SAND2018-13120PE

The Use of In-cylinder Soot Diagnostics to Understand Shortcomings of PMI for Stratified-Charge SI Combustion

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AEC Program Review Meeting at USCAR

August 14-16, 2018

Abstract

Extensive testing using 9 different fuels reveals that PMI sometimes can be a poor predictor of soot emission for lean stratified-charge SI combustion. When wall-wetting occurs, PMI tends to underestimate particulate mass (PM) for ethanol-containing fuels. In contrast, for boosted conditions with minimal wall wetting, PMI underestimates PM for ethanol-containing fuels, and other discrepancies exist. To start unraveling why PMI fails to predict soot emission for various types of fuels under boosted conditions, both direct flame imaging and diffuse-back illumination (DBI) soot diagnostics are applied. The focus is on three fuels; E30 and High-Olefin Co-Optima Core fuels, and a diisobutylene-blend. It is found that the average peak combustion luminosity scales well with the exhaust PM level, but large cycle-to-cycle variations exist for all fuels. Consistent with this, the DBI technique reveals high cycle-to-cycle variability of the in-cylinder soot mass. In particular, the diisobutylene blend shows occasional cycles with very slow late-cycle soot decay rate, possibly suggesting that those cycles contribute disproportionately to a PM level that is higher than expected based on PMI. Furthermore, two other possible shortcomings of PMI in the context of stratified-charge combustion are identified. First, differences in stoichiometric air-fuel ratio can influence the local fuel-air equivalence ratio (ϕ), affecting the amount of mass that is located at sufficiently high ϕ to produce soot. Second, the PMI value is highly influenced by the volatility of the fuel, as appropriate for the port-fuel injected engines for which PMI was developed. However, the importance of volatility for PM may be reduced for stratified-charge operation that utilize late injection into a dense charge that has been heated by compression.

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U.S. DEPARTMENT OF ENERGY

Co-Optimization of Fuels & Engines

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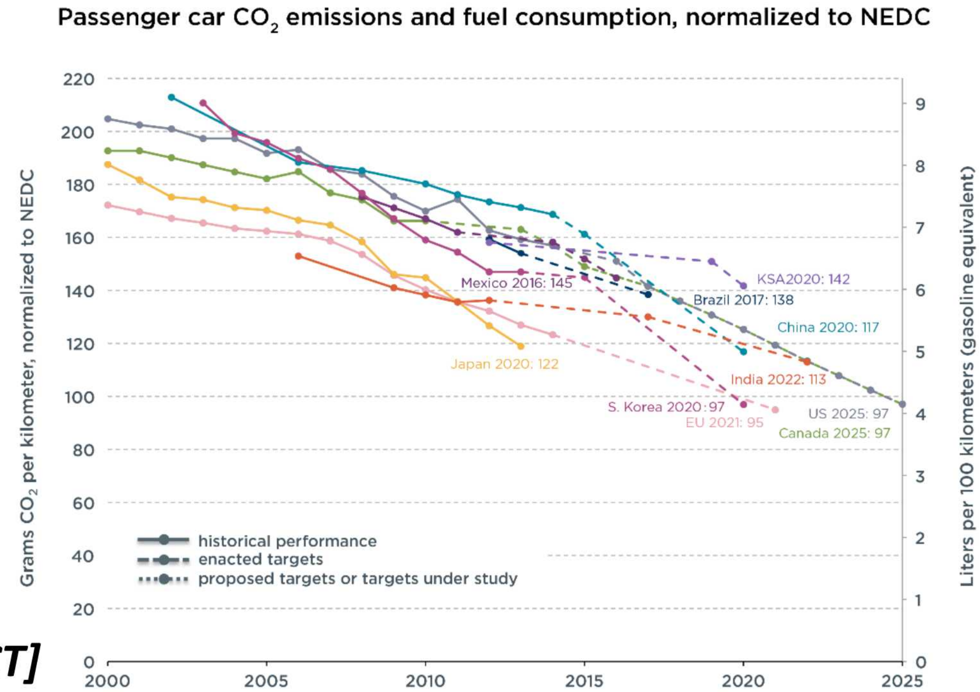
Outline

1. Motivation
2. Fuel effects on engine-out PM for different operating conditions
3. In-cylinder soot diagnostics
4. Conclusions

Regulation on CO_2 Emission from PV

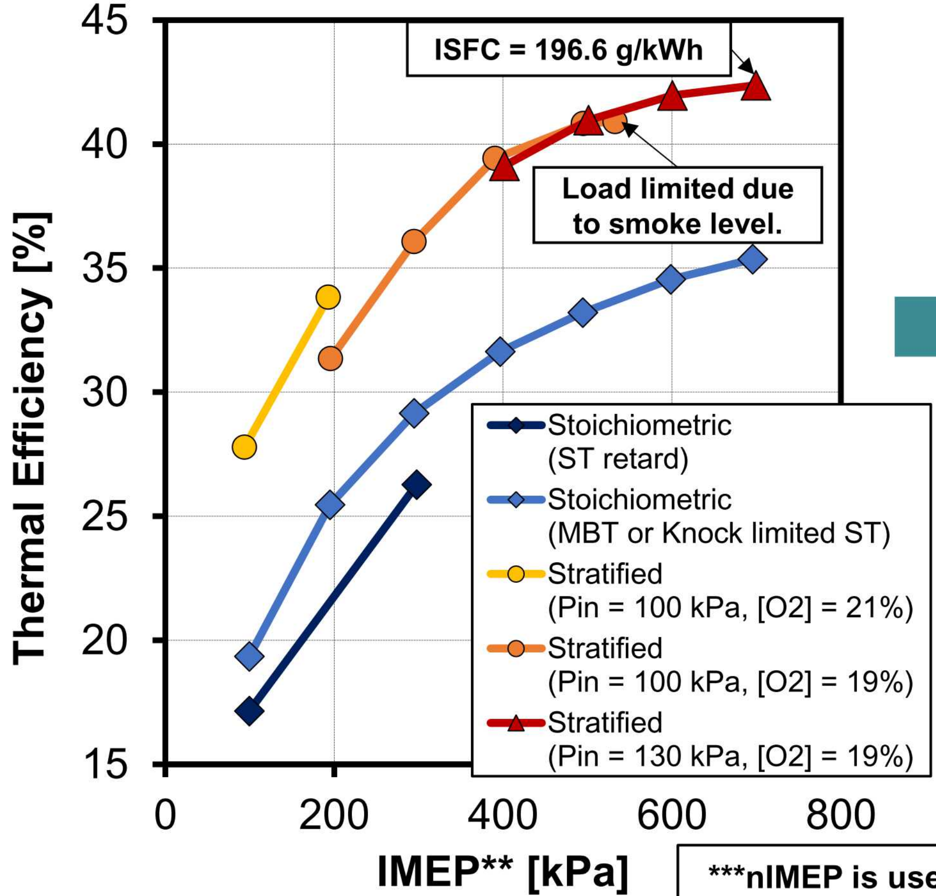
- The regulation on CO_2 emission from passenger vehicle (PV) is becoming very stringent.
- Especially for the US, the portion of gasoline-fueled vehicles that comprises the vehicle sales is very large.
- Thus, it is crucial to improve efficiency of gasoline engines.
- Stratified-charge operation can be an option due to its potential for efficiency improvement.

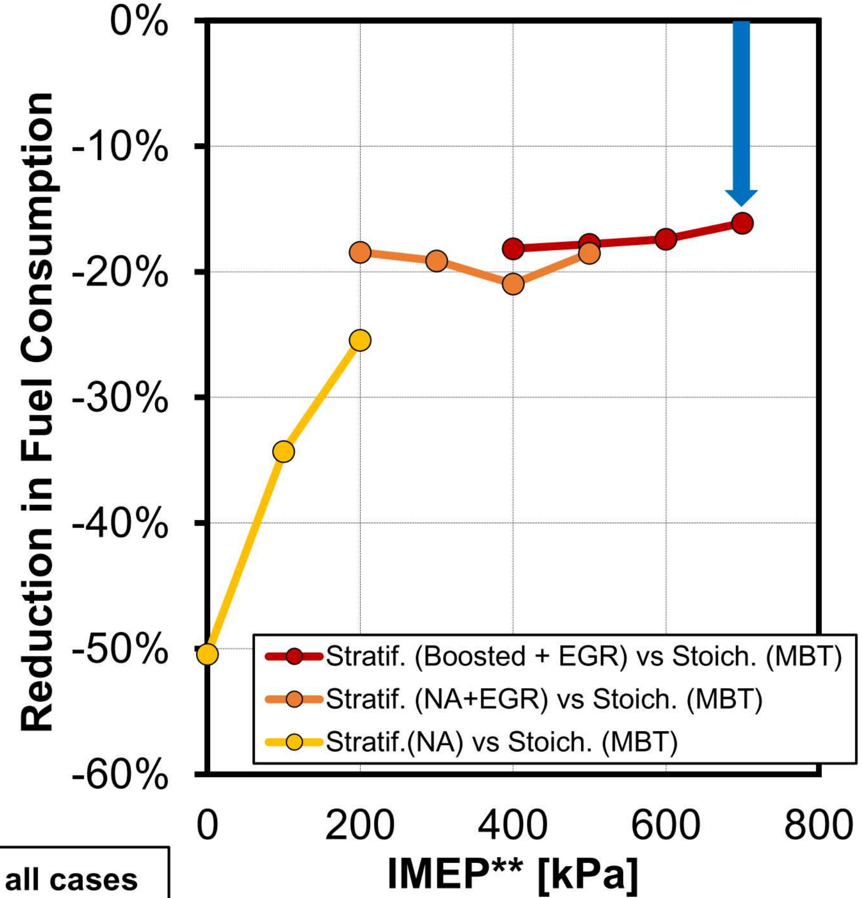


[ICCT]

Merit of Stratified Combustion

- Fuel used for these results: High Cycloalkane (RON 98)
- Over the broad range of engine load, significant gain in efficiency can be realized without optimization of hardware and calibration.
- A dramatic reduction in fuel consumption under very low load condition.

