of ignitability in turbulent flowing systems?**

Flame Ignition Limits: Motivation

- Time-averaged concentration field



- Contour Levels
  - Red – 10.4%
  - Orange – 8.5%
  - Green – 5.1%
  - Blue – 2.6%

H_2 Concentration Data from:
Dr. Michael Swain
Fuel Cell Summit Meeting
June 17, 2004

Jet Conditions:

Flowrate = 20 scfm, Hole Dia. = 9.44 mm

Exit Mach Number = 0.1 (Unchoked Flow)

- ***Swain determined that hydrogen in turbulent jets could not be ignited at concentrations less than 8%.***
- ***Why does this ignition limit differ from the traditional LFL of H_2 of 4%?***
- ***Possible explanations:***
  - ***The LFL of H_2 is not well known***
  - ***Ignition limits in turbulent jets are not well-represented by the time-averaged concentration field***

- *Which volume fraction contour is relevant:*
  - *lean flammability limit? … 4% or 8%*
  - *detonation limit? … 18%*
  - *a fraction of the lowest lean flammability limit? … 1%*

Flammability Limits for H_2

Upward Flame Propagation (4%)

Tube Dimensions, cm		Firing end	Limits, percent		Water Vapor Content	Reference
Diameter	Length		Lower	Higher		
7.5	150	Closed	4.15	75.0	Half-saturated	356
5.3	150	Open	4.19	74.0	Dried	94
5.3	150	“				
5.3	150	“				
5.0	150	Close				
5.0	150	Open				
4.8	150	“				
4.5	80	Close				
4.5	80	“				

Horizontal Flame Propagation (7.2%)

Tube Dimensions, cm		Firing end	Limits, percent		Water Vapor Content	Reference
Diameter	Length		Lower	Higher		
7.5	150	Closed	6.5	-----	Half-saturated	356
5.0	150	“	6.7	-----	“	356
2.5						

Downward Flame Propagation (9.5%)

cm		end				
Diameter	Length		Lower	Higher		
21.0	31	Open	9.3	----		
8.0	37	Closed	8.9	68.8		
7.5	150	“	8.8	74.5		
7.0	150	“	-----	74.5		
6.2	33	Open	8.5	----		
6.0	120	“	9.45	----	“	325

Propagation in a Spherical Vessel

Capacity, cc	Firing end	Limits, percent		Water Vapor Content	Reference
		Lower	Higher		
Not stated	Closed	9.2	----	Saturated	271
Not stated	“	8.5	67.5	“	82
1,000	“	8.7	75.5	“	95
810	“	5.0	73.5	“	349
350	“	4.6	70.3	“	368
35	“	9.4	64.8	“	297

- ***Flammability limits of H_2 are sensitive to propagation direction but are well established***

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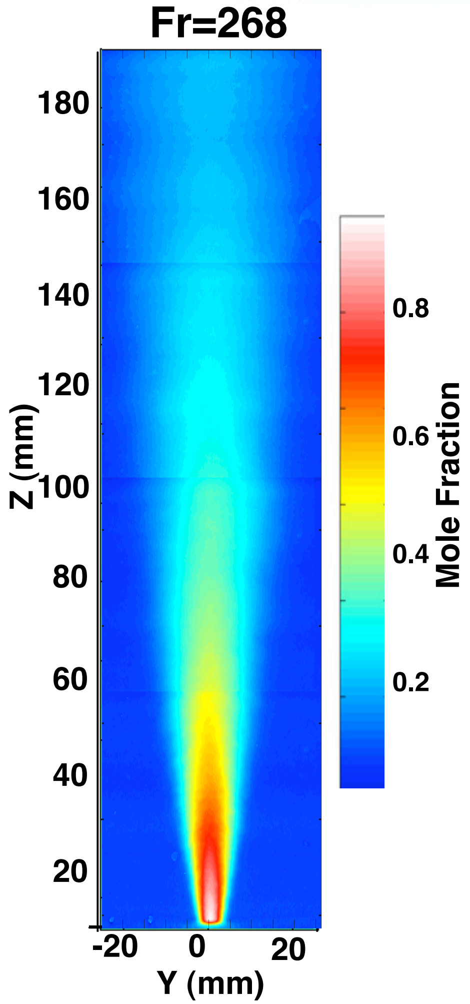
Flame Ignition Limits: Approach

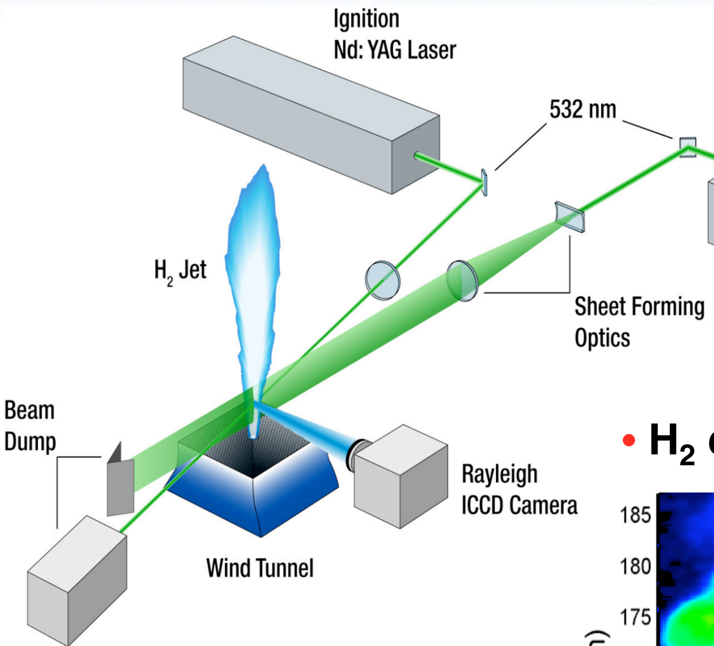
- Vertical H_2 Jet (d_j=1.9 mm)



- **Objective**
  - Develop the understanding of turbulent H_2 releases needed to identify most suitable criteria for ignitability of H_2 releases.
- **Approach**
  - Experimentally determine the ignition characteristics of turbulent H_2 jet flows.
  - Determine time-averaged flow quantities so ignition characteristics can be related to CFD-modeled quantities.
  - Characterize instantaneous flow quantities and establish best measure of ignitability.
  - Incorporate findings into a CFD model that can predict ignition characteristics in H_2 releases.

