

# Mixture Formation and Combustion in a Hydrogen-Fueled Internal Combustion Engine

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# H<sub>2</sub>ICEs: A bridge to the hydrogen economy

- **Technology is available today and economically viable in the near-term.**
- **Number of test/demo vehicles: Ford, BMW among others (see below).**
  - demonstrated efficiencies in excess of today's gasoline engines.
  - operate cleanly (NO<sub>x</sub> is the only emission pollutant)
- **Fewer constraints concerning H<sub>2</sub> storage compared to fuel cells.**
  - relative ease of a dual-fuel option (H<sub>2</sub>/gasoline).
  - impurities are a non-issue



# U.S. DOE's interest in the H<sub>2</sub>ICE

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- H<sub>2</sub>ICEs are part of DOE's transitional strategy towards a hydrogen economy.
  - [www.hydrogen.energy.gov/pdfs/hydrogen\\_posture\\_plan.pdf](http://www.hydrogen.energy.gov/pdfs/hydrogen_posture_plan.pdf)
- DOE's near-term goals for the H<sub>2</sub>ICE (same as for fuel cell vehicle):
  - peak brake thermal efficiency (BTE)  $\geq 45\%$ .
  - Tier2/bin5 emissions or better ( $\text{NO}_x \leq 0.07\text{g/mile}$ ).
  - power densities greater than present-day gasoline engines.
- Research is required to resolve technical barriers to meet these goals.
  - fundamental research of in-cylinder combustion and transport processes.
  - $\text{NO}_x$  emissions and control.
  - advanced H<sub>2</sub>ICE concepts and related technical issues:
    - pressure boosting (preignition, CR effects, heat transfer, etc)
    - direct-injection (in-cylinder mixing, injector durability, etc) **MOST PROMISING**

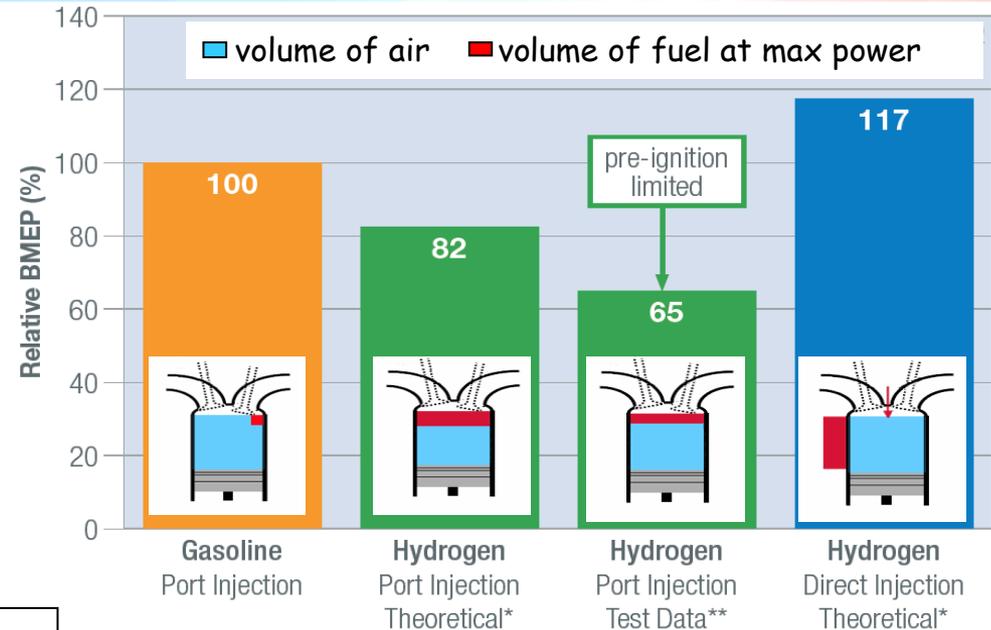
# Direct-injection (DI) H<sub>2</sub>ICEs

## Benefits:

- power density improvement  
→ no displacement of air by H<sub>2</sub>
- mitigate preignition  
→ optimize injection timing
- multiple degrees of freedom  
→ improved efficiency  
→ reduced emissions

## Technical challenges:

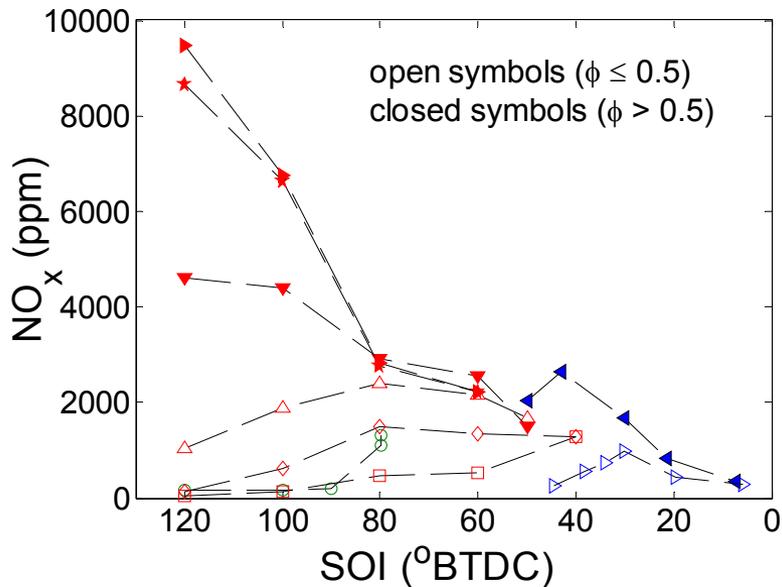
- high-pressure, high-flow rate injector  
→ durability issues
- short available mixing times  
→ 1–20 ms depending on engine speed and injection timing.



**Mixture distribution at onset of combustion is critical to engine performance and emissions.**

# Mixture stratification in a DI-H<sub>2</sub>ICE

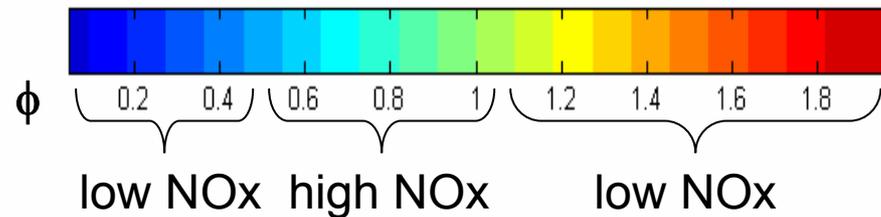
## Effect of start-of-injection on NO<sub>x</sub> emissions



**Conjecture:**  
**Mixture inhomogeneities**



Mixture formation	$\phi = 0.3$	$\phi = 0.8$
well-mixed		
stratified		



# Sandia H<sub>2</sub> research engine facility



## Optical test engine

### GM single-cylinder head

- 4 valves, central spark plug
- 560 cm<sup>3</sup> displacement
- CR: 9.1 (flat piston)

### Optical access

- interchangeable quartz liner
- interchangeable quartz piston

### Hydrogen fueling

- side direct injection (Westport Innov.)