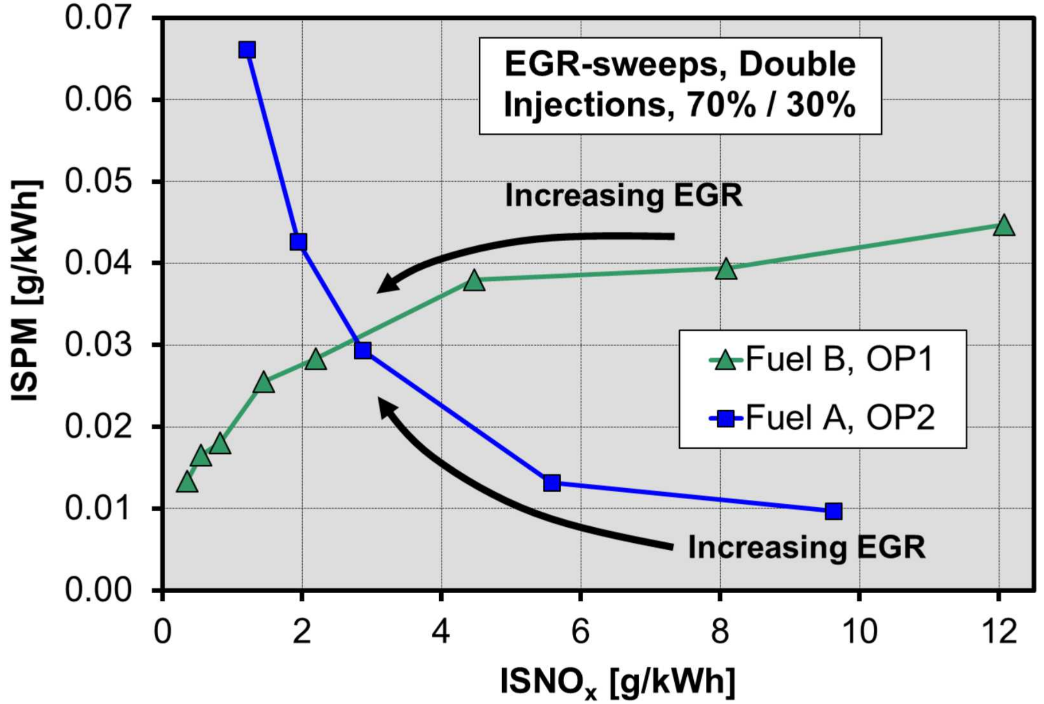




***nIMEP is used for all cases except for boosted conditions.

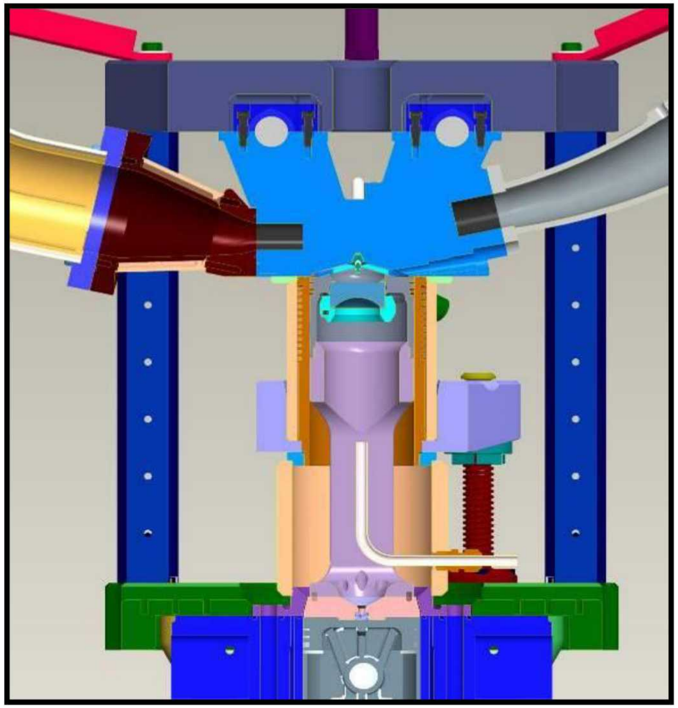
NO_x / Soot Trade-off

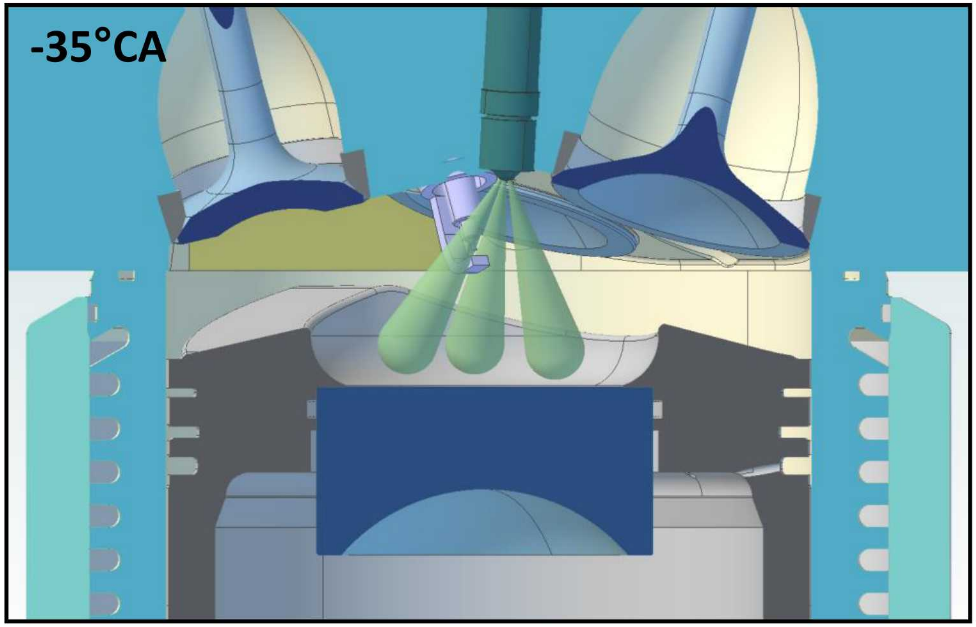
- For lean stratified operation, three-way catalyst can not be utilized to reduce NO_x.
- Thus, EGR needs to be applied to reduce engine-out NO_x.
- However, EGR can increase soot emission as EGR generally impedes oxidation of soot.
- Depending of fuels and operating point, the application of EGR can lead to either increasing or decreasing smoke.
- The soot formation mechanisms / pathways appear to be very different for these two examples.

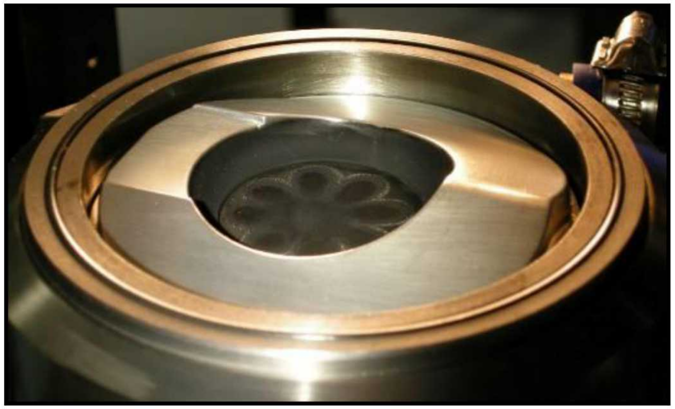


Research Engine

- Drop-down single-cylinder engine.
- Automotive size. 0.55 liter swept volume.
- Identical geometry for **All-metal** and **Optical.**
- Designed for spray-guided stratified-charge operation ⇒ Piston bowl.







Fuel Matrix

- One E10 regular gasoline, and eight RON = 98 fuels were studied.
- Octane sensitivity, compositions, boiling points, heat of vaporization and PMI vary greatly.

	E10 RD5-87	Alkylate	E30	High Aromatic	High Cycloalkane	High Olefin	Diisobutyl-ene Blend	2-Butanol Blend	Isobutanol Blend
RON	92.1	98.0	97.9	98.1	97.8	98.3	98.3	98.2	98.1
MON	84.8	96.7	87.1	87.6	86.9	87.9	88.5	89.1	88.0
Octane Sensitivity	7.3	1.3	10.8	10.5	11.0	10.4	9.8	9.1	10.1
Oxygenates [vol.%]	10.6	0.0	30.6	0.0	0.0	0.0	0.0	28.4	24.1
Aromatics [vol.%]	20.9	0.7	13.8	39.8	33.2	13.4	20.1	17.9	19.0
Alkanes [vol.%]	49.4	98.1	40.5	46.2	40.6	56.4	56.3	50.1	53.1
Cycloalkanes [vol.%]	11.3	0.0	7.0	8.0	24.2	2.9	0.0	0.0	0.0
Olefins [vol.%]	4.9	0.1	5.6	4.5	1.6	26.5	23.6	3.6	3.8
T10 [°C]	57	93	61	59	56	77	63	63	63
T50 [°C]	98	100	74	108	87	104	-	-	-
T90 [°C]	156	106	155	158	143	136	111	111	111
Net Heat of Combustion [MJ/kg]	41.9	44.5	38.2	43.0	43.2	44.1	43.2	40.1	40.6
Heat of Vaporization [kJ/kg]	412	308	532	361	373	333	337	415	412
AFR Stoichiometric	14.1	15.1	12.9	14.5	14.5	14.8	14.7	13.6	13.8
HoV [kJ/kg stoichiometric charge]	27.3	19.1	38.4	23.3	24.0	21.1	21.5	28.5	27.9
Particulate Matter Index	1.68	0.22	1.28	1.80	1.54	1.00	0.47	0.37	0.40

Introduction to PMI

- Test fuels used by Honda for the development of PMI correlation were prepared by blending indolene and additives listed below.
- The amount of oxygenated hydrocarbon blended with indolene was limited.

Additive	FBP** [K]	DBE
2,2,4- Trimethylpentane	372	0
Dodecane	489	0
Ethylbenzene	409	4
α-Methylstyrene	436	5
1,2,4-Trimethylbenzene	442	4
Divinylbenzene	468	6
Naphthalene	491	7
Indene	455	6
Ethanol	351	0

**FBP = final boiling point

Characteristics of the test fuel	
Aromatic content [wt. %]	21.4 ~ 44.9
Oxygen content [wt.%]	0 ~ 3.6
FBP [K]	424 ~ 557
PMI [-]	0.9 ~ 3.0

[Aikawa and Jetter, IJER, 2014]

$$DBE = \frac{2C + 2 - H}{2}$$

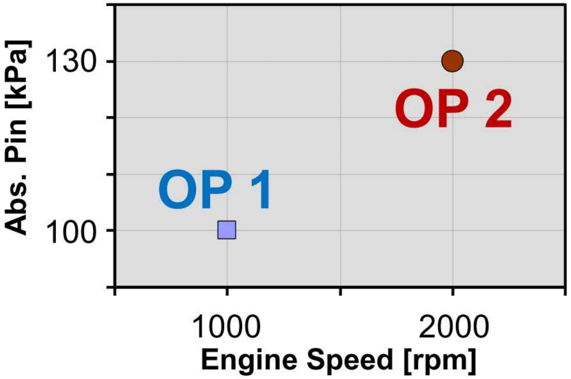
$$PMI = \sum_{i=1}^{n} I_{[443K]} = \sum_{i=1}^{n} \left(\frac{DBE_i + 1}{VP\ (443K)_i} \times Wt_i \right)$$

DBE_i : double bond equivalent
$VP\ (443K)_i$: Vapor pressure at 443K
Wt_i : Mass fraction

Experimental Conditions for All Metal Operation

- Two different operating conditions were chosen because previous study revealed that those operating conditions result in different soot formation pathways.

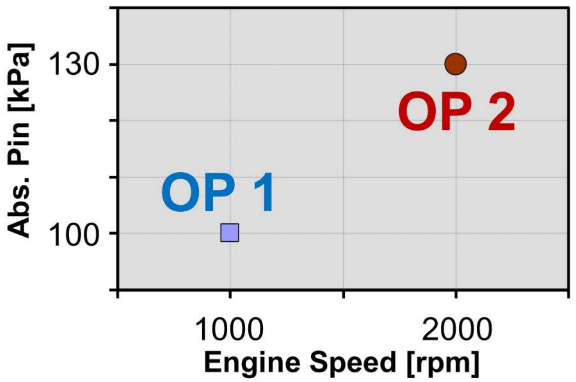
CR	12	
Valve Timings	For minimal residual level	
$T_{coolant}$	75 ºC	
T_{intake}	28~30 ºC	
Mass-based equivalence ratio (ϕ_m)	0.33	
Injection pressure	170 bar	
# of Injections	Double (70%/30% split ratio)	
Engine speed	1000 rpm	2000 rpm
Intake Pressure	100 kPa	130 kPa
Start of Injection (SOI_{a1}/SOI_{a2})	-40 / -25 ºCA aTDC	-65 / -35 ºCA aTDC
Spark Timing (ST)	-22 ºCA aTDC	-29 ºCA aTDC
$[O_2]_{intake}$	19.0 ~ 14.0%	19.0 ~ 16.0%
$IMEP_g$	340~390 kPa	455~510 kPa
	OP 1	OP 2