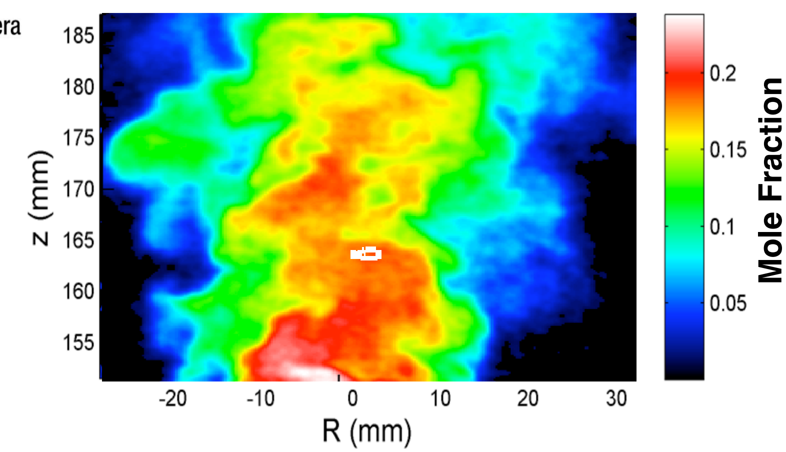
Jet Ignition Probability: Ignition Point Concentration Contours

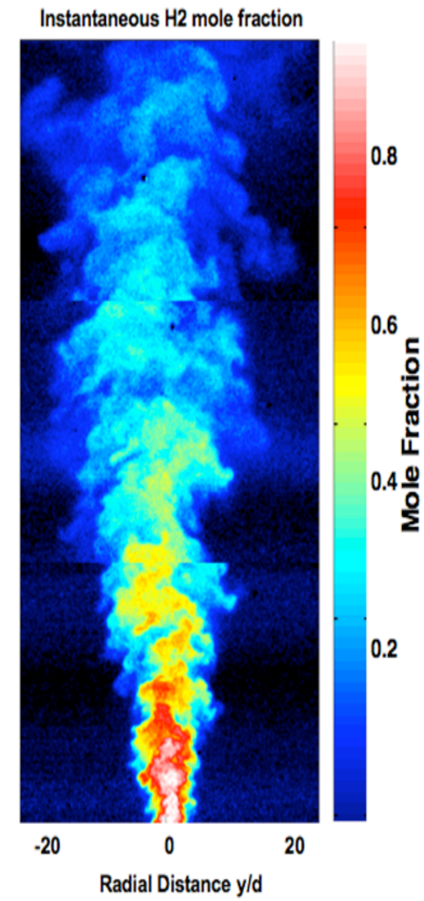
- **Simultaneous Planar Laser Rayleigh Scattering (PLRS) and laser ignition**



- **Rayleigh laser occurs 320 μsec before ignition laser pulse.**

- **H_2 distribution in ignition region**





• Use simultaneous Rayleigh imaging and laser ignition to characterize H_2 concentration distribution at ignition point.

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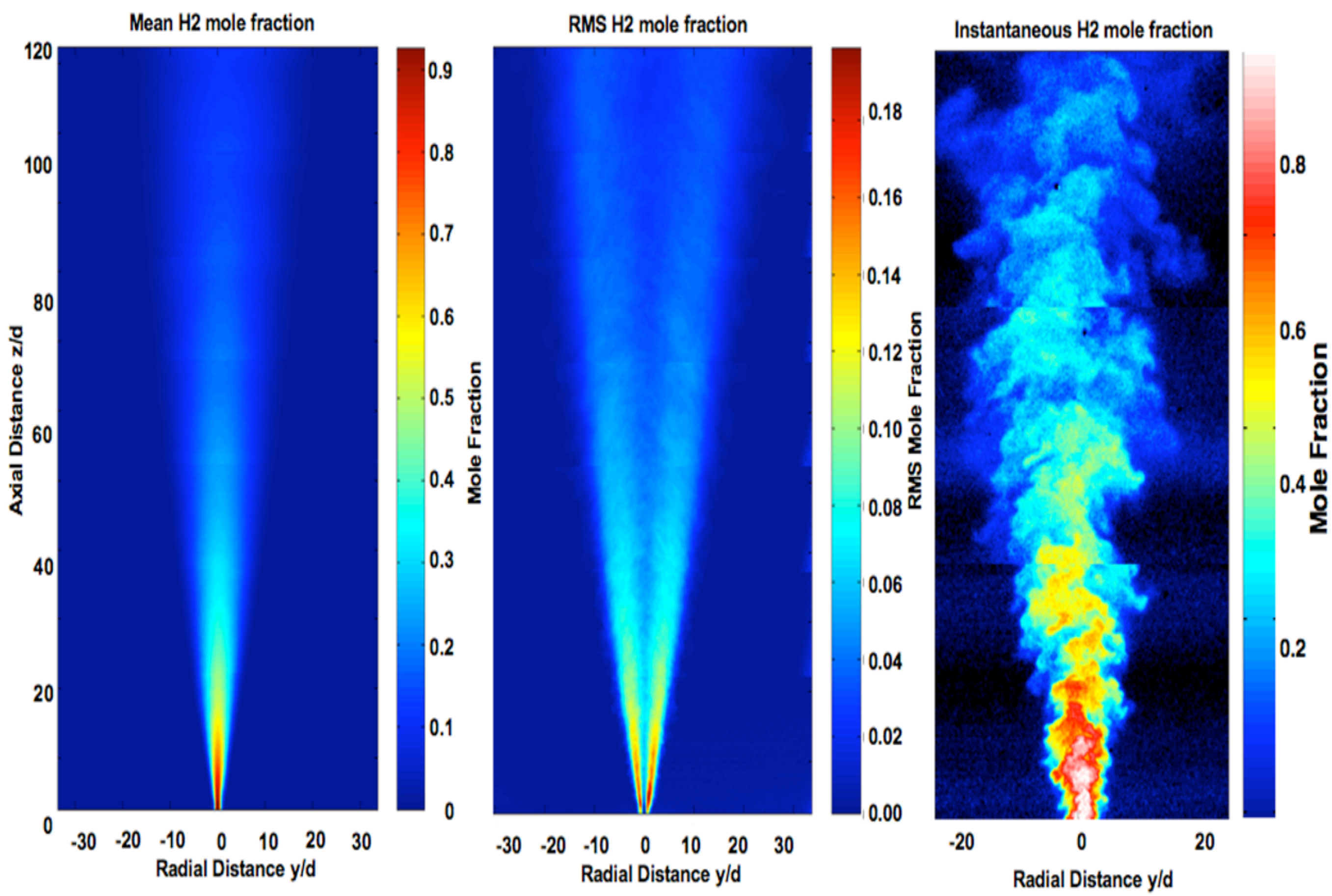
Small Unignited Releases: Vertical Jets

- Vertical H_2 Jet (d_j=1.9 mm)



- Time-averaged mean and fluctuating concentration field provides validation data and link to CFD modeled quantities.
- Single-shot images reveal instantaneous flow structure.
- Significant temporal fluctuations in H_2 at all locations in flow.