## Approach

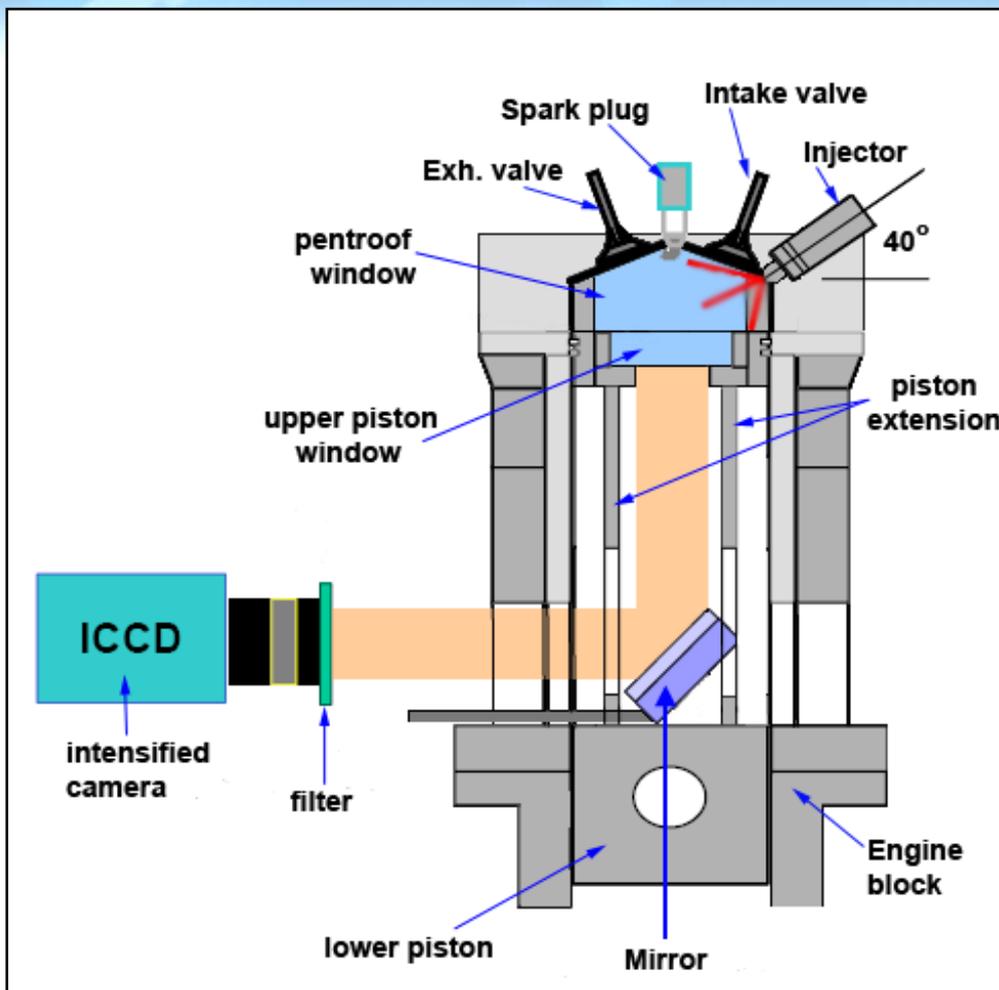
- focus on evaluation of in-cylinder mixing processes in a DI-H<sub>2</sub>ICE
- systematic experiments
  - OH chemiluminescence imaging
  - planar laser induced fluorescence (PLIF)
  - particle image velocimetry (PIV)

# OH chemiluminescence experiment

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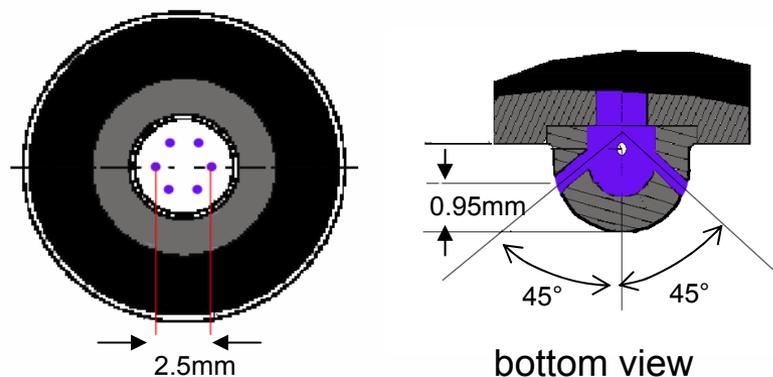
- **Relatively simple experimental technique.**
  - Natural flame luminosity due to chemical reaction that creates excited state OH.
  - OH\* has a unique emission spectra with a peak about 308 nm.
- **Characterize flame front propagation characteristics**
  - OH\* is a combustion intermediary that tracks heat-release (i.e. flame front)
- **Evaluate mixture formation for DI operation using premixed operation as a baseline.**
  - use OH chemiluminescence intensity as a metric for equivalence ratio.
    - ⇒ intensity increases exponentially with equivalence ratio
  - use OH chemiluminescence distribution as a metric for mixture homogeneity.
- **Limitations**
  - line-of-sight measurement
  - qualitative (at best semi-quantitative)
  - time integrated (weak signal  $\approx$  1 CAD at 1200 rpm)