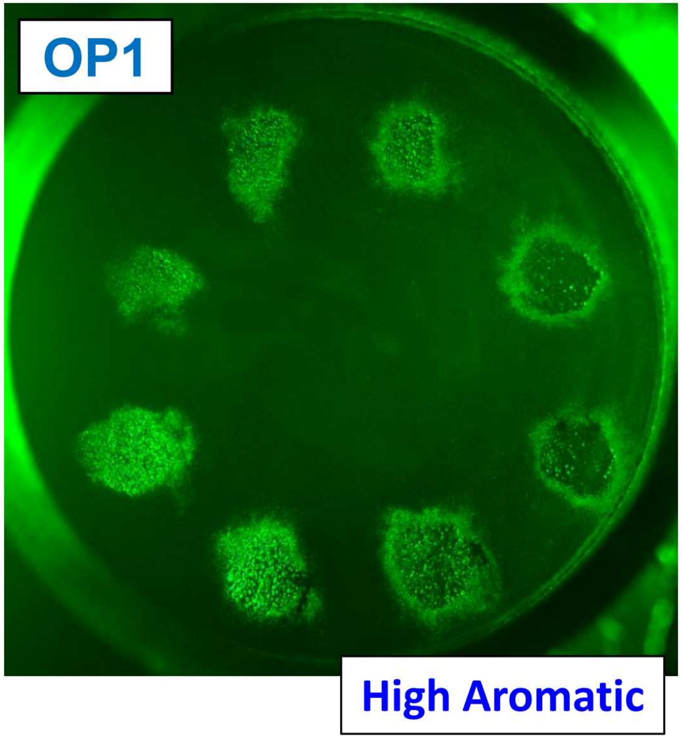


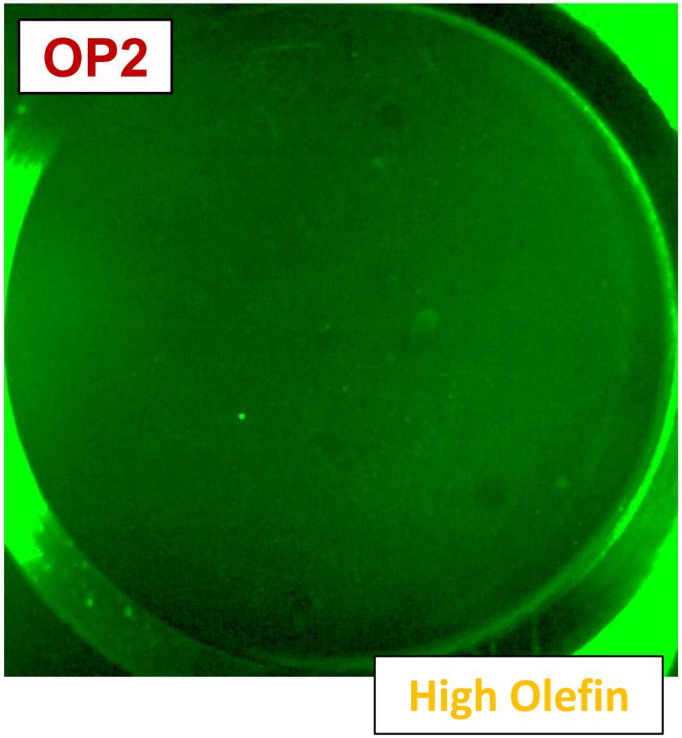
$$\phi_m \equiv \frac{\left(F/C\right)_{Actual}}{\left(F/A\right)_{Stoichiometric}}$$

Wall Wetting Issue

- RIM technique was utilized to visualize spray impingement and resultant fuel film formation.
- The result indicates that wall wetting becomes less important factor for soot emission for OP2.

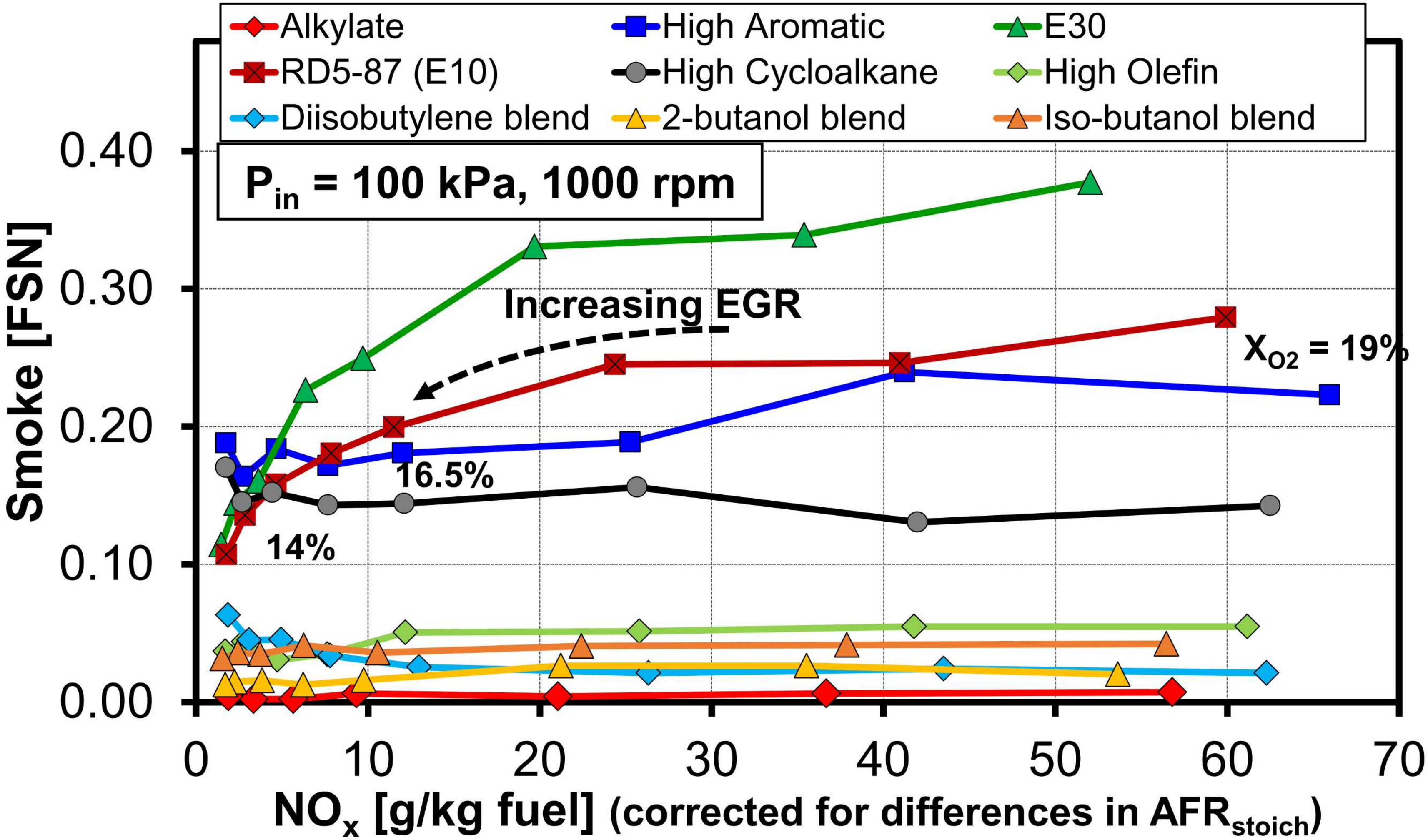






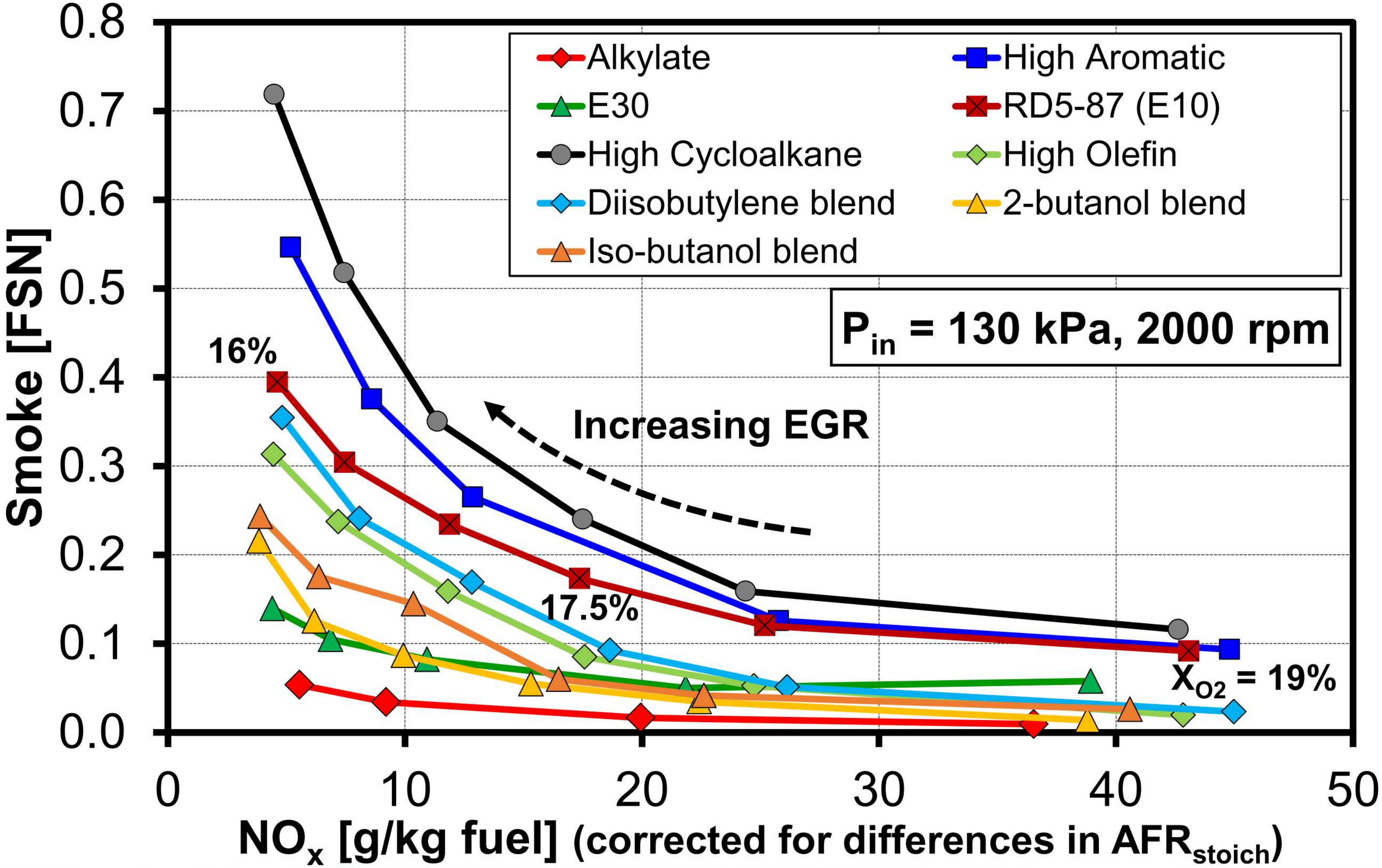
NO_x vs Smoke @[OP 1]

- Strong reduction of NO_x with EGR for all fuels.
- E30 and E10 show marked reduction of smoke with EGR.
  – Due to suppression of pool-fires, as discussed during AEC meeting in Jan 2018.



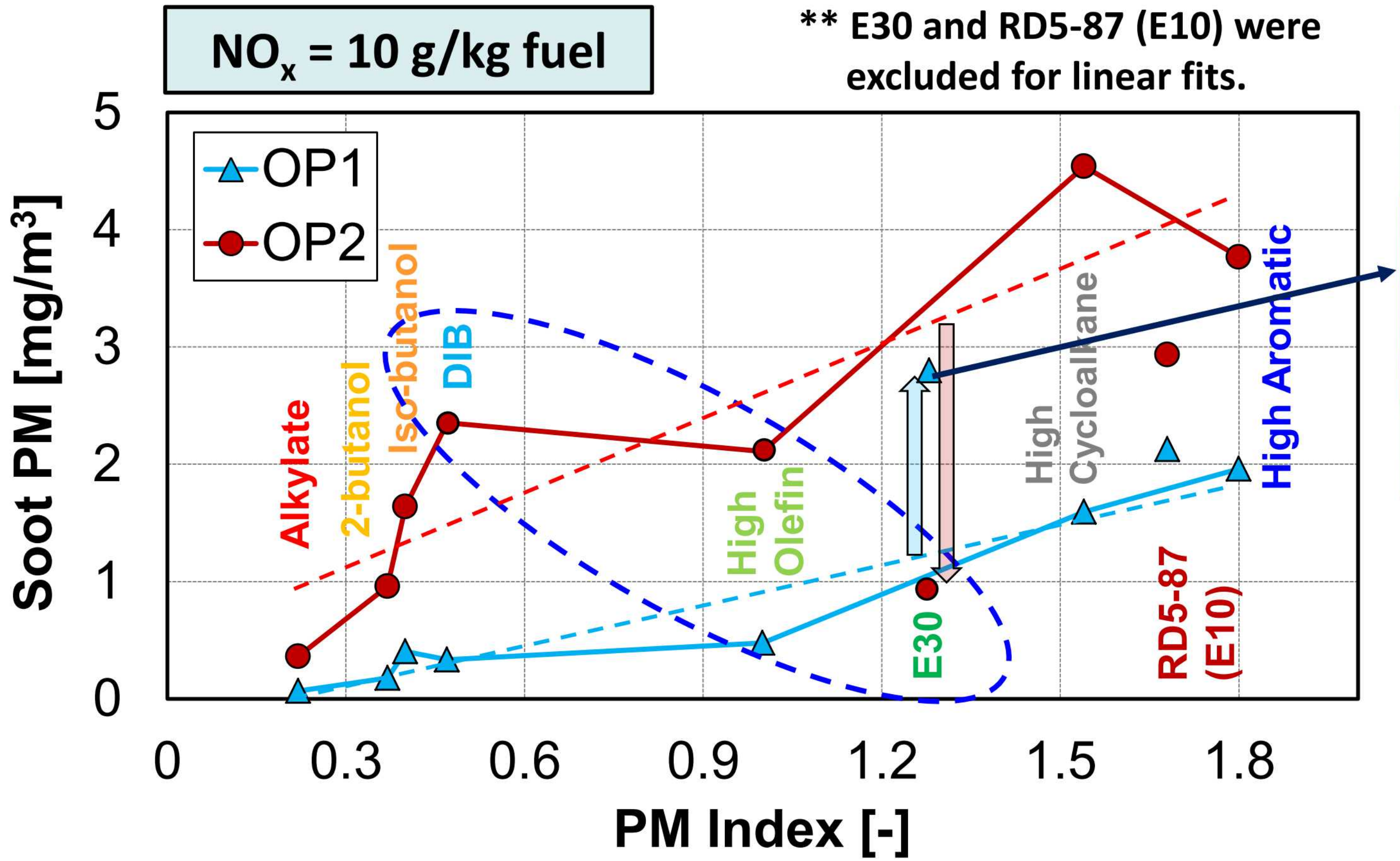
NO_x vs Smoke @[OP 2]