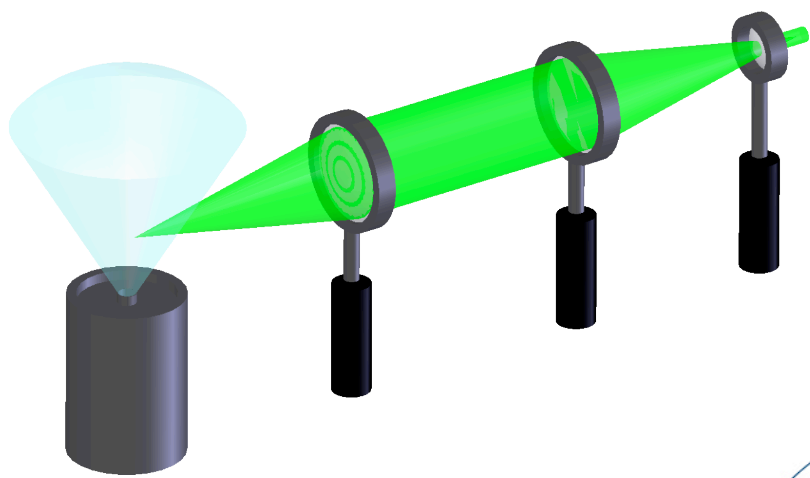
Jet Ignition Probability: Application to Unintended Releases

STRATEGY

- Rayleigh Data can be used to quantify time-averaged concentration field.
- Ignition experiments have been performed to determine ignitability characteristics of turbulent H_2 jet flows.
- A CH_4 jet has been investigated in order to compare work with earlier Birch et al. studies to validate experimental approach.

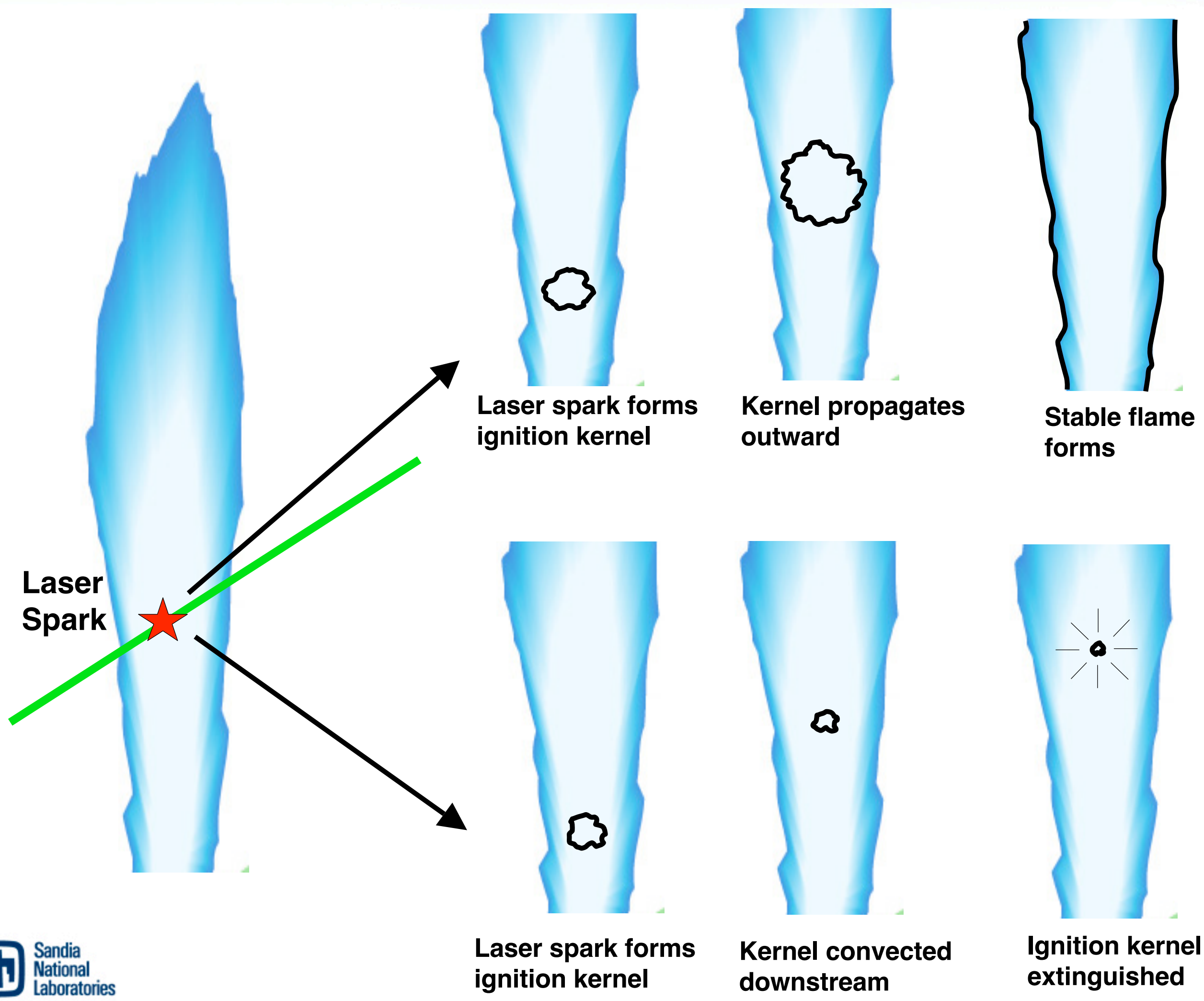
OPTICAL SPARK ARRANGEMENT

- Laser Spark generation possesses advantages over traditional spark generation (Birch studies)
  - Non-intrusive
  - Spark duration instantaneous compared to smallest turbulent scale
  - Laser energy greater than MIE
  - 532 nm Nd:YAG laser beam, with a pulse energy and duration of up to 1 Joule and 9-nsec, respectively, is focused using suitable optics to a 0.2 mm diameter spot, providing 100 mJ

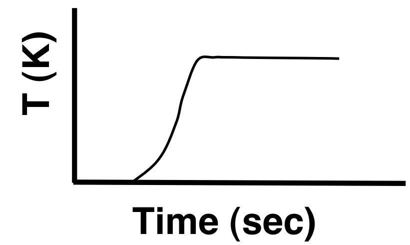


Jet Ignition Probability: Definitions

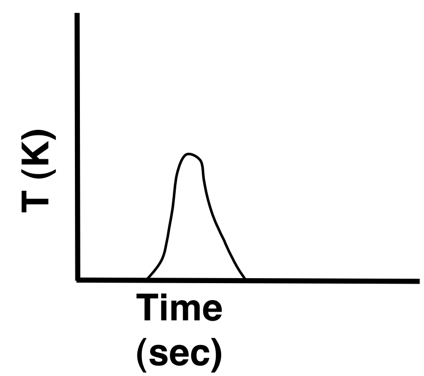
- **Methane jet studies revealed both local ignition and total flame lightup.**