# OH chemiluminescence experimental set-up



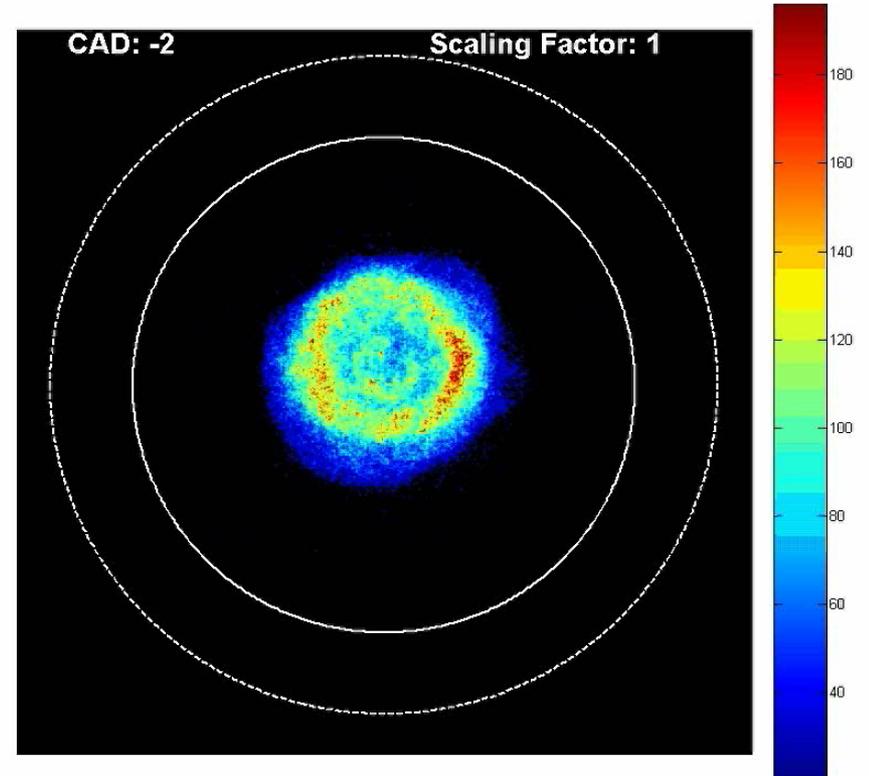
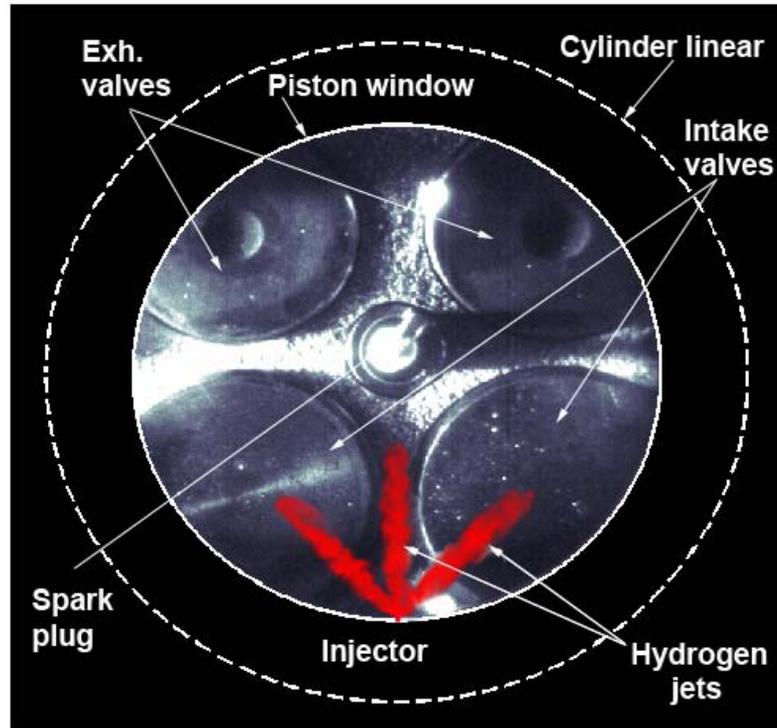
## H2 DI Injector (Westport Innov.)

- Solenoid type injector
- six hole,  $D = 0.56\text{mm}$
- jet angles  $45^\circ$  wrt to injector axis



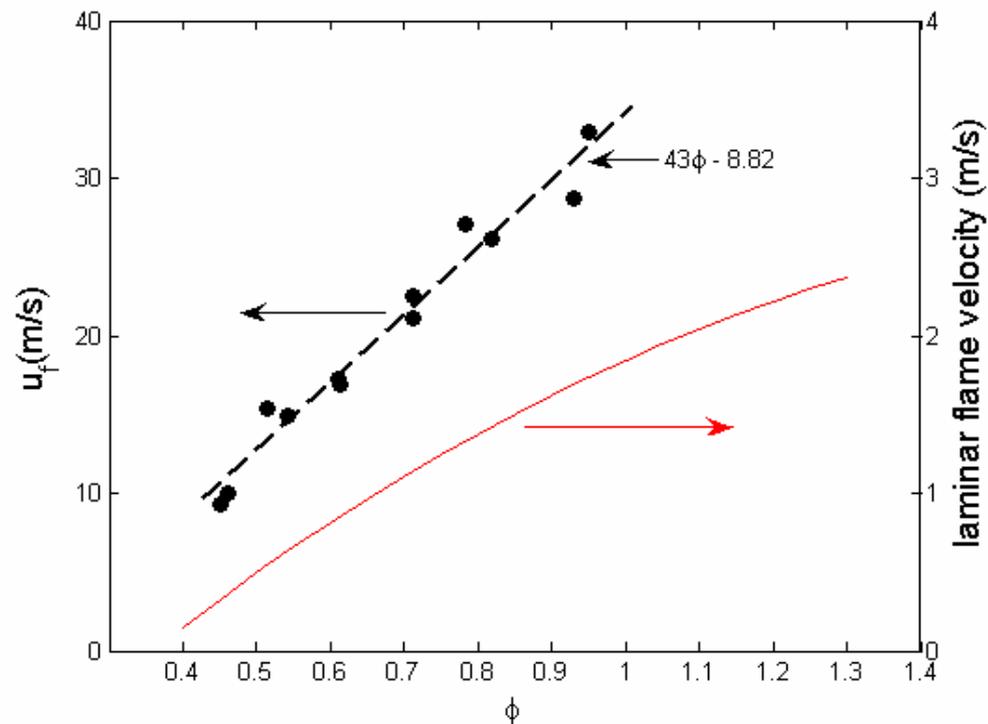
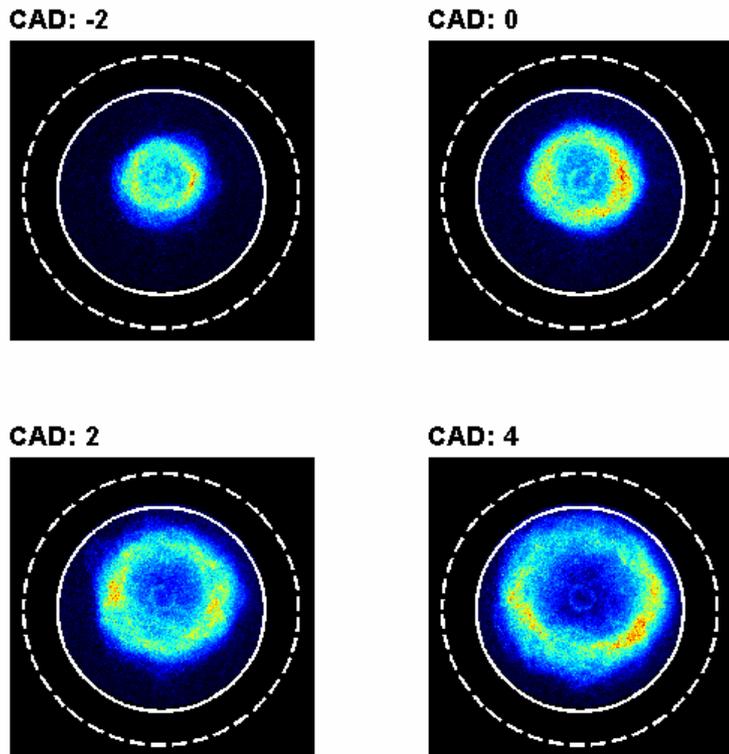
Engine Speed	1200 rpm
Intake air pressure (BDC)	50 kPa
"Premixed" fueling (SOI/EOI)	-270/-240 CAD
Direct injection fueling (SOI)	Later than -112 CAD

