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Ability of PMI to Predict Soot Emissions from Lean Stratified-Charge and Well-Mixed Stoichiometric SI Operation using Alternative Fuels

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U.S. DEPARTMENT OF ENERGY

Co-Optimization of Fuels & Engines

Abstract

Direct fuel injection is becoming increasingly common for modern automotive spark-ignited (SI) engines since it offers benefits like improved cold starting and catalyst heating, faster response to load transients, better anti-knock performance, and the ability to create a stratified charge for lean operation. However, the use of direct injection can lead to issues with increased particulate matter (PM) emissions. This is a particular concern in the context of alternative gasoline formulations that deviate substantially from typical E0-E10 market gasolines.

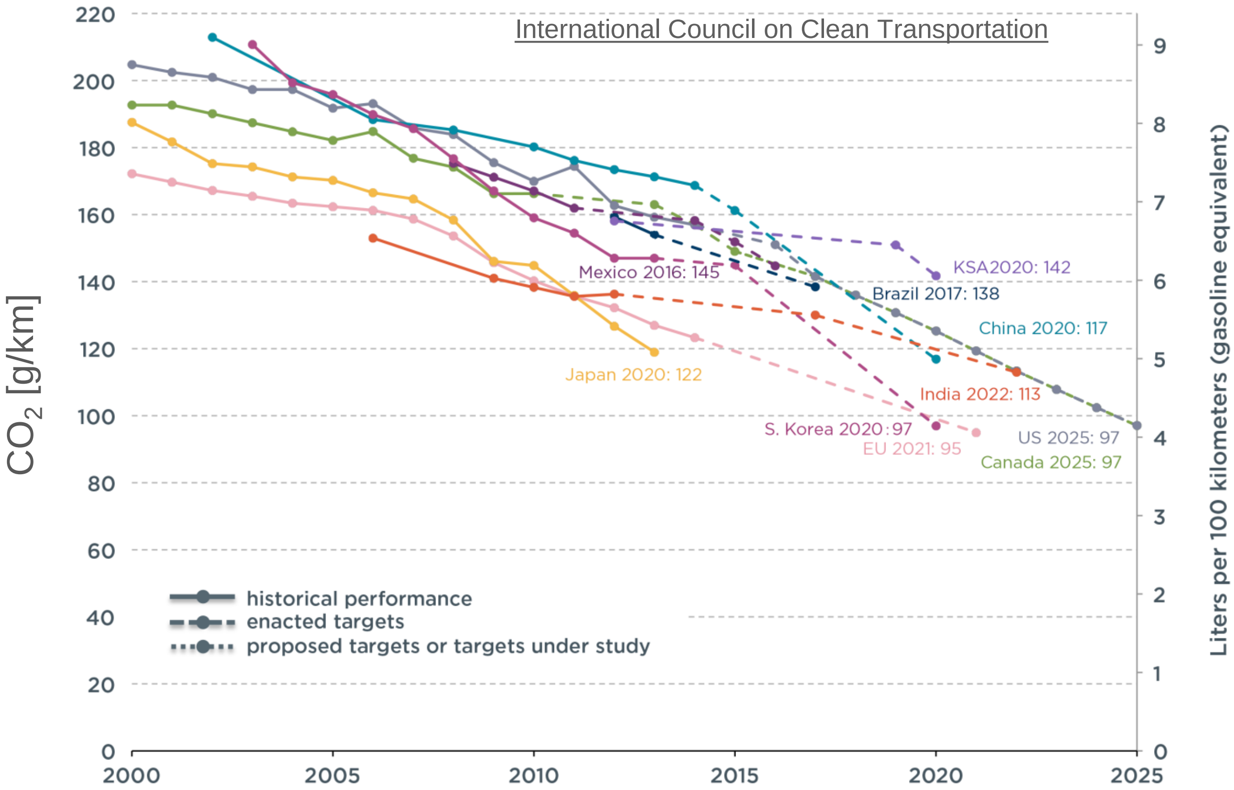
To help ensuring that future fuel formulations are well compatible with the requirement of low exhaust PM of direct-injection spark-ignition (DISI) engines, fuel-property metrics that capture sooting propensity need to be evaluated and potentially developed further. Here, the ability of one such metric, namely Particulate Matter Index (PMI), to rank order fuel performance in terms of exhaust soot is evaluated for eight gasoline-type fuels used in a single-cylinder DISI research engine. It can be noted that PMI was originally developed for port-fuel injection (PFI) SI engines to capture total particulate number (PN) and PM over a drive cycle, and only low levels of oxygenates were considered, namely ethanol up to E10.

This preliminary assessment of PMI is focused on stoichiometric well-mixed operation, but also includes lean fully stratified operation for three of the eight fuels. The exhaust soot was measured with an AVL Smoke Meter 415S, which converts filter paper blackening to soot mass concentration. It was found that fuel effects on exhaust PM can be very strong for both well-mixed stoichiometric and lean stratified-charge SI operation. For the rather limited test ranges examined here, it was found that PMI is a reasonable predictor of the relative exhaust PM level for steady-state well-mixed stoichiometric operation at 1400 rpm, and also for steady-state moderately boosted stratified operation at 2000 rpm. However, it was discovered that PMI is a poor predictor of the relative exhaust PM level for transient well-mixed stoichiometric operation, which has lower in-cylinder surface temperatures compared to the steady-state operation.