- **Downstream Temperature Sensor Readout.**

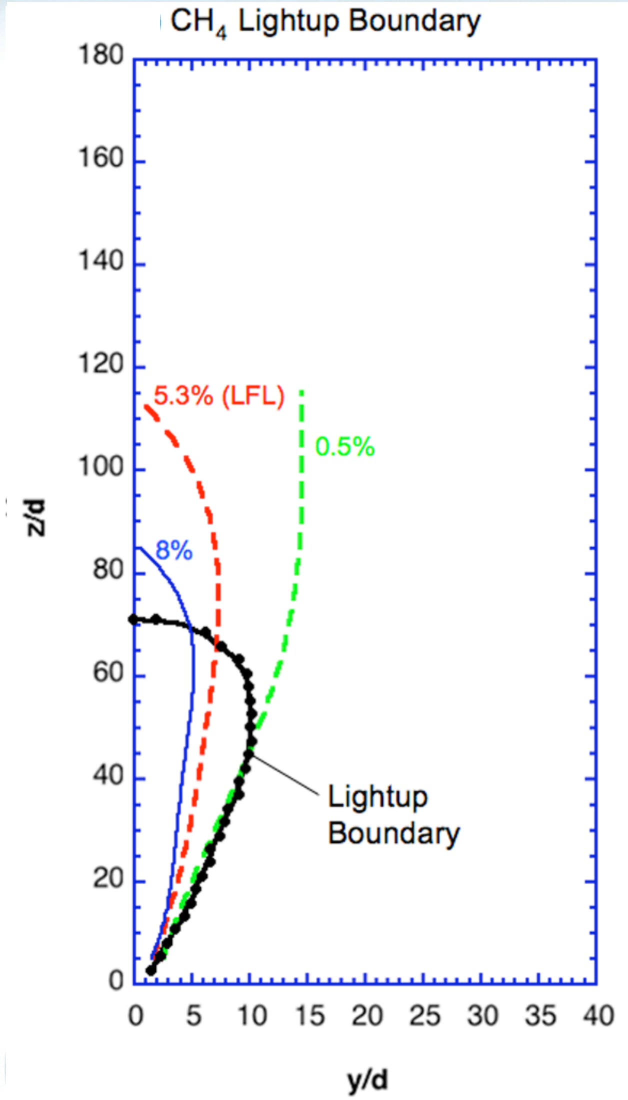


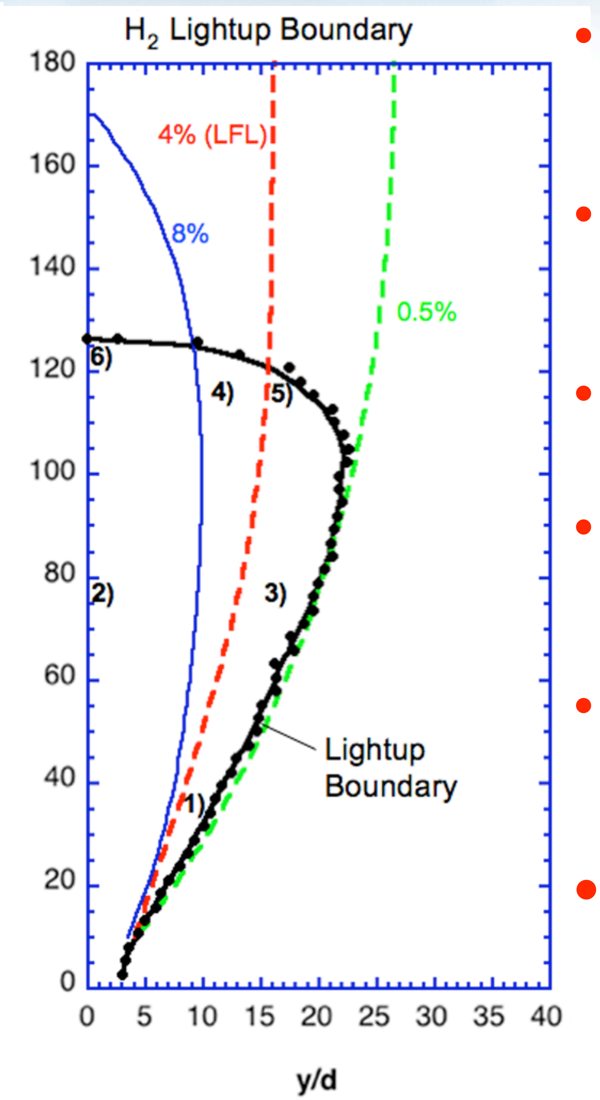
- **Define Lightup Probability, P_L, as probability stable jet flame forms.**



- **Define Ignition Probability, P_I, as probability of local ignition event.**

Jet light-up is possible over an interesting range of average concentration.





- **Flame light-up is defined as an ignition event that leads to stable flame.**
- **Jet Reynolds numbers are 2,384 and 3,406 for H_2 and CH_4 jets, respectively.**
- **H_2 jet ignition characteristics are similar to CH_4 jet.**
- **No flame lightup observed near jet centerline for H_2 volume fraction < 10% (in agreement with Swain).**
- **At outer radial locations flame lightup boundary closely follows 0.5% H_2 (<< LFL_{H2}).**
- *Important: contours are ensemble-averaged mean values*