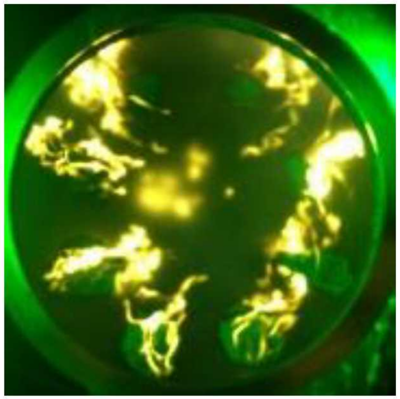
- Sensitivity to EGR rate for smoke is different significantly from fuel to fuel.
- Rank order of fuel differs compared to that of the other operating condition.



PMI vs Soot

- Engine-out soot generally agrees with PMI when fuels containing ethanol are excluded.
- Deviation between actual soot emission and PMI increases with ethanol content.
- High Olefin fuel generally results in less amount of soot compared to the predicted amount based on its PMI value.

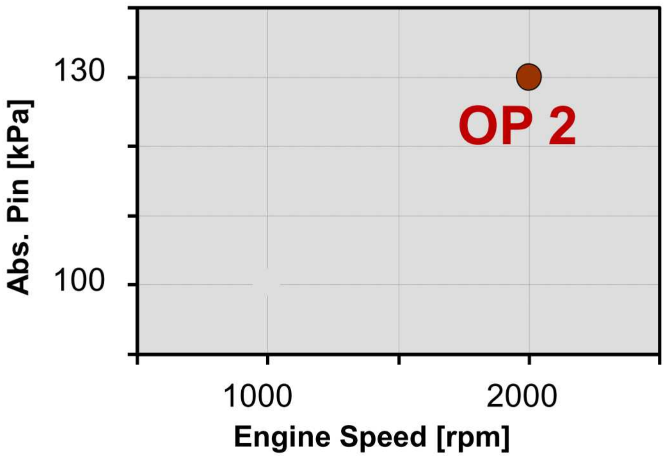




Experimental Conditions for Optical Mode

- Optical diagnostics were conducted at 2000 rpm, 130 kPa intake pressure (OP2).
- Skip-firing strategy was applied. (3 out of 12 cycles were fired)

Engine speed	2000 rpm
Intake pressure	130 kPa
$T_{coolant}$	90 ºC
Test fuel	Diisobutylene Blend, High Olefin, E30
Injection pressure	170 bar
# of Injections	Double (70%/30% split ratio)
Start of Injection (SOI_{a1}/SOI_{a2})	-65 / -35 ºCA aTDC
Spark Timing (ST)	-29 ºCA aTDC
Mass-based equivalence ratio (ϕ_m)	0.33
$[O_2]_{intake}$	**17.0%**
Equivalence ratio (ϕ)	0.40



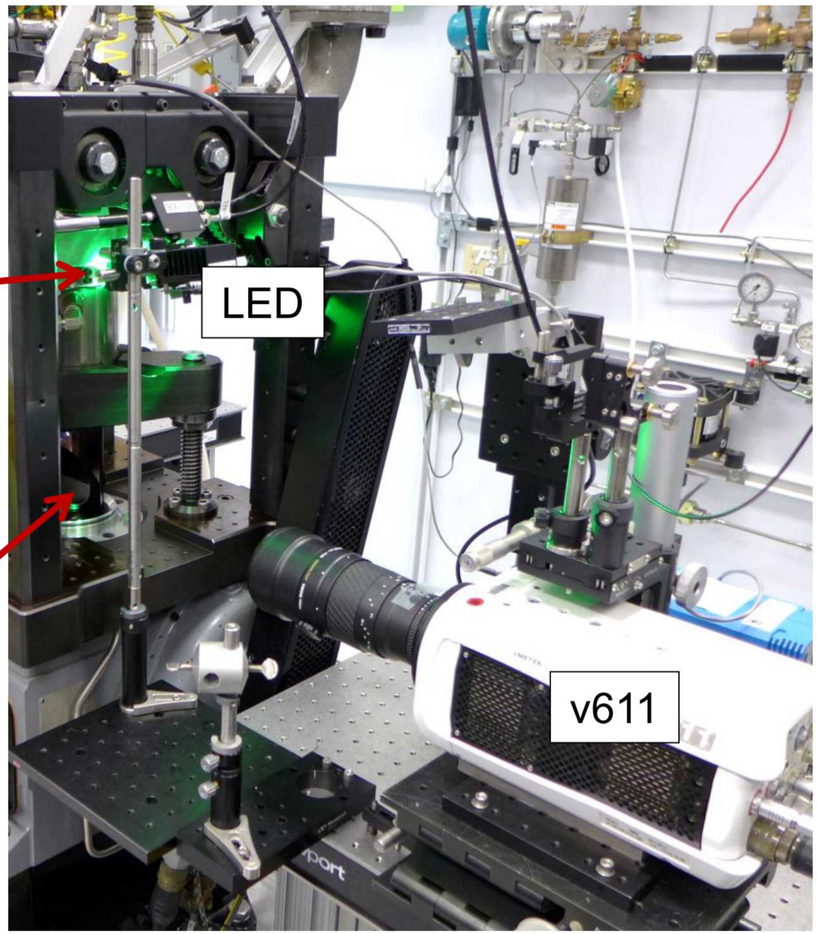
$$\phi_m \equiv \frac{\left(F/C\right)_{Actual}}{\left(F/A\right)_{Stoichiometric}}$$

Optical Setup for Natural Luminosity Imaging

- Image acquisition rate: 20 kHz (0.6°CA) with 512 x 512 resolution.

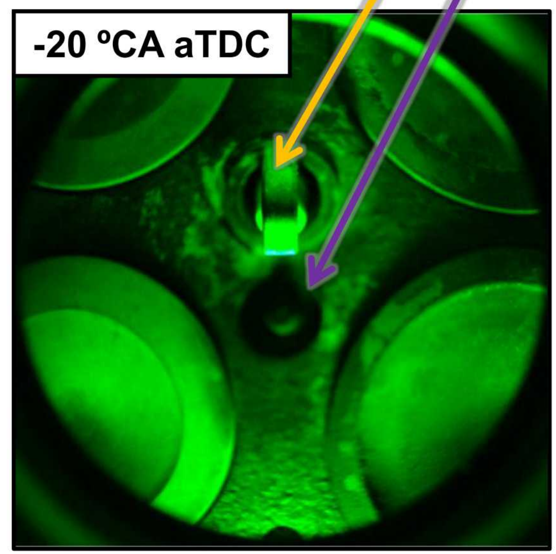
Pent-roof side window

45° Bowditch Mirror



Spark plug

Injector tip



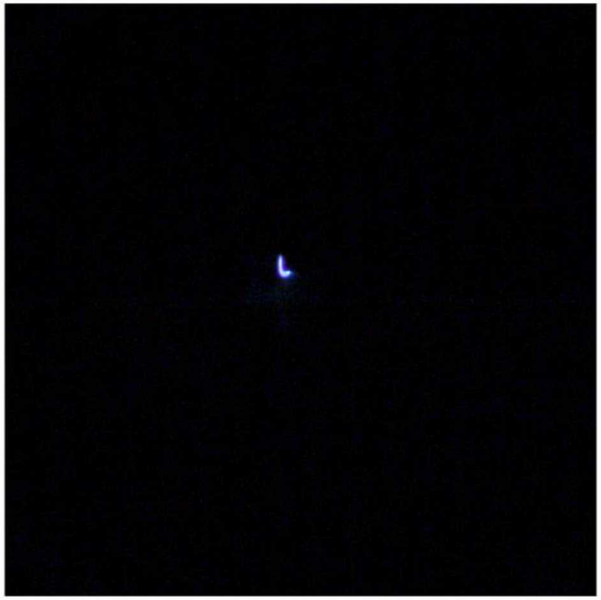
Exhaust ***Intake***

Imaging Result - Natural Luminosity

- Flame luminosity structures are similar in shape and evolution, but size and intensity vary.
- Large quantity of soot cloud appears to remain in the intake side.
  - Caused by tumble-induced fuel-vapor asymmetry, as discussed in *Zeng et al.*, Proc. Comb. Inst., 2017.

Diisobutylene Blend (PMI = 0.47)

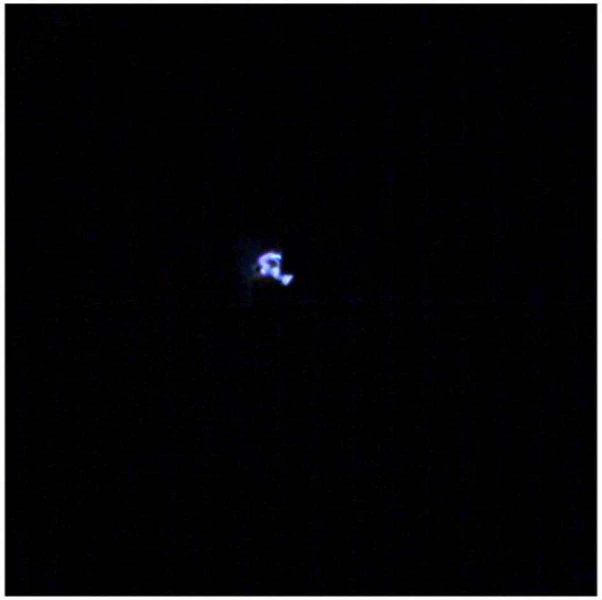
-24.0 °CA aTDC



Exhaust ***Intake***

High Olefin (PMI = 1.00)

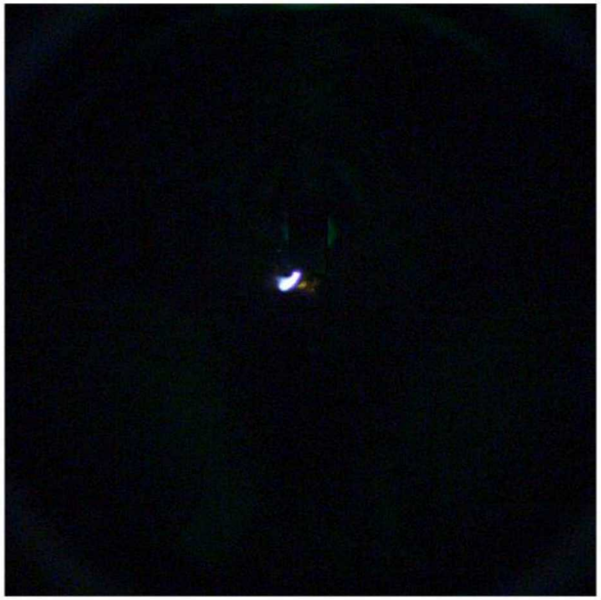
-24.0 °CA aTDC



Exhaust ***Intake***

E30 (PMI = 1.28)