Furthermore, PMI was not able to correctly predict relative exhaust PM level for steady-state naturally aspirated stratified operation at 1000 rpm, and this was attributed to excessive wall wetting for the E30 fuel. Overall, elevated soot PM for fuels with ethanol, iso-butanol and 2-butanol points to the importance of vaporization and co-vaporization properties, and to the inability of PMI to correctly capture these effect.

Lastly, a recently developed wall-wetting diagnostics based on refractive index matching (RIM) was demonstrated for engine operation with an E30 and an Alkylate fuel. This optical technique shows promise to be one of the tools used in future work aimed at clarifying the shortcoming of PMI, and potentially also in future work that target enhancements to PMI or other fuel-property metric that reliably can predict relative PM exhaust emissions for new fuel formulations.

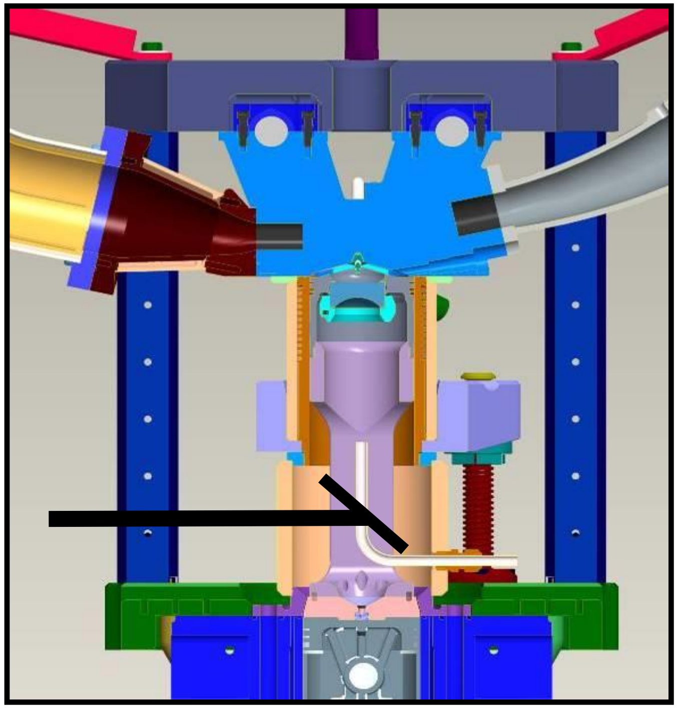
Introduction

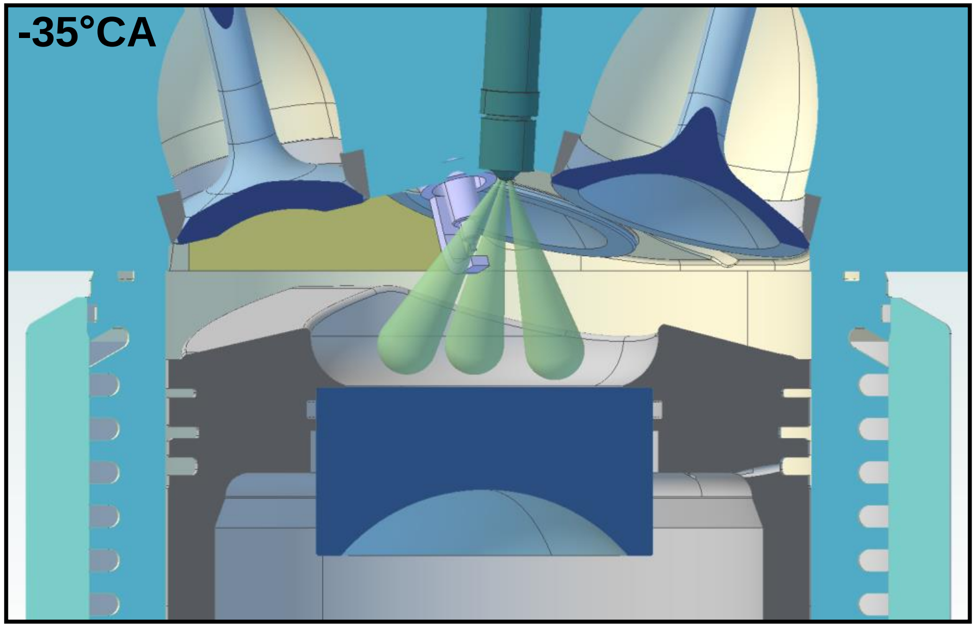


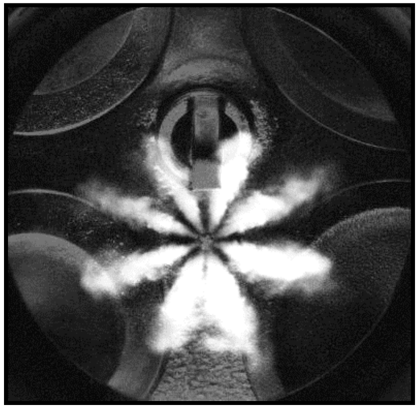
- Strong pressure to reduce CO_2 emissions.
- Improved engine efficiency is one key factor.
- Stoichiometric SI operation is standard for gasoline-type engines.
- Onset of knock limits CR and overall efficiency.

Research Engine

- Designed for spray-guided stratified-charge operation ⇒ Piston bowl.
- 8-hole injector. P_{in} = 170 bar.
- Drop-down single-cylinder engine.
- Automotive size. 0.55 liter swept volume.
- Identical geometry for **All-metal** and **Optical.**







Fuels Matrix