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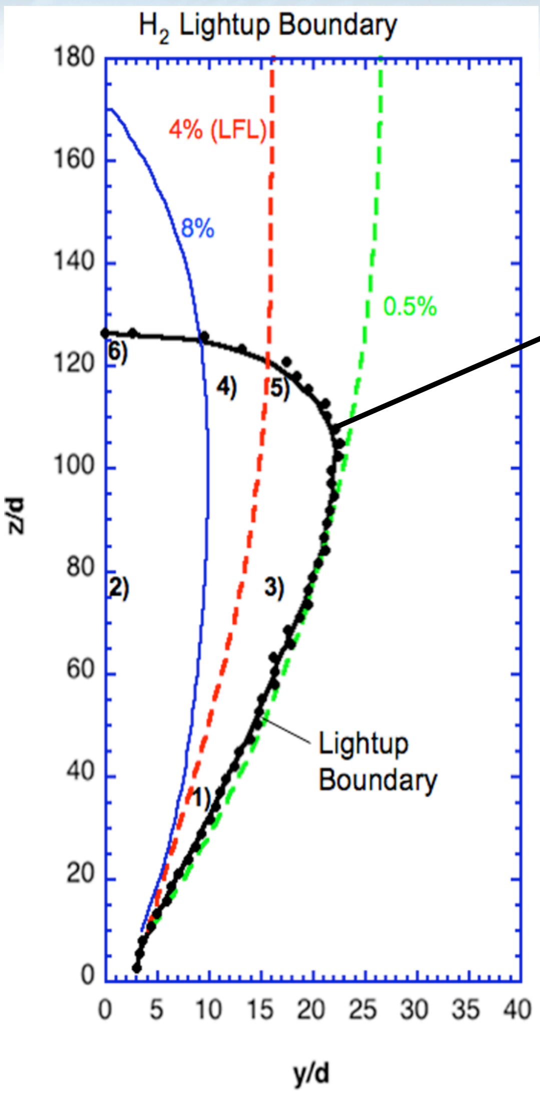
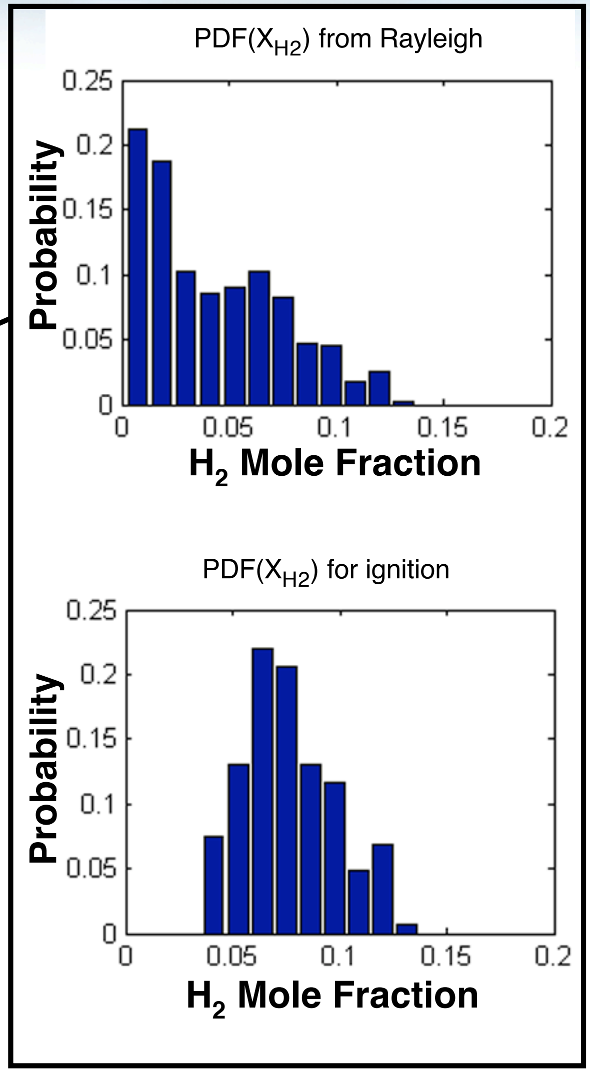
Ignition only occurs when concentration is within flammability limits.

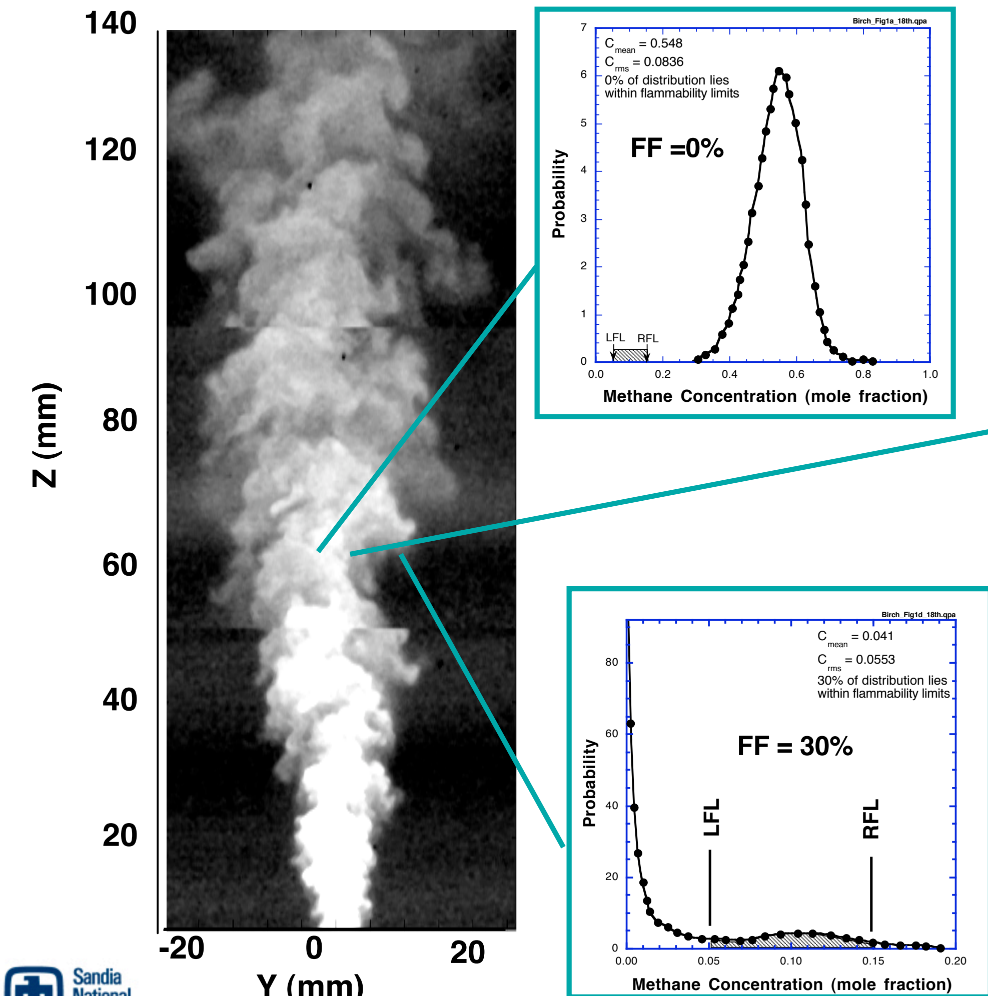




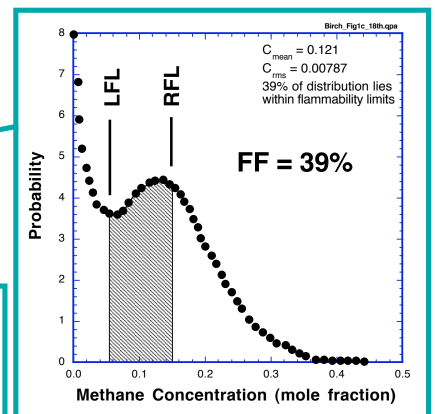
- **Unconditional PDF's of H_2 concentration at <u>outer radial locations</u> show significant contribution from pure air.**
- **Since at most times pure air occupies ignition location, time-averaged H_2 concentration is well below LFL.**
- **PDF's conditional on ignition show that ignition only occurs when the local concentration is within the H_2 flammability limits.**
- **Similar findings at other flow locations.**
- **Flammability limit concepts are valid at the location and time of ignition, but cannot be applied based on mean concentrations in turbulent flows.**

Jet Ignition Probability: Definitions

- **Methane jet into ambient air (Birch et. al., 1981)**



- **Concluded time-averaged concentration data are not a good measure of ignitability in turbulent flows.**
- **Probability distributions quantify intermittent nature of turbulent flows and must be used to determine ignition probability.**



Flammability Factor is defined as the cumulative probability of a potentially flammable mixture occurring at a given point.