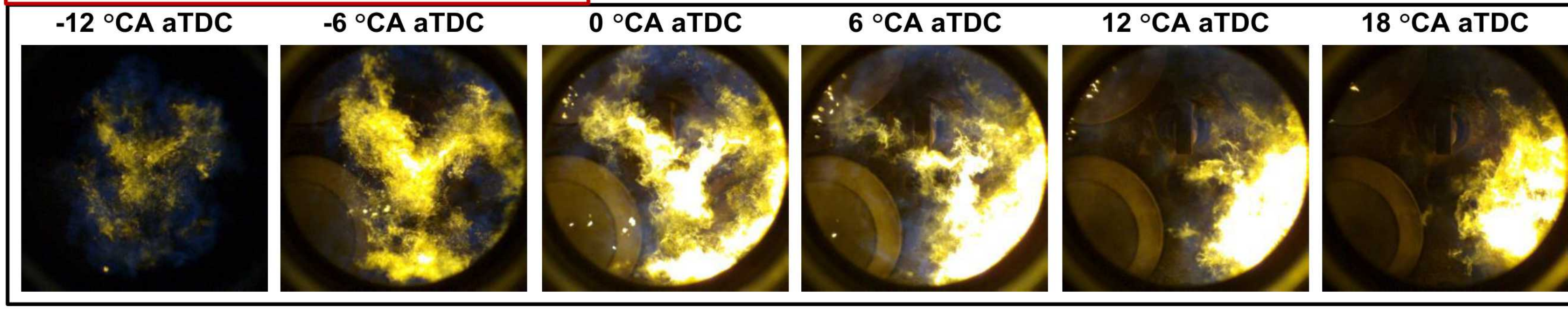
-24.0 °CA aTDC



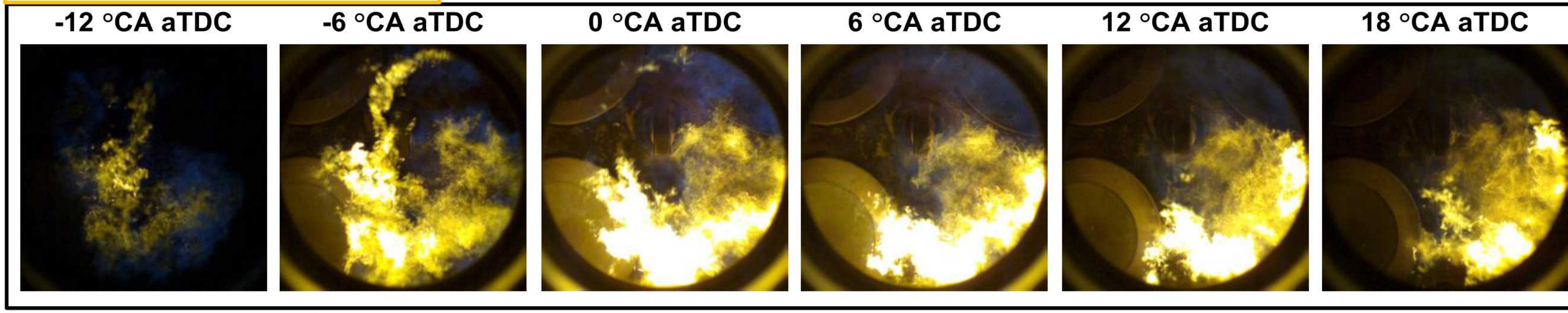
Exhaust ***Intake***

Images from Representative Cycles

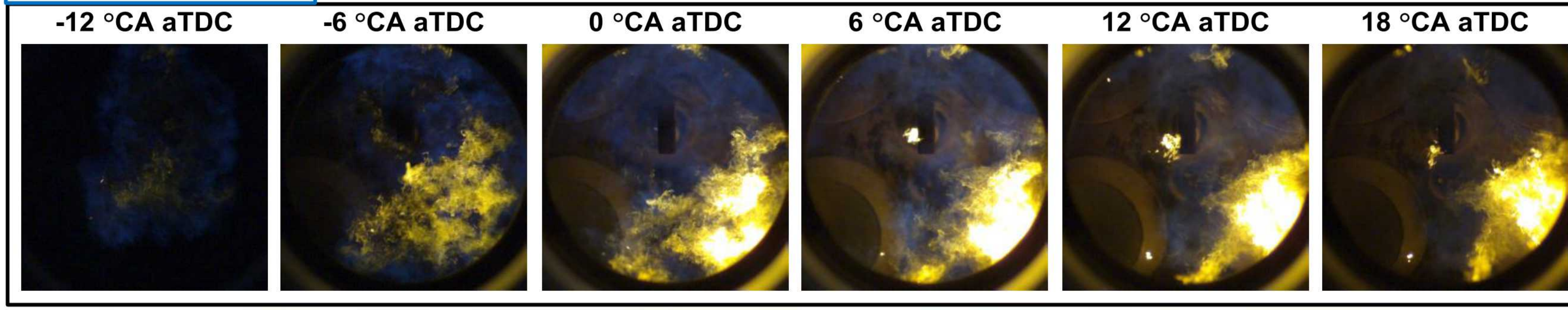
Diisobutylene Blend (PMI = 0.47)



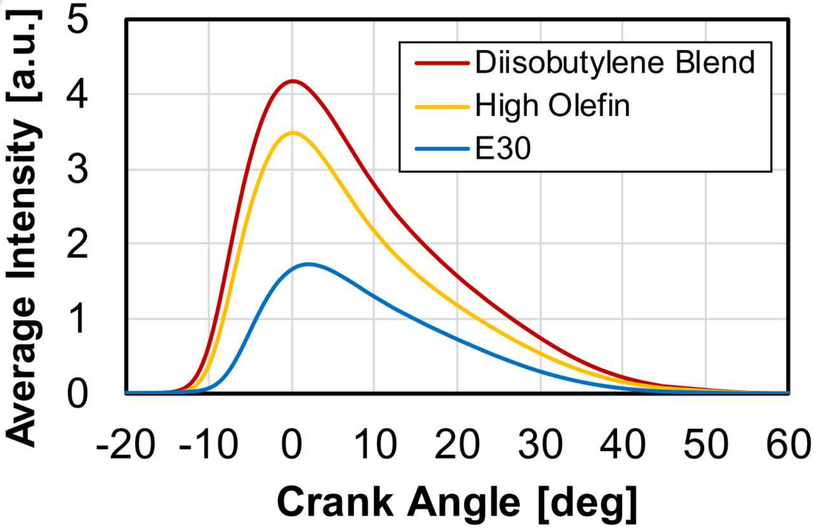
High Olefin (PMI = 1.00)

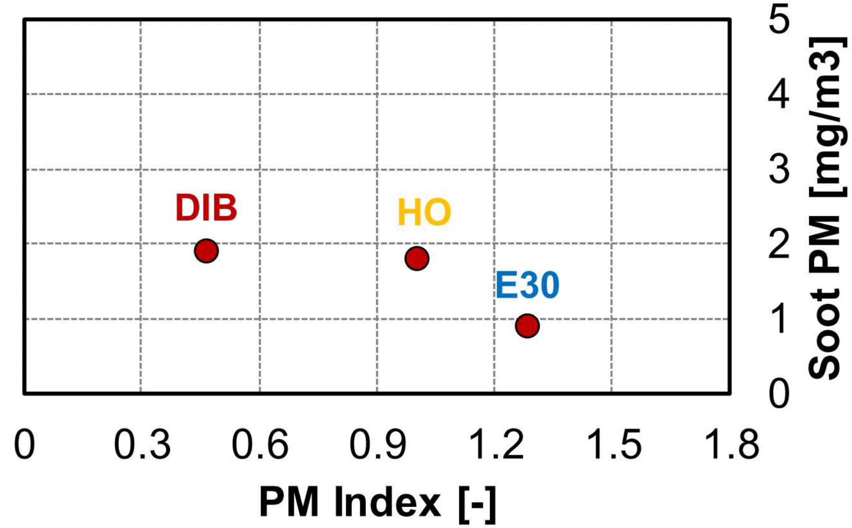


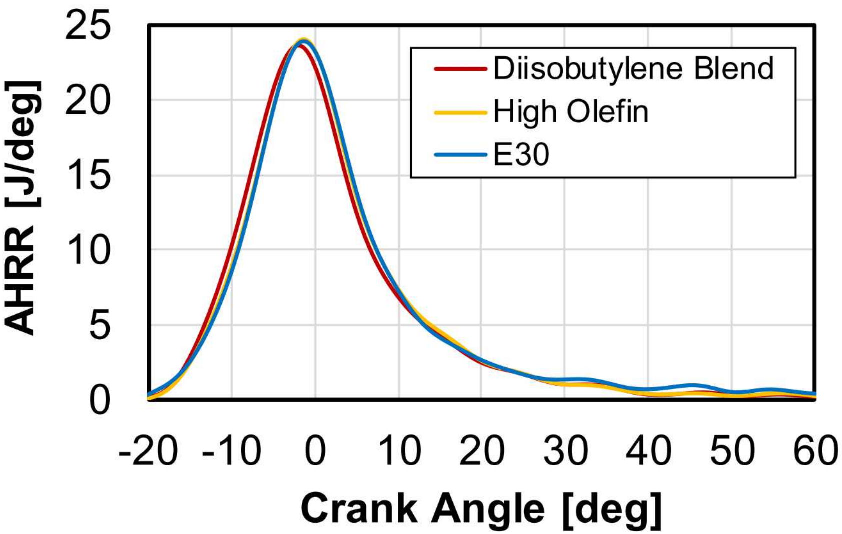
E30 (PMI = 1.28)