# Ensemble-averaged OH\* image movie: $\phi = 0.51$ (premixed); spark = -11CAD;



Color bar corresponds to OH chemiluminescence intensity

# Flame front expansion speed (“premixed”)



$$u_f = \frac{dr_f}{dCAD} \cdot \frac{dCAD}{dt}, \text{ where } r_f \text{ is the flame radius and } t \text{ is time.}$$

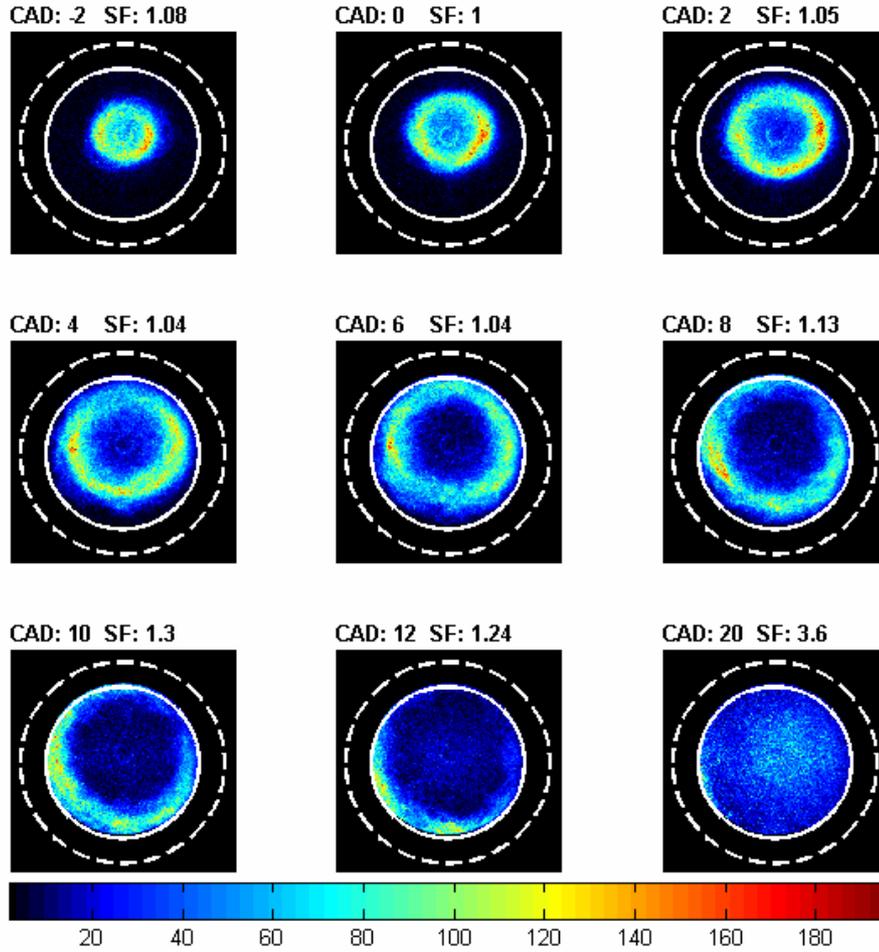
Note:  $u_f$  approximates the burned gas expansion speed

# Experimental conditions for DI operation

Case	H <sub>2</sub> Inj. Press (MPa)	MBT Spark (CAD)	Images at CAD	SOI (CAD)	EOI (CAD)	global $\phi$
i	2.5	-8	0, 1, 2, 3, 4, 5, 6, 7, 11	-112	-62	0.56
ii	2.5	-11	-3, -2, -1, 0, 1, 2, 4, 8, 12	-90	-40	0.56
iii	2.5	-11	-3, -2, -1, 0, 1, 3, 4, 8, 12	-77.5	-27.5	0.58
iv	10	-8	0, 1, 2, 3, 4, 5, 6, 7, 16	-112	-99.5	0.53
v	10	-8	0, 1, 2, 3, 4, 5, 6, 11, 16	-90	-77.5	0.53
vi	10	-5	0, 1, 2, 3, 4, 5, 6, 11, 16,	-70	-57.5	0.54
vii	10	-11	-3, -1, 1, 3, 8, 12, 16, 20, 28	-50	-37.5	0.53
viii	10	-11	-3, -1, 1, 3, 8, 12, 16, 20, 28	-40	-27.5	0.53

- Global equivalence ratio  $\approx 0.55$  (near the knee in NO<sub>x</sub> curve).
- Two injection pressures:
  - $P_{inj} = 25$  bar and  $\Delta_{inj} = 50$  CAD
  - $P_{inj} = 100$  bar and  $\Delta_{inj} = 12.5$  CAD
- SOI sweep (IVC is at -112 CAD).

# Baseline ensemble-averaged images: $\phi = 0.51$ (premixed); spark = -11CAD;



Color bar corresponds to OH chemiluminescence intensity

- Radial “flame” development
- “Flame” front is beyond field-of-view after 8 CAD.
- Peak intensities 190 counts.  
– fairly low signal!
- SF is a multiplicative scaling factor based on maximum intensity (utilize the same color bar)

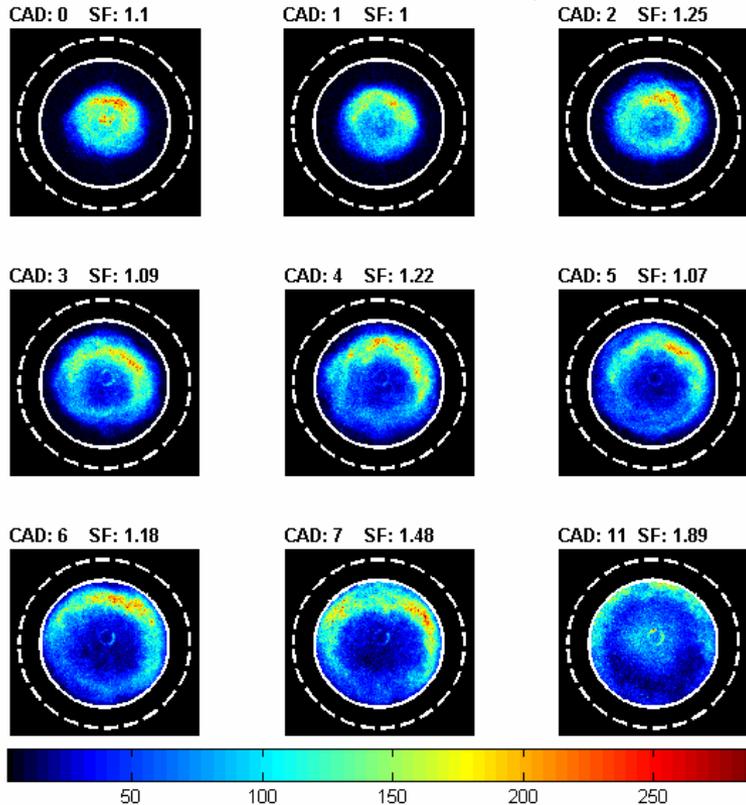
## Next few slides:

**Evaluate mixture formation for DI compared to premixed operation.**

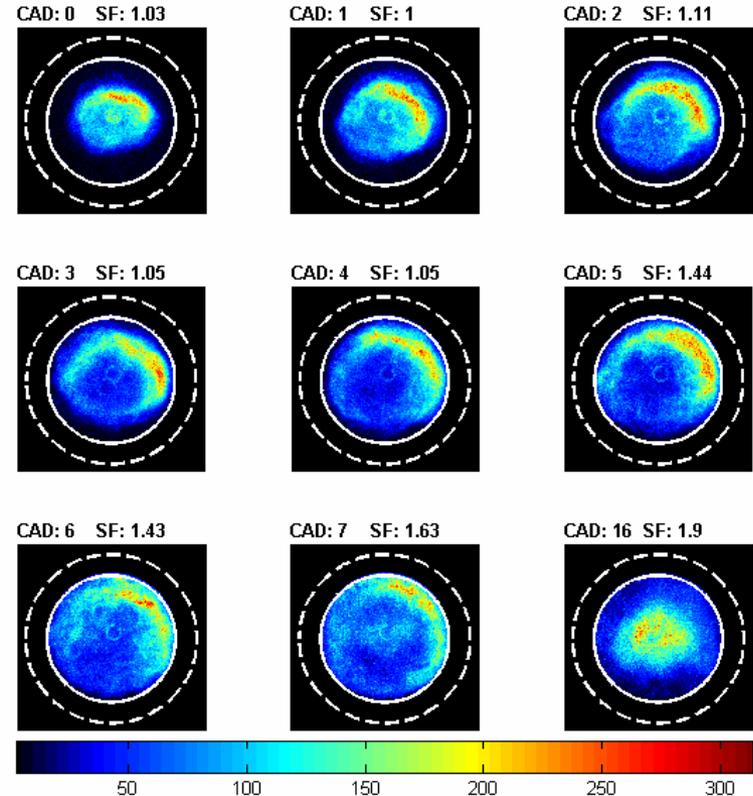
- (1) use OH chemiluminescence intensity as a metric for equivalence ratio.
- (2) use OH chemiluminescence distribution as a metric for mixture homogeneity.

# Early Injection: SOI at IVC, spark = -8CAD

$P_{inj} = 25 \text{ bar}$ ,  
SOI(-112)/EOI(-62),  $\phi_{global} = 0.56$



$P_{inj} = 100 \text{ bar}$ ,  
SOI(-112)/EOI(-99.5),  $\phi_{global} = 0.53$



## Main observations

- Intensity scale similar to premixed case.  
→  $\phi_{local} \approx \phi_{global}$
- Radial “flame” development.
- High intensities opposite injector.

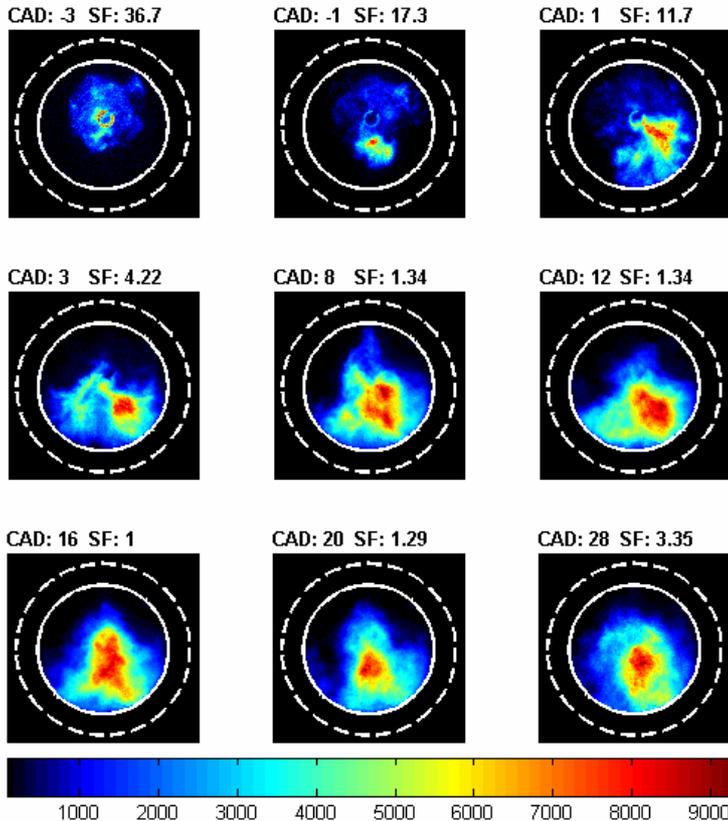


## Summary:

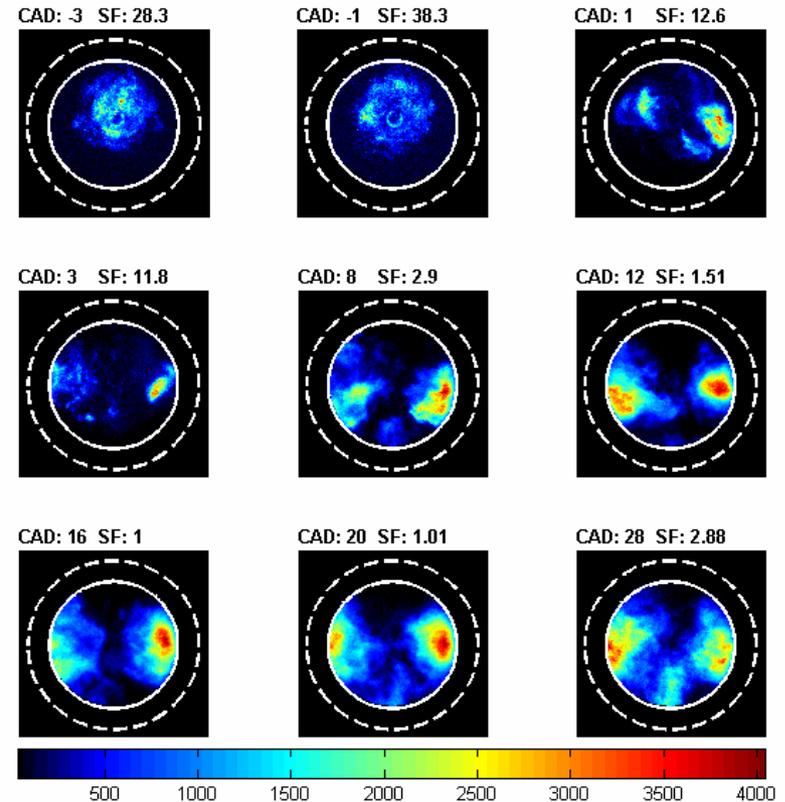
- Near-homogeneous mixture
- Similar characteristics as premixed case
- Little difference with injection pressure