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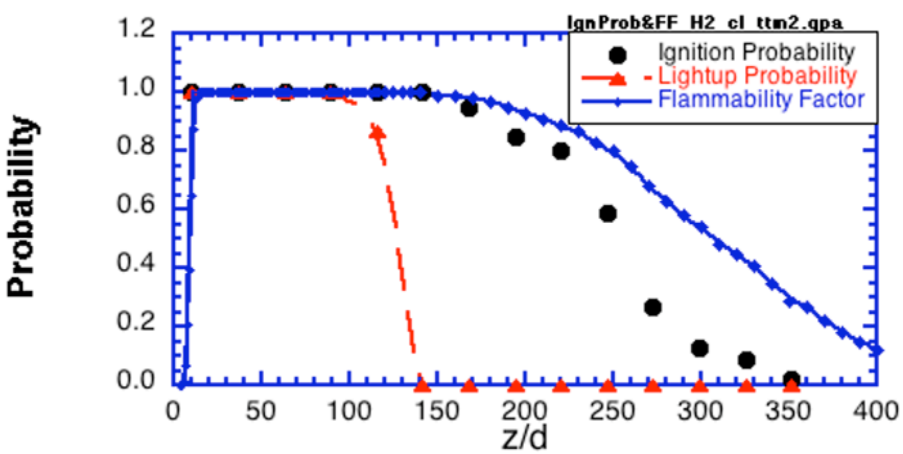
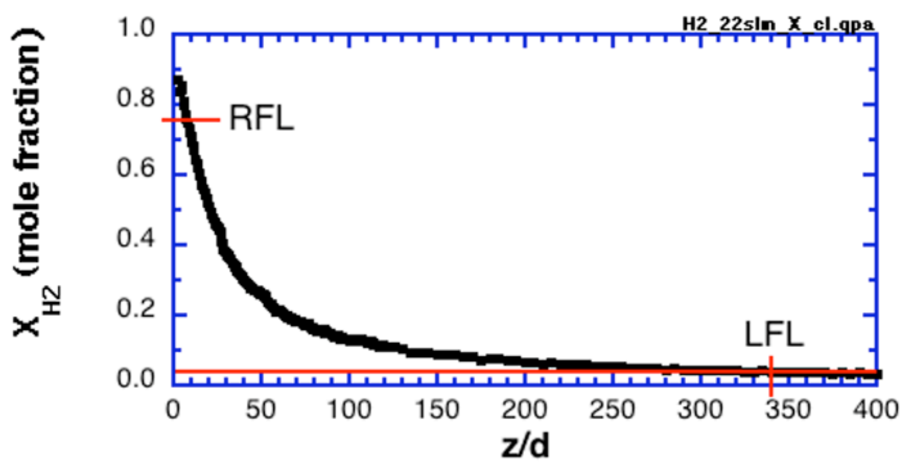
Jet Ignition Probability: Centerline Profiles

- Hydrogen jet (d_j=1.91 mm)

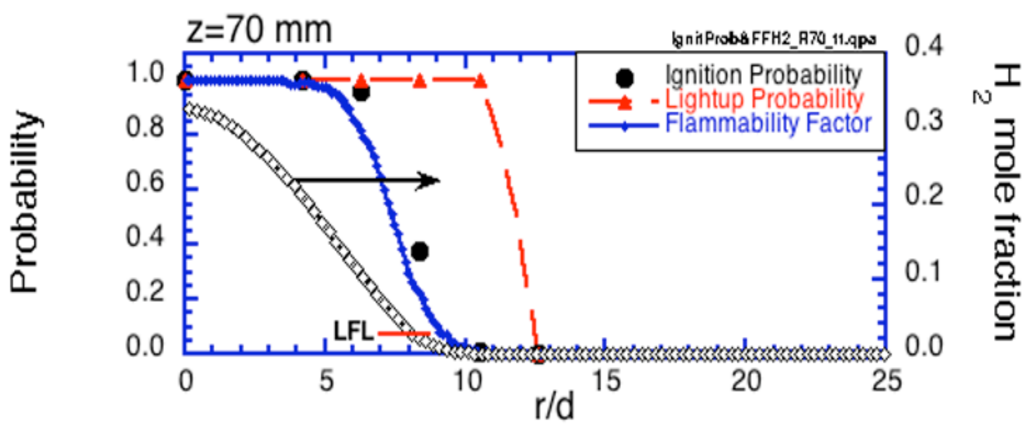


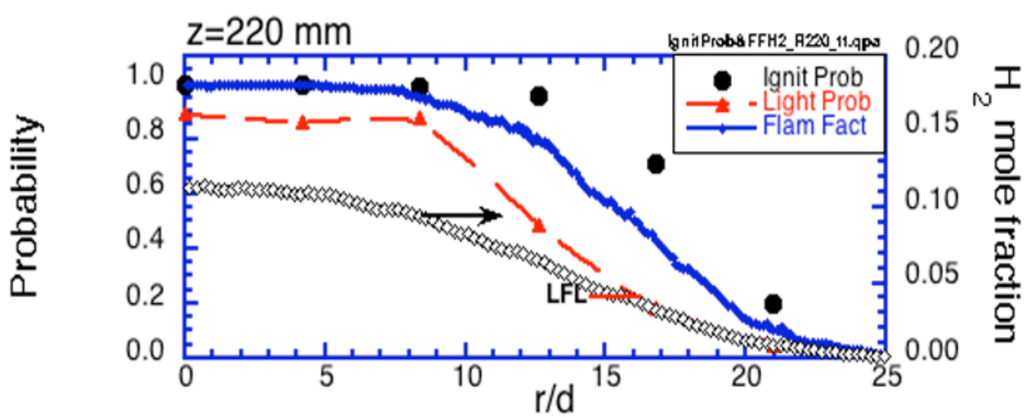


- Both P_L and P_I increase rapidly to unity downstream of jet exit.
- Between 5 < z/d < 120, both P_I and P_L are unity and every ignition leads to lightup.
- P_L decreases to zero at z/d=140 which corresponds to X_{H2}=0.10 (>2*LFL).
- Between 140 < z/d < 350 P_I is nonzero while P_L is zero and all ignitions are extinguished.
- Flammability Factor provides reasonable measure of ignitability upstream but falls off more gradually than P_I.