Natural Luminosity vs PMI



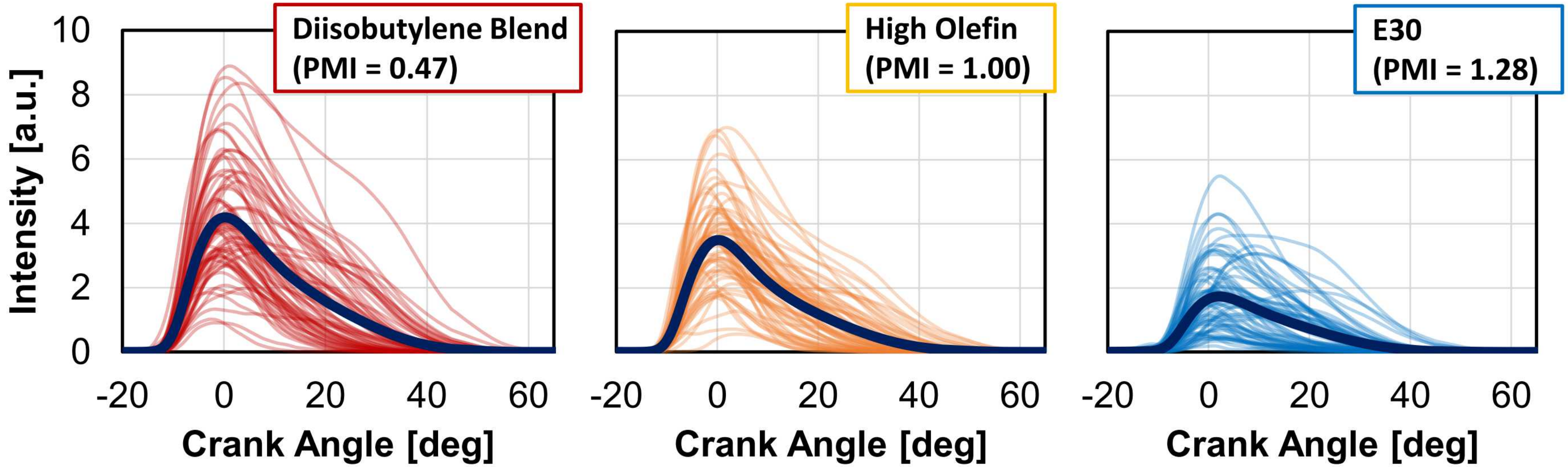


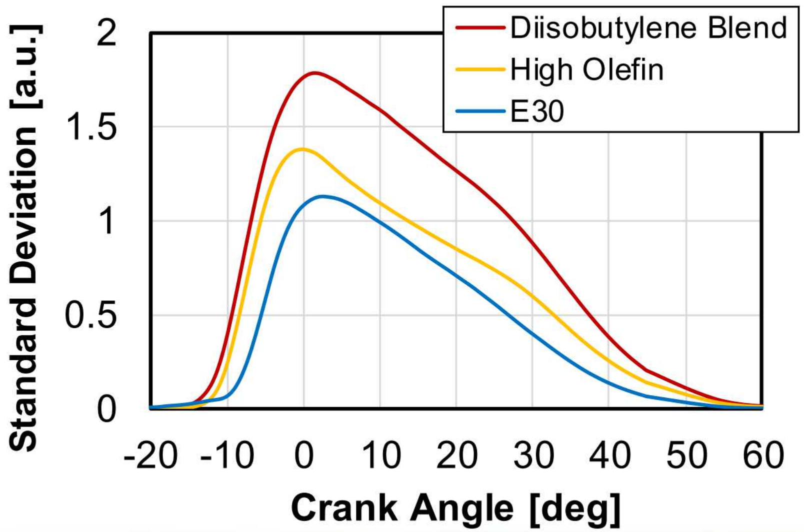


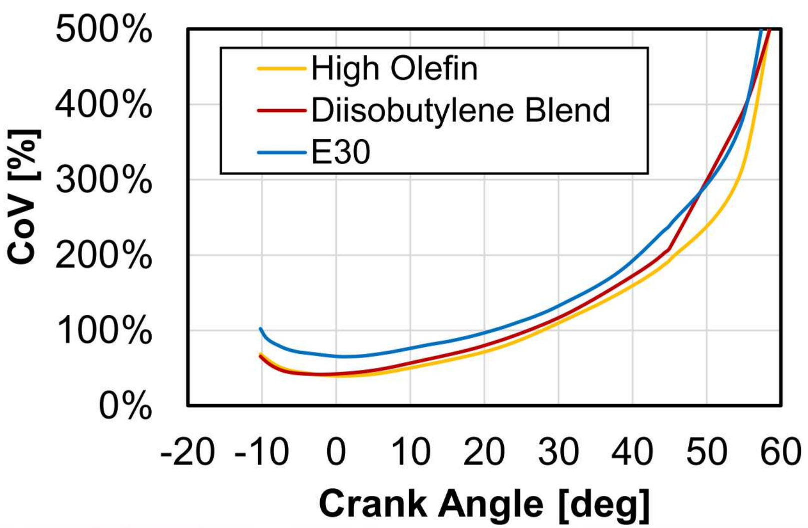
- Peak of average intensity from natural luminosity agrees well with the trend in measured soot PM.
- Despite having the highest value of PMI, average intensity of natural luminosity is the lowest for E30 .
- Average intensity reaches its peak value close to the timing when peak of AHRR is reached.

Variability in Natural Luminosity

- Relative variability in measured intensity from images becomes very high later in cycle.







Effect of Stoichiometric AF Ratio on Local ϕ

- For lean stratified operation, air-fuel mixing is concurrent with combustion.
- Stoichiometric AF ratio of E30 is lower than those of the other fuels. ($AFR_{stoich,\ E30} \approx 12.8$ vs $AFR_{stoich,\ Diisobutylene} \approx 14.7$)
- Difference in AFR_{stoich} would influence local ϕ.
  - For example, assume that the same degree of mixing of air and fuel is achieved in a region.

    m_{air} = 1 [mg], m_{fuel} = 0.15 [mg] → $AFR_{local} \approx 6.67$

    $\phi_{local,\ diisobutylene} \approx 2.21$, $\phi_{local,\ High\ Olefin} \approx 2.22$ vs $\phi_{local,\ E30} \approx 1.92$

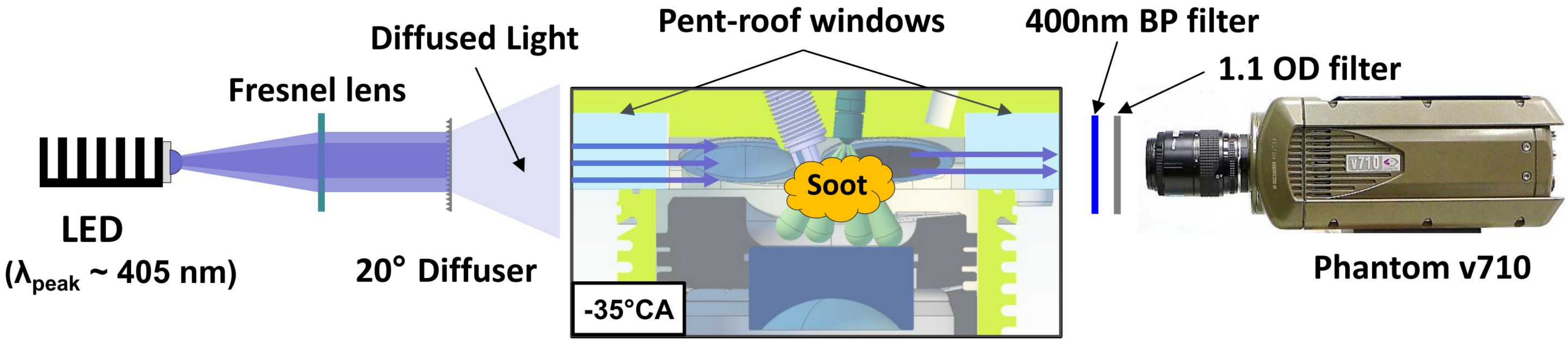
- Lower AFR_{stoich} of E30 can contribute to reduced soot formation during combustion event.
- PMI does not consider differences in AFR_{stoich}.

$$PMI = \sum_{i=1}^{n} I_{[443K]} = \sum_{i=1}^{n} \left(\frac{DBE_i + 1}{VP\ (443K)_i} \times Wt_i \right)$$

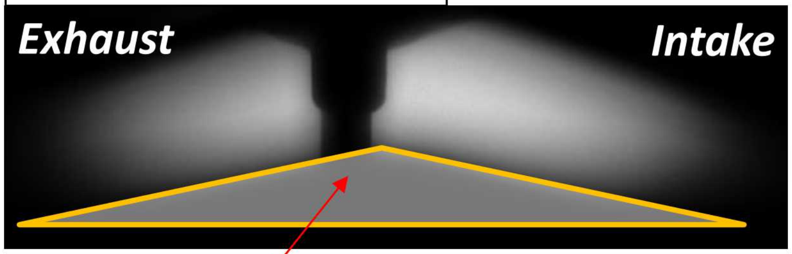
DBE_i *: double bond equivalent*
$VP\ (443K)_i$: *Vapor pressure at 443K*
Wt_i : *Mass fraction*

Optical Setup for DBI Imaging

- Diffuse back-illumination (DBI) technique was employed for in-cylinder soot diagnostics via pent-roof windows.
- Possible to measure evolution of soot quantity for a given cycle at high speed.
- Skip-firing strategy (3 fired/12 cycles), 24kHz frame rate

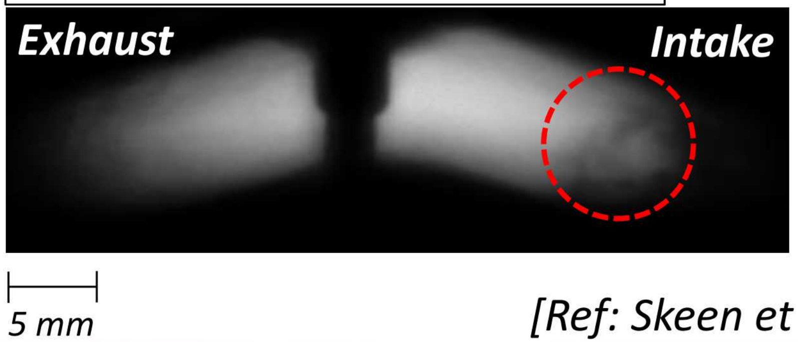


Reference image (I_0)



Reduction of view depends on piston position

Raw image with combustion (I)

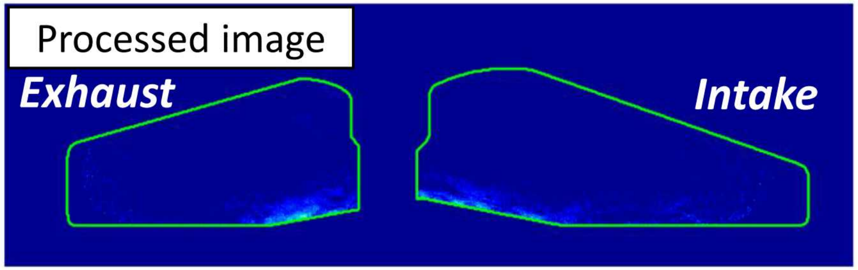


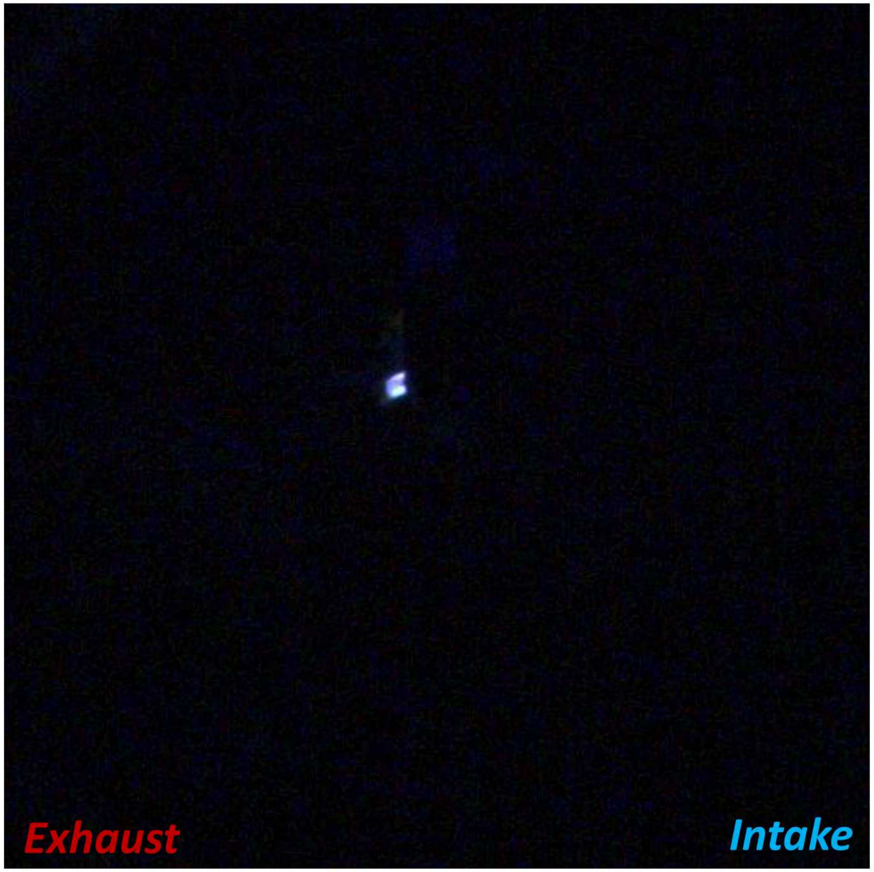
[Ref: Skeen et al.]

Imaging Results - DBI

- Test fuel: High Olefin
- Extinction due to soot was imaged and processed to obtain KL.
- Even at TDC, it was possible to detect extinction due to soot despite a significant reduction of available viewing area due to piston motion.