# Late Injection: EOI at -27.5CAD, spark = -11CAD

$P_{inj} = 25$  bar,  
SOI(-77.5)/EOI(-27.5),  $\phi_{global} = 0.57$

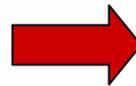


$P_{inj} = 100$  bar,  
SOI(-40)/EOI(-27.5),  $\phi_{global} = 0.53$



## Main observations

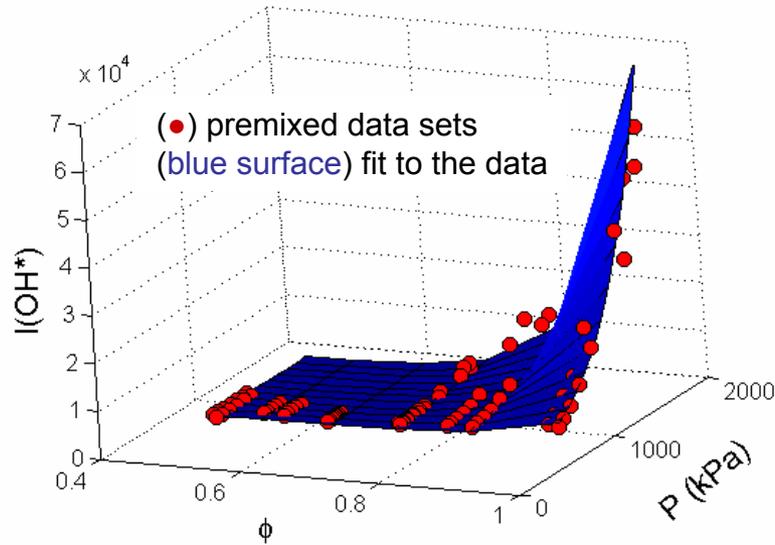
- Intensity scale greater than premixed case.
  - $\phi_{local} > \phi_{global}$
- No clear flame front.
- High intensity local regions.



## Summary:

- Strongly heterogeneous mixture
- Significant difference with injection pressure
  - intensity scale
  - spatial distribution

# Empirical relationship



## Four parameter fit:

$$I = AP^B \exp(CP^D \phi)$$

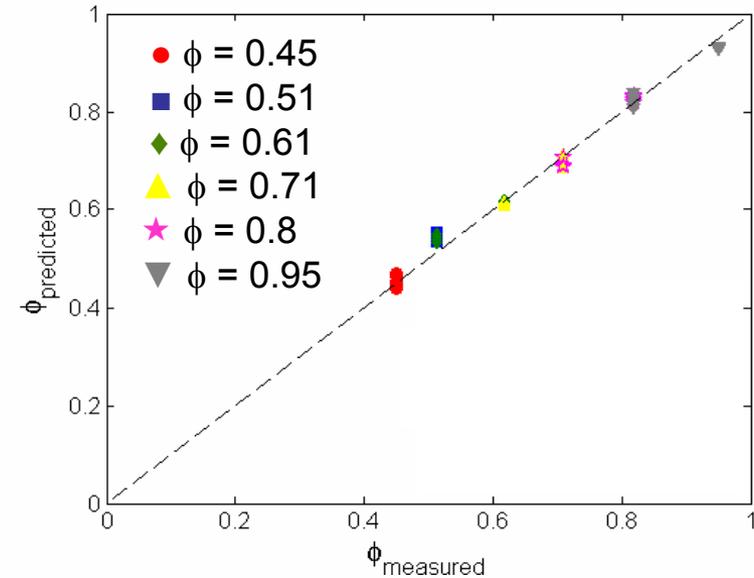


$$\phi_{\text{predicted}} = \frac{\ln(I / AP^B)}{CP^D}$$



Evaluate  $\phi_{\text{local}}$  during combustion from measurement of  $I$  and  $P$ .

## Premixed data sets

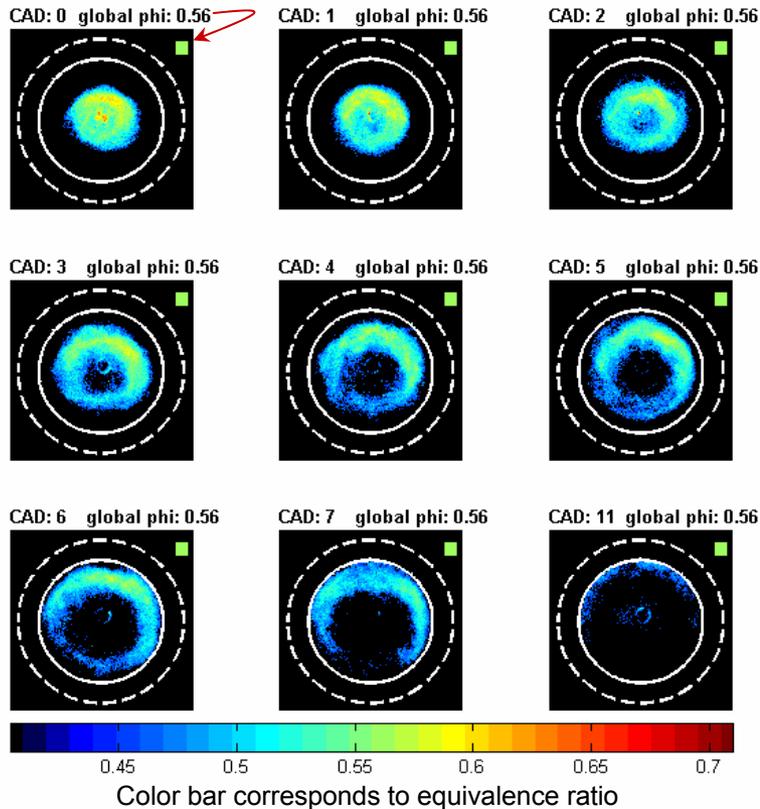


- measure of how well the empirical relationship fits the data.
- % difference is within  $\pm 8\%$