Jet Ignition Probability: Radial Profiles

- **Hydrogen jet (d_j=1.91 mm)**

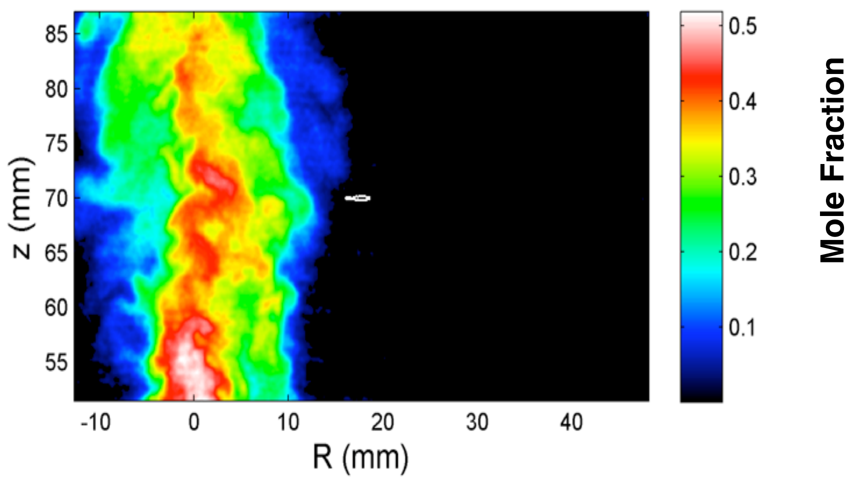




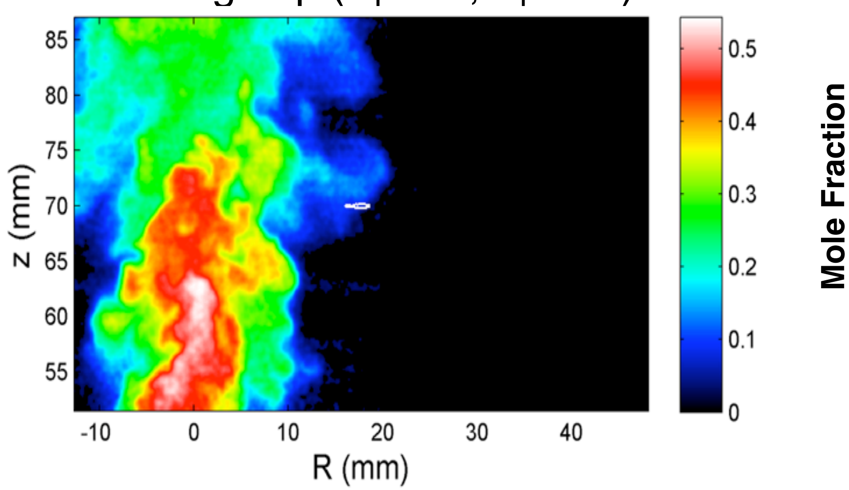
- **P_I and P_L are both unity in central jet and decrease to zero at outer radial locations due to mixing with excess air.**
- **Width of region where ignition occurs increases with downstream distance.**
- **Both ignition and lightup are observed at radial locations where mean H_2 concentration is below static flammability limits.**
- **Flammability factor provides a good measure of ignitability at outer radial locations.**

Jet Ignition Probability: Ignition Point Concentration Contours

- No Lightup (P_I=0.1; P_L=1.0)



- Jet Lightup (P_I=0.1; P_I =1.0)



- **Instantaneous concentration distribution near ignition point at radial location in outer jet shear layer.**
- **In the upper image no local ignition occurred since pure air occupied the ignition volume.**
- **In the lower image both local ignition and jet lightup occurred since mixed H_2/air was present at the ignition point and within the flammability limits.**

A modeling approach has been developed to predict the ignition probability in a turbulent jet flow.

Goals:

- **Construct and validate a relatively simple model to predict ignition probability of H_2 in turbulent flows;**
- **If successful, use the model to create comparison maps between ignition probability and static flammability limits of H_2 in complex flows (e.g., impinging and recirculating flows), providing a technical basis for safety distances in hydrogen codes and standards.**

Background:

- **Lower and Upper (lean and rich) Flammability Limits (LFL and UFL) are known for static, homogeneous mixtures of fuel and air.**
- **Use of average concentration of fuel (e.g., mole fraction $\overline{X}_{\text{fuel}}$) to evaluate LFL and UFL is not valid for a turbulent flow due to differences between mean and instantaneous values caused by turbulent fluctuations.**

Procedure:

- **A statistical approach to prediction of ignition probability (PI) has been shown to work well for turbulent jet flows of natural gas, propane, and town gas (Birch et al., 1981; Smith et al., 1986)**

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The method is based on using probability density functions to compute the flammability factor.

- **Flammability Factor (FF) is defined as the integral of a probability density functi (PDF) over the static flammability limits of the fuel:**

$$\mathrm{FF} = \int_{X_{\mathrm{fuel}_{\mathrm{LFL}}}}^{X_{\mathrm{fuel}_{\mathrm{UFL}}}} \mathrm{P}(X_{\mathrm{fuel}})dX_{\mathrm{fuel}}$$

- **A Gaussian (normal) PDF works well along the centerline of a turbulent jet flow because the intermittency factor γ=1**

$$\mathrm{P}_{\mathrm{G}}(X_{\mathrm{fuel}}) \equiv \frac{1}{\sqrt{2\pi \overline{X'^2_{\mathrm{fuel}}}}} \exp\left[-\left(X_{\mathrm{fuel}} - \overline{X}_{\mathrm{fuel}}\right)^2 \Big/ \left(2\overline{X'^2_{\mathrm{fuel}}}\right)\right]$$

- **Off jet centerline γ<1 and a composite PDF includes a delta function to describe the finite probability of occurrence of pure air:**

$$P_c(X_{fuel}) = (1-\gamma)\delta(\varepsilon)[H(X_{fuel}) - H(X_{fuel} - \varepsilon)] + \gamma P_G(X_{fuel})[H(X_{fuel}) - H(X_{fuel} - 1)]$$

- **Parameters, $\overline{X}_{\mathrm{fuel}}$ (mean), $\overline{X'^2_{\mathrm{fuel}}}$ (variance), and γ obtained either from experiment o modeled transport equations; $H(x)$ is the Heaviside step function where $H(x) = 0$ for $x < 0$; $H(x) = 1$ for $x \geq 0$; ε is a small and δ is defined such that:**

$$\int_0^1 \mathrm{P}_{\mathrm{c}}(X_{\mathrm{fuel}})dX_{\mathrm{fuel}} = 1 \qquad \gamma = \frac{K+1}{\overline{f'^2}/\overline{f}^2 + 1} \; ; \; K = 0.25$$