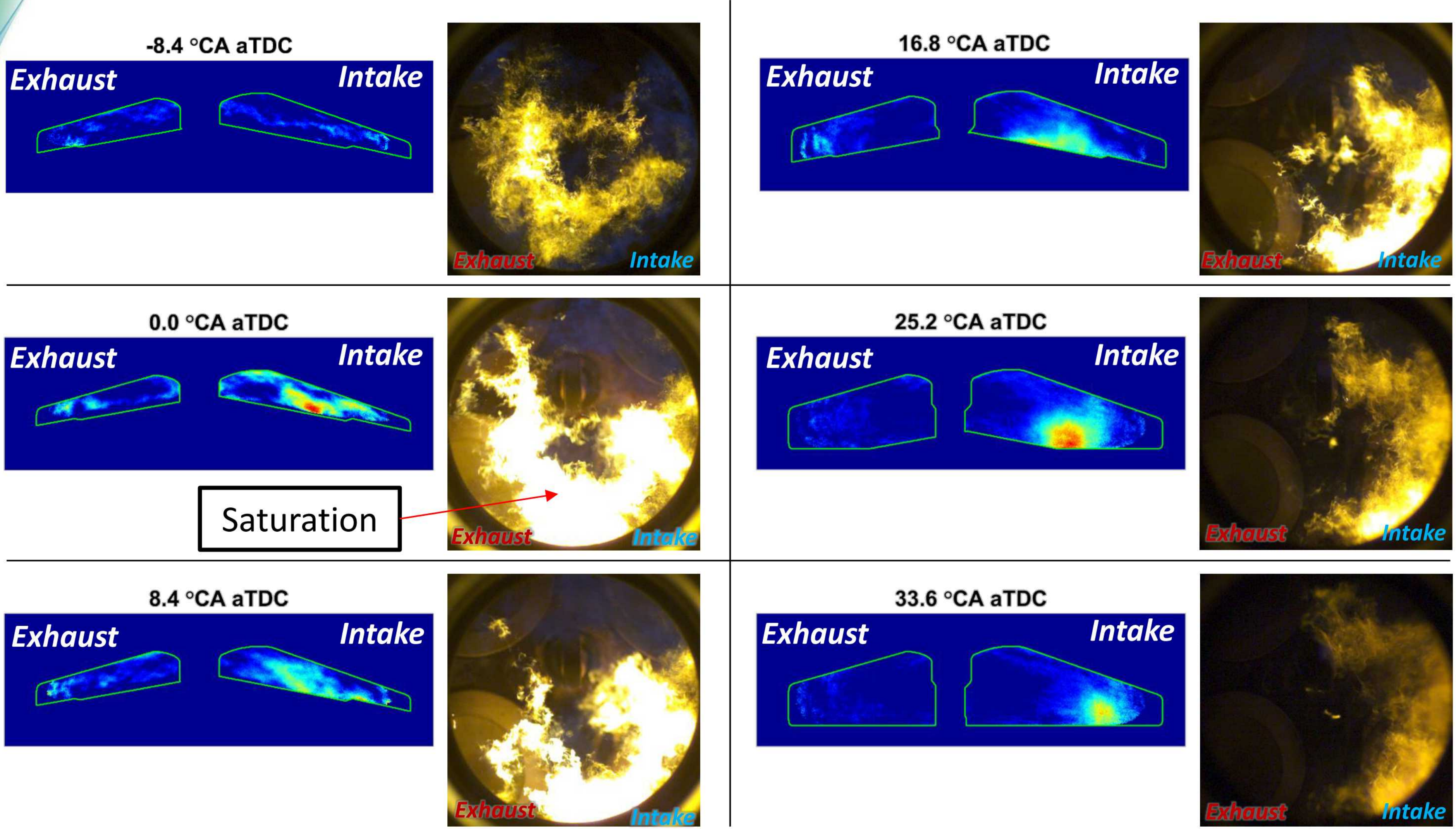
-25.8 °CA aTDC





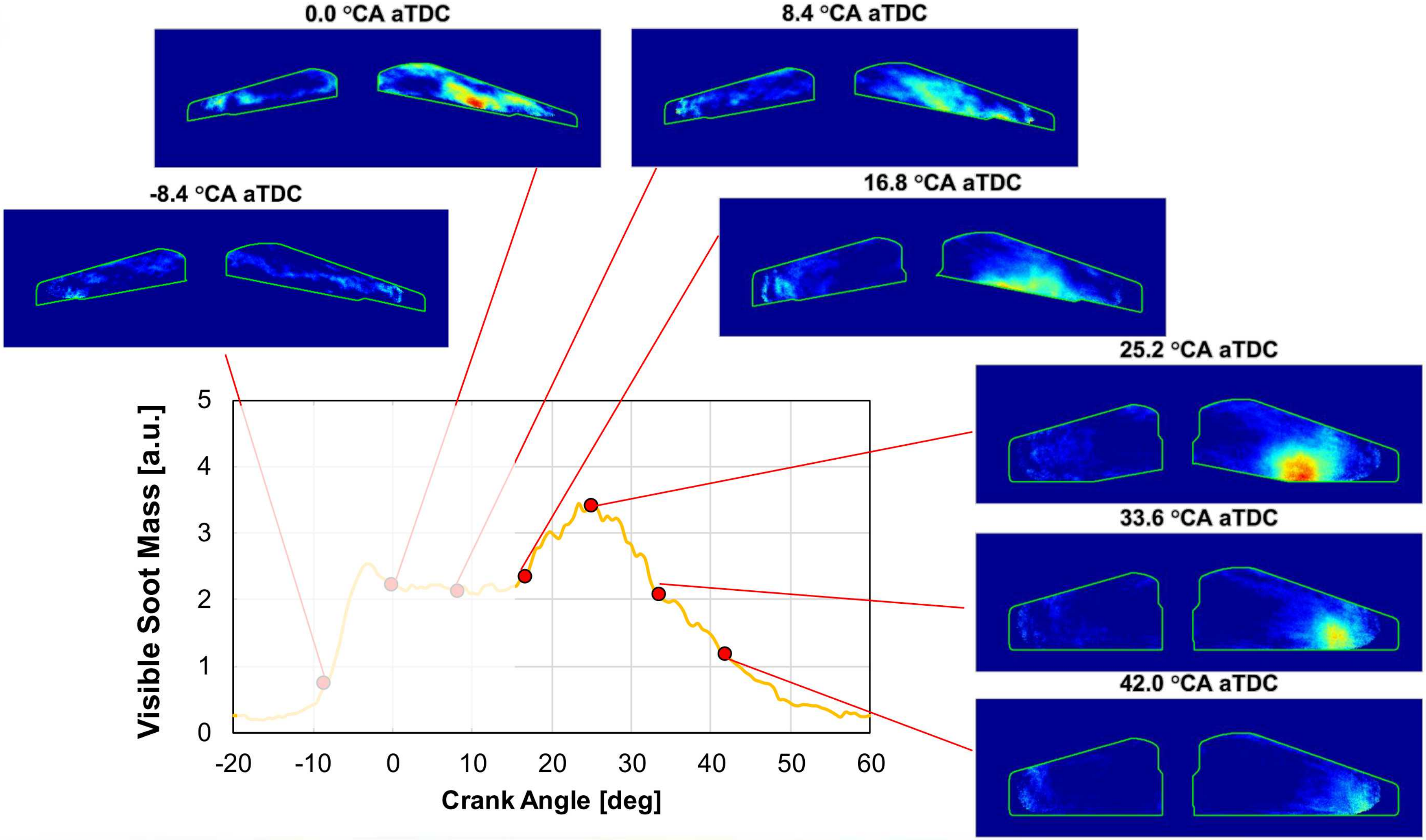
Natural Luminosity vs DBI

- DBI results can provide more information on temporal evolution of visible soot cloud which may not be captured well from natural luminosity.

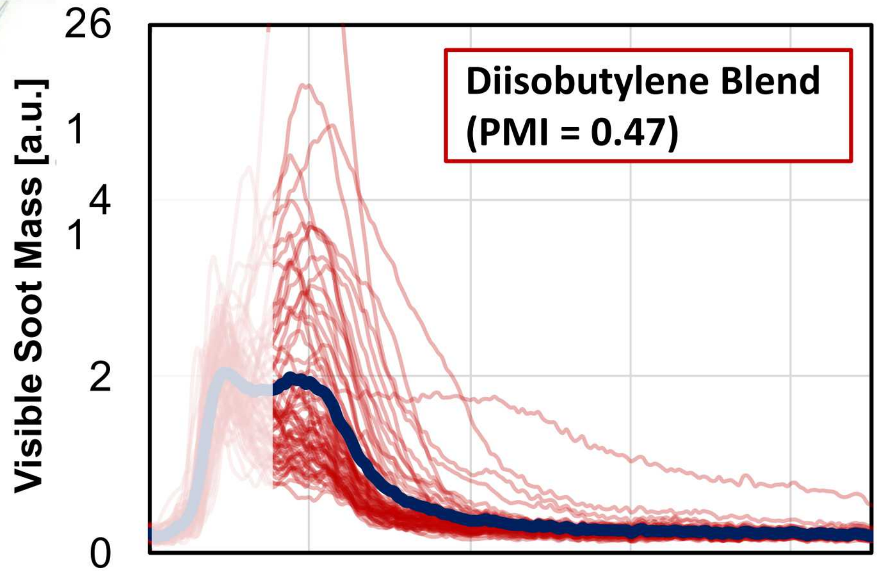


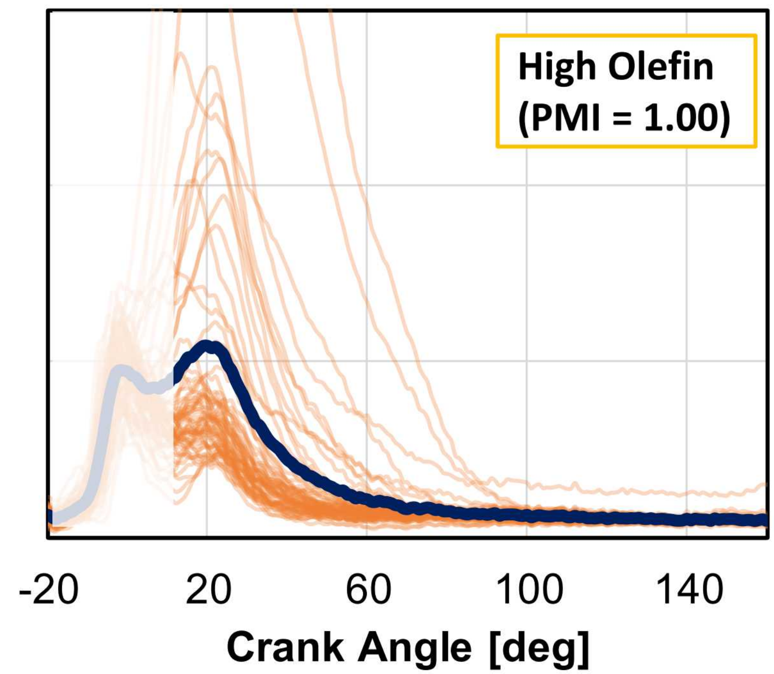
Imaging Results - DBI

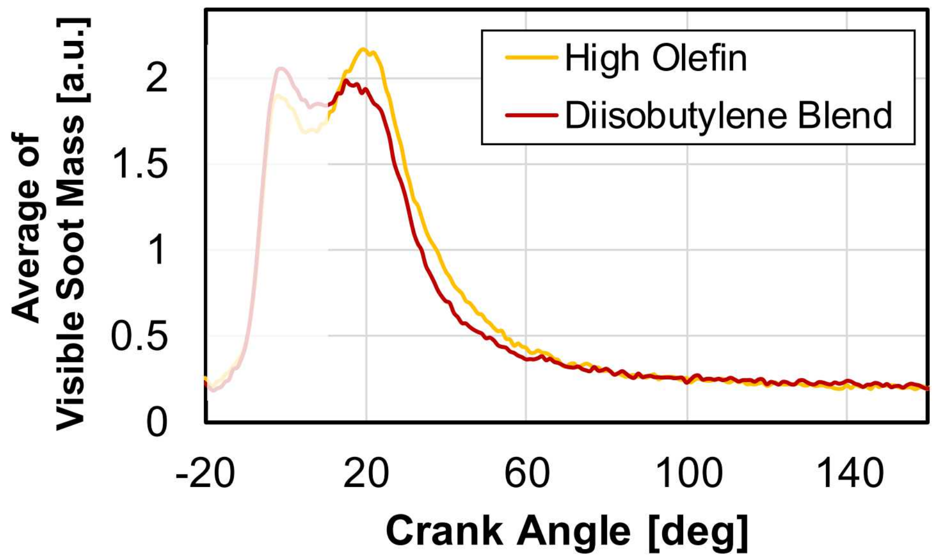
- Comparison between evolution in semi-quantitative soot mass and processed images shows that soot mass starts to increase from 16.8 ºCA aTDC because piston moves out of the view.