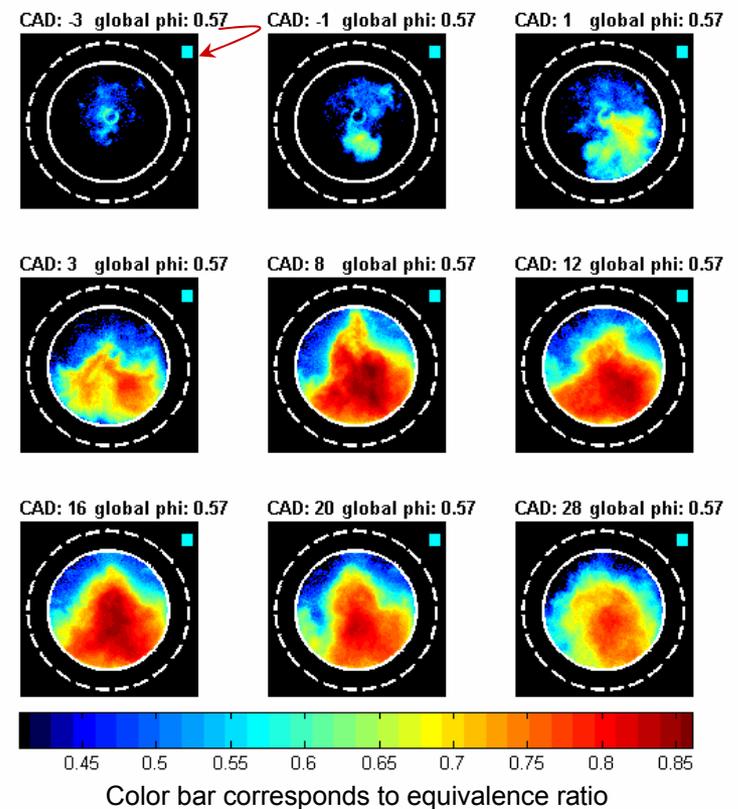
$$\% \text{ difference} \equiv (1 - \phi_{\text{predicted}} / \phi_{\text{measured}}) \times 100$$

# Evaluation of $\phi$ from $I(\text{OH}^*)$ for DI data-sets

$P_{\text{inj}} = 25 \text{ bar}$ ,  
 SOI(-112)/EOI(62),  $\phi_{\text{global}} = 0.56$



$P_{\text{inj}} = 25 \text{ bar}$ ,  
 SOI(-77.5)/EOI(-27.5),  $\phi_{\text{global}} = 0.57$



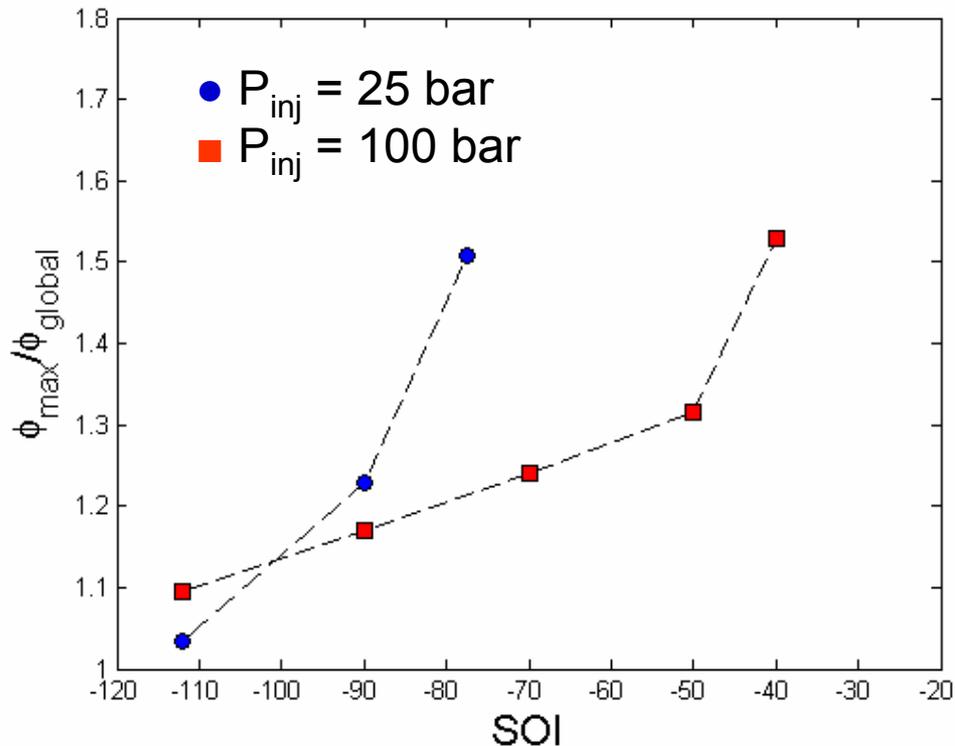
## Main observations

- Method is valid only for max  $\phi$  on flame front.
  - inherent limitation of the method.
- equivalence ratio on flame front similar to global equivalence ratio (credence to method)

## Main observations

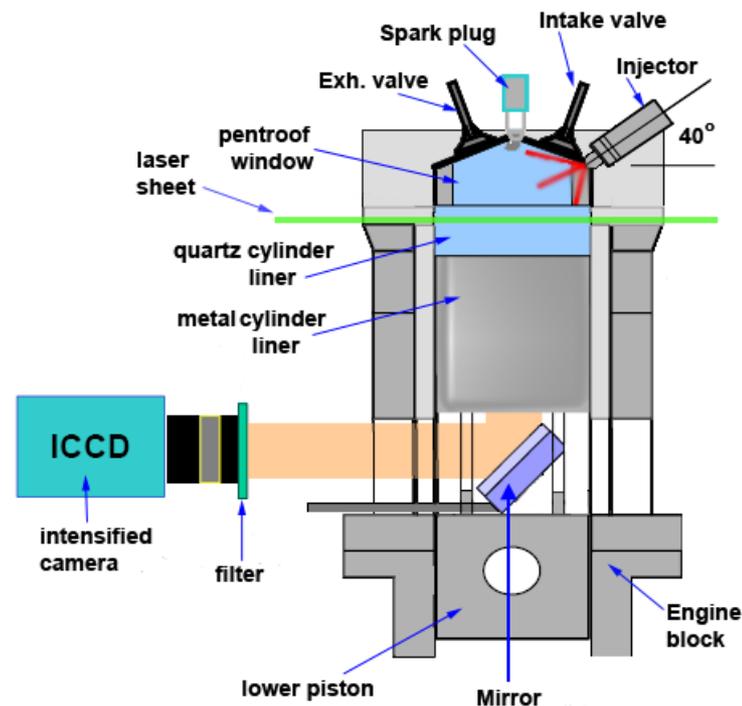
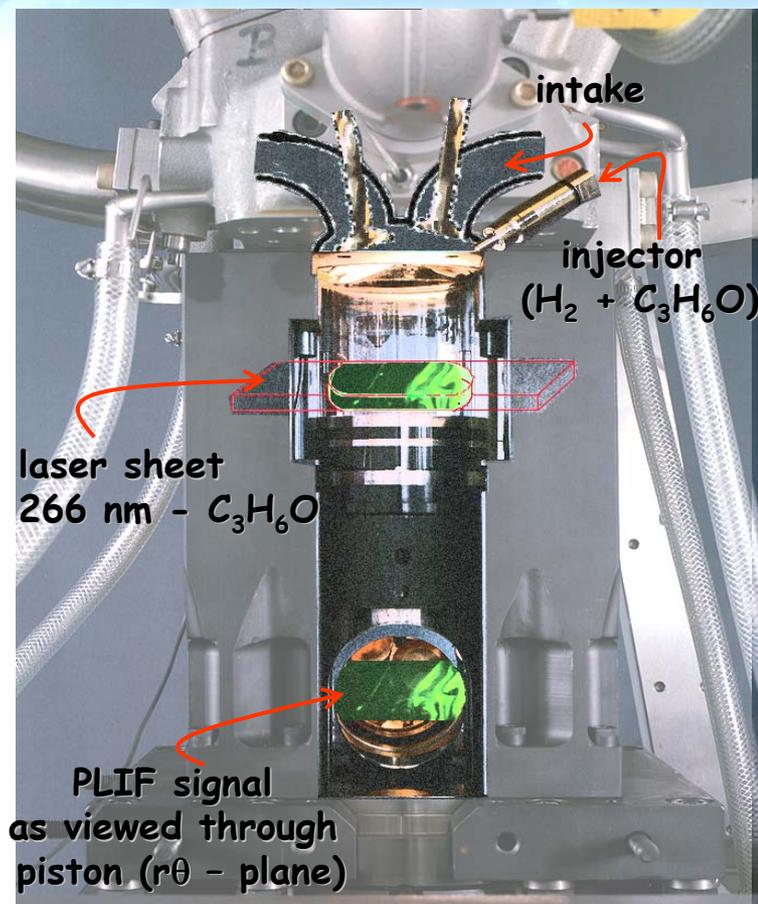
- No clear flame front (interpretation difficult)
- Limited to looking at max  $\phi$  during cycle