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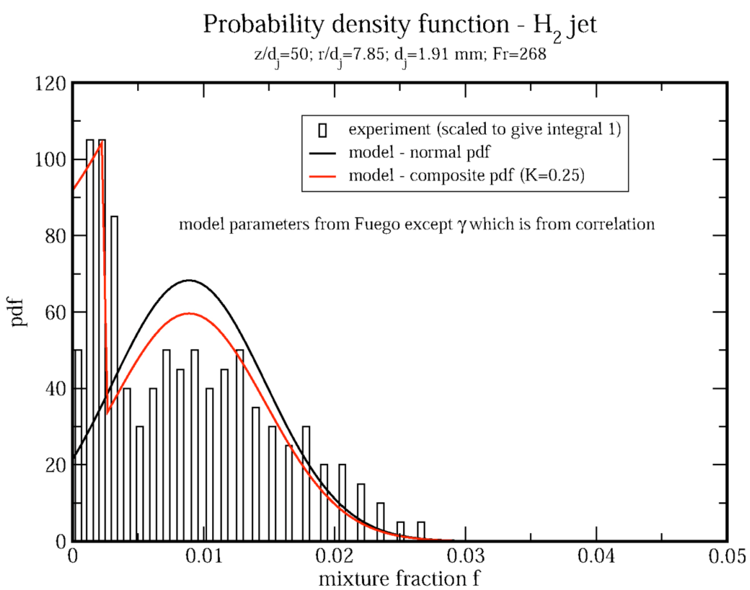
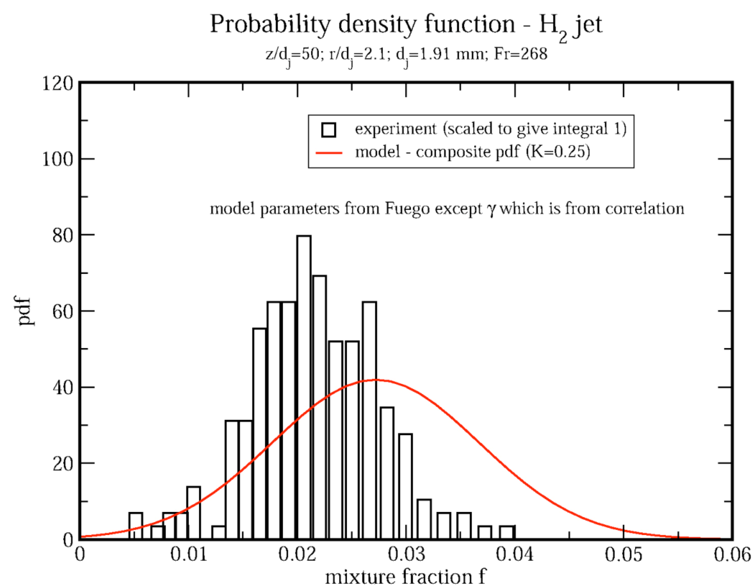
A bimodal PDF is required in regions of intermittency.

- **Composite PDF agrees well with measured PDF in shear layer of H_2 jet at r/d_j=7.85, z/d_j=50 (here the empirical relation for γ gives γ=0.87)**
- **Closer to jet centerline, at r/d_j=2.1, PDF is approximately Gaussian and γ=1**
- **FF is integral of PDF; errors in PDF may get averaged out**

bimodal at r/d_j=7.85; γ=0.87



approx. Gaussian at r/d_j=2.1; γ=1.0



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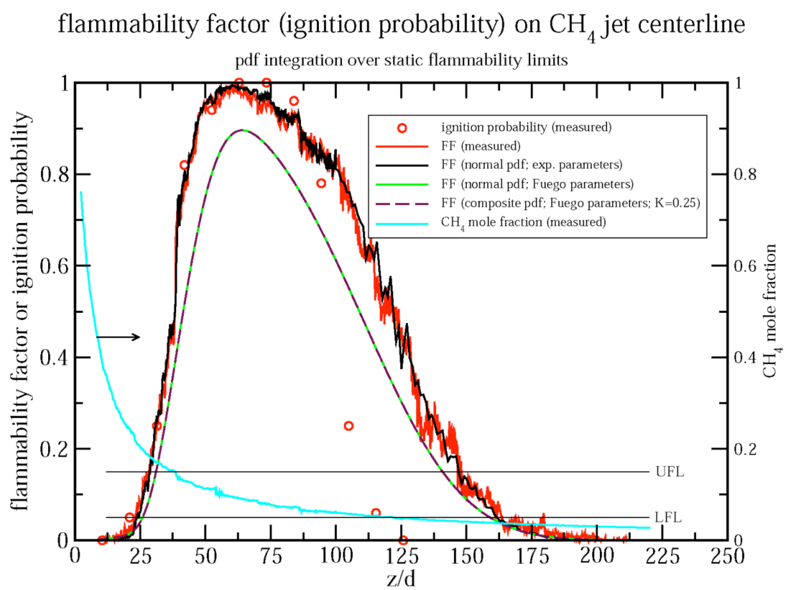
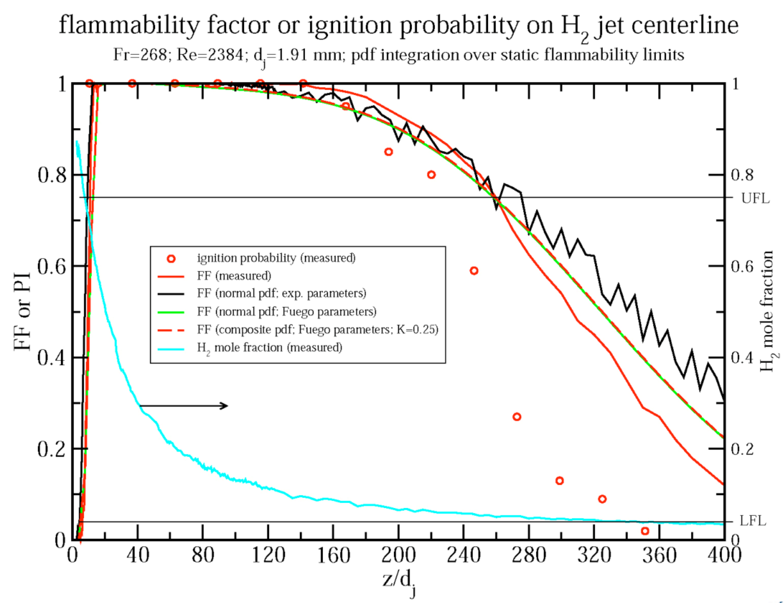
The ignition model has been validated for turbulent jet flows.

- **Good agreement between FF computed using parameters (mean $\bar{X}_{\text{fuel}}$ and rms $\sqrt{\overline{X'^2_{\text{fuel}}}}$) obtained from either experiment or from the solution of transport equations along centerlines of turbulent jets of CH_4 and H_2**

- **No difference along centerline of jet between FF computed with either Gaussian or composite PDFs (Note: $\gamma \approx 1$ on centerline)**





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Jet Ignition: Summary and Future Work

- Hydrogen flammability limits are well established in static systems. New flammability limit studies are not needed.
- Time-averaged concentration contours and static flammability limits are not a good measure of ignitability in turbulent flows.
- Flammability Factor is a more realistic measure of ignitability in turbulent flows.
- Conditional concentration distributions at time and location of ignition shows that local H_2/air mixture must be within static flammability limits for ignition to occur.
- Whether local ignition leads to flame lightup likely depends on local turbulence characteristics (length and time scales, turbulence intensity and strain rates) that results in flame extinction.
- Validation of a model for predicting flammability factor (FF) or probability of ignition (P_I) in a turbulent jet flow has been carried out
    - Extension of the model to more complex flows is a primary goal