Imaging Results - DBI

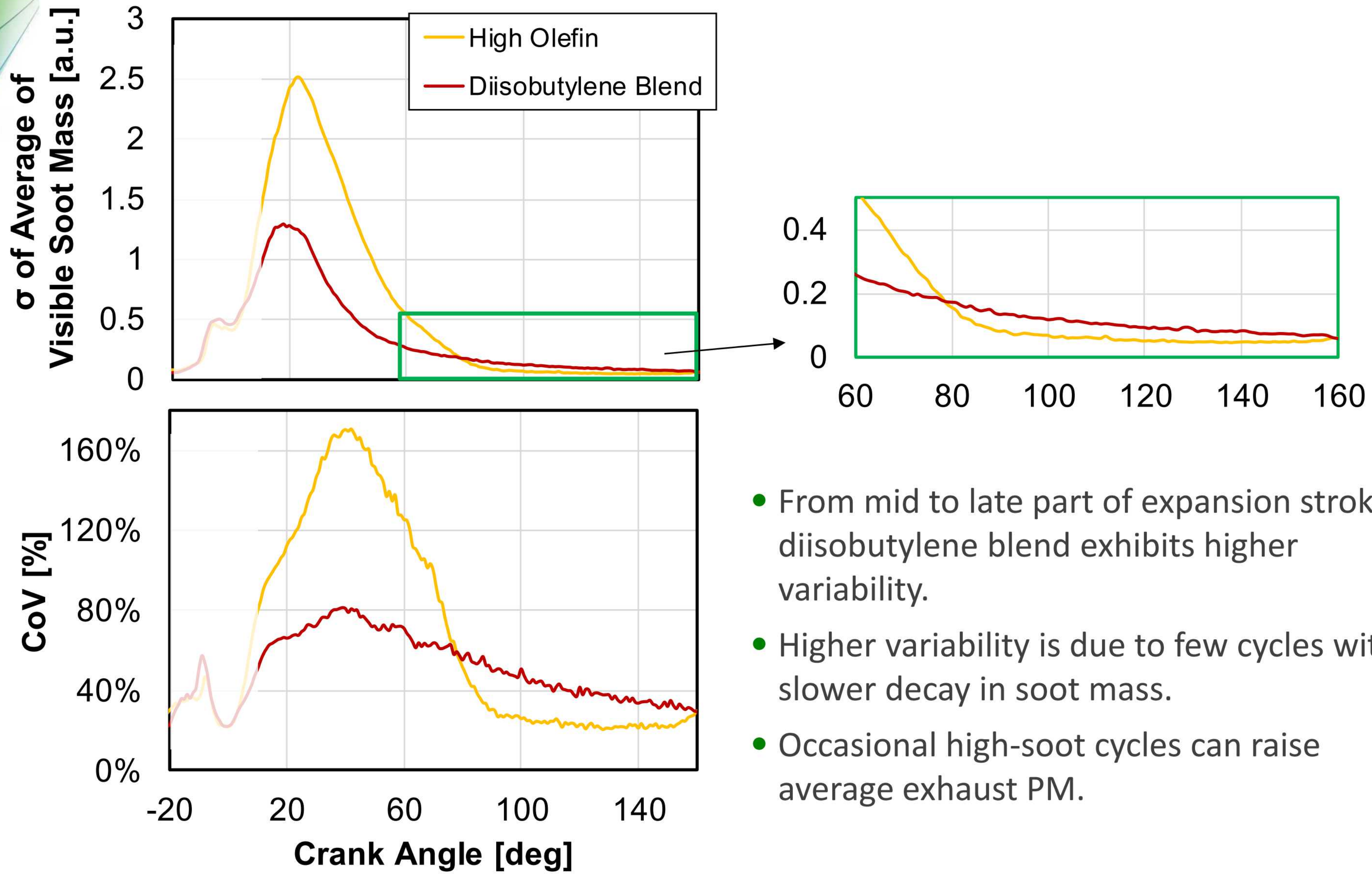






- Result from High Olefin fuel shows several cycles which shows extremely large amount of soot.
- Few extreme cycles are contributing to increase in average soot mass.
- At later phase of expansion stroke, few cycles from diisobutylene blend shows slower decay rate in soot mass.

Imaging Results - DBI

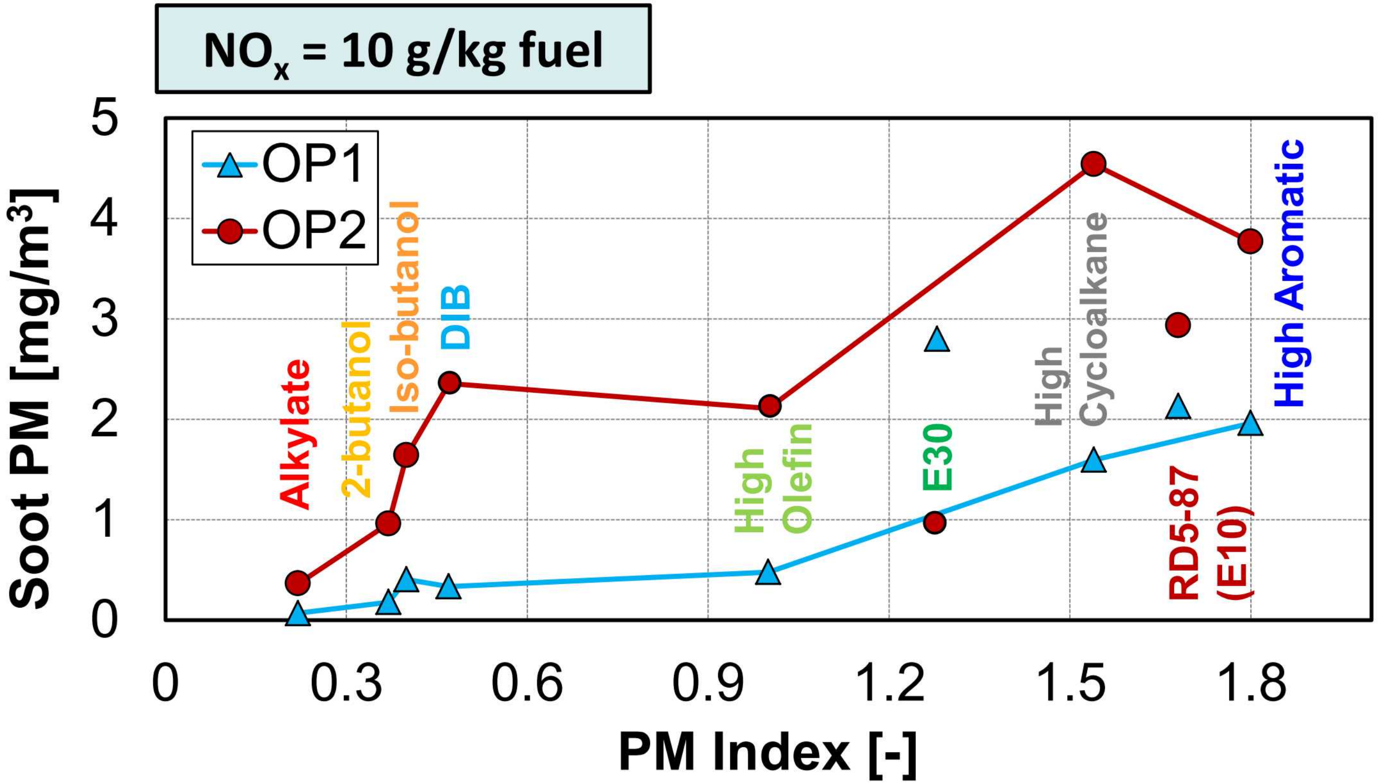


- From mid to late part of expansion stroke, diisobutylene blend exhibits higher variability.
- Higher variability is due to few cycles with slower decay in soot mass.
- Occasional high-soot cycles can raise average exhaust PM.

PMI vs Soot

- Occasional high-soot cycles can raise average exhaust PM for diisobutylene blend.
- Diisobutylene blend has lower PMI than High Olefin fuel, despite higher aromatics content.
- Higher volatility contributes to this.

	High Olefin	Diisobutylene Blend
Alkanes [vol.%]	56.4	56.3
Cycloalkanes [vol.%]	2.9	0.0
Aromatics [vol.%]	**13.4**	**20.1**
Olefins [vol.%]	26.5	23.6
T90 [°C]	136	111



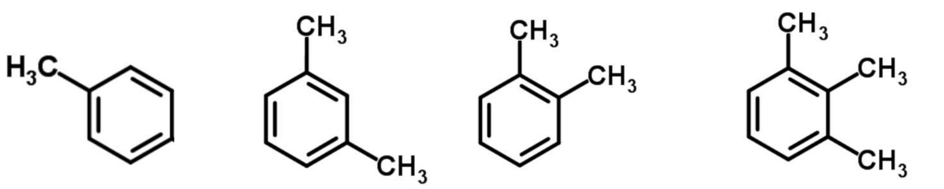
Effect of Vapor Pressure on PMI

- Contribution to PMI for each compound is inversely proportional to its vapor pressure at 443K.

$$PMI = \sum_{i=1}^{n} I_{[443K]} = \sum_{i=1}^{n} \left(\frac{DBE_i + 1}{VP\ (443K)_i} \times Wt_i \right)$$

DBE_i : *double bond equivalent*
$VP\ (443K)_i$: *Vapor pressure at 443K*
Wt_i : *Mass fraction*

- For operating conditions with insignificant wall wetting, effect of vapor pressure may become less influential to sooting propensity.
- PMI of toluene is much smaller than other species with similar molecular structure due to its higher vapor pressure.



Toluene **m-Xylene** **o-Xylene** **1,2,3-Trimethyl-benzene**

`	C	H	DBE	VP [kPa]	PMI_m
Toluene	7	8	4	424.5	1.18
m-Xylene	8	10	4	217.3	2.30
o-Xylene	8	10	4	189.4	2.64
1,2,3-Trimethy-lbenzene	9	12	4	85.5	5.85

- Sooting propensity of diisobutylene blend may have been underestimated by vapor pressure considered in computation of PMI.

COMPONENT	PMI_m	%WGT	PMI_i
Hexene-1	0.164	3.7	0.006
2,2,4-Trimethylpentane	0.190	41.8	0.079
n-Heptane	0.177	11.3	0.020
Toluene	**1.178**	23.9	**0.281**
diisobutylene-1	0.409	14.4	0.059
diisobutylene-2	0.439	4.8	0.021

Summary and Conclusions

- Stratified-charge SI operation offers high efficiency, but maintaining low soot emissions is one of the implementation challenges.
- Fuel effects on soot emission are strong for the nine fuels studied here.
- Engine-out soot can be reasonably well correlated with the fuels' PMI, but with two noteworthy shortcomings:

A. For conditions <u>with</u> wall wetting, ethanol-containing fuels produce much higher soot than indicated by their PMI.
   - Larger injected fuel mass and higher HoV $\Rightarrow$ pool fires.

B. For boosted conditions <u>without</u> significant wall wetting, E30 fuel produces much less soot than indicated by its PMI, while a diisobutylene blend (DIB) produces more.
   - These two fuels were investigated optically, along with a High-Olefin fuel.

- Analysis of natural luminosity indicates similar soot-cloud evolution for these three fuels.
- Average peak natural luminosity correlates well with engine-out soot for **E30, DIB and High-Olefin** fuel, but strong cycle-to-cycle variability exists for all three fuels.
- DBI diagnostic reveals higher cycle-to-cycle soot-mass variability for DIB in late expansion stroke, suggesting that some cycles contribute disproportionally to the engine-out soot.
- Further contributions to shortcomings of PMI for lean stratified SI operation may come from:
  - Disregard for differences in stoichiometric air-fuel ratio between fuels.
  - Excessive importance of vapor pressure (in PMI formula) for conditions with late fuel injection.

Acknowledgements

The authors would like to thank Alberto Garcia, Gary Hubbard, Keith Penney, and Tim Gilbertson for their dedicated support of the DISI laboratory.

The work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. This research was conducted as part of the Co-Optimization of Fuels & Engines (Co-Optima) project sponsored by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE), Bioenergy Technologies and Vehicle Technologies Offices. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.