# Maximum equivalence ratio verses SOI



- Maximum local equivalence ratio increases monotonically with retard of SOI for both injection pressures.
- Results agree with trends of  $\text{NO}_x$  emission with retard of SOI (in the literature).
- Excellent “starting point” for advanced laser-based diagnostics.

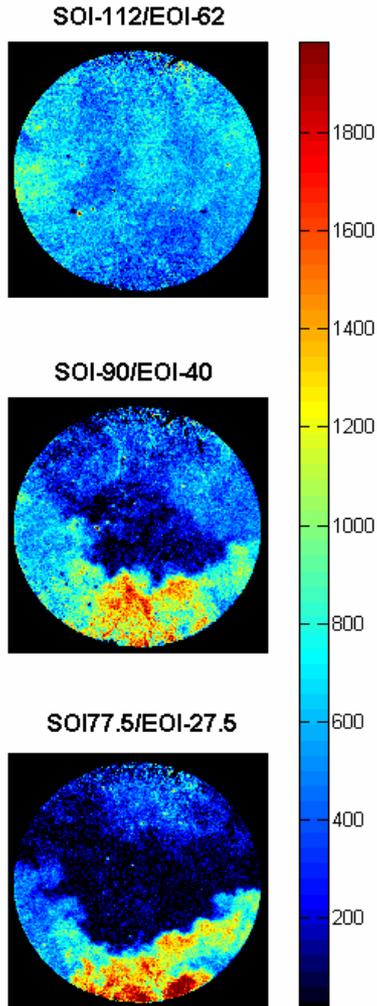
# PLIF experimental set-up



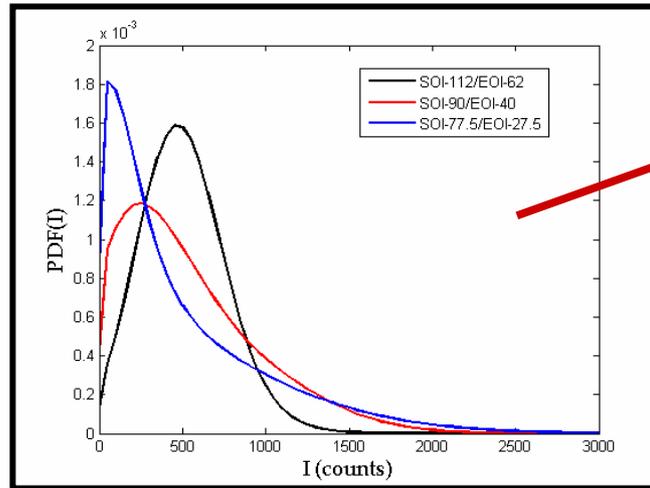
Engine Speed	1200 rpm
Intake air pressure (BDC)	50 kPa
$P_{inj}$	25 bar
global_φ	0.55
Acetone mole fraction	$5 \times 10^{-3}$

# PLIF Results

Representative Images  
(100 images per SOI)

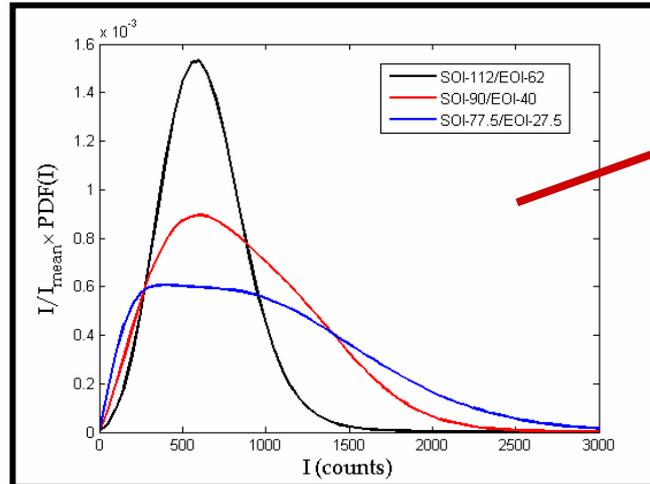


## PDF of Intensity



Retard of SOI produces increasing regions of low and high intensity

## Weighted PDF of Intensity



**Proportional to fuel mass distribution:**  
With retard of SOI fuel mass is increasingly concentrated in small volumes that are locally "rich".

# Summary and Conclusions

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- Measured flame front propagation speeds for “premixed” hydrogen-air mixtures for various equivalence ratios.
- DI operation with SOI at IVC produces similar results as premixed operation.
  - little difference between low and high injection pressures.
- Developed a method to evaluate  $\phi_{\text{local}}$  from OH chemiluminescence images.
- Showed that the maximum  $\phi_{\text{local}}$  increases monotonically with retard of SOI from IVC for both injection pressures.
  - however temporal and spatial distribution differs significantly.
- PLIF images are consistent with results/conclusions from the OH\* chemiluminescence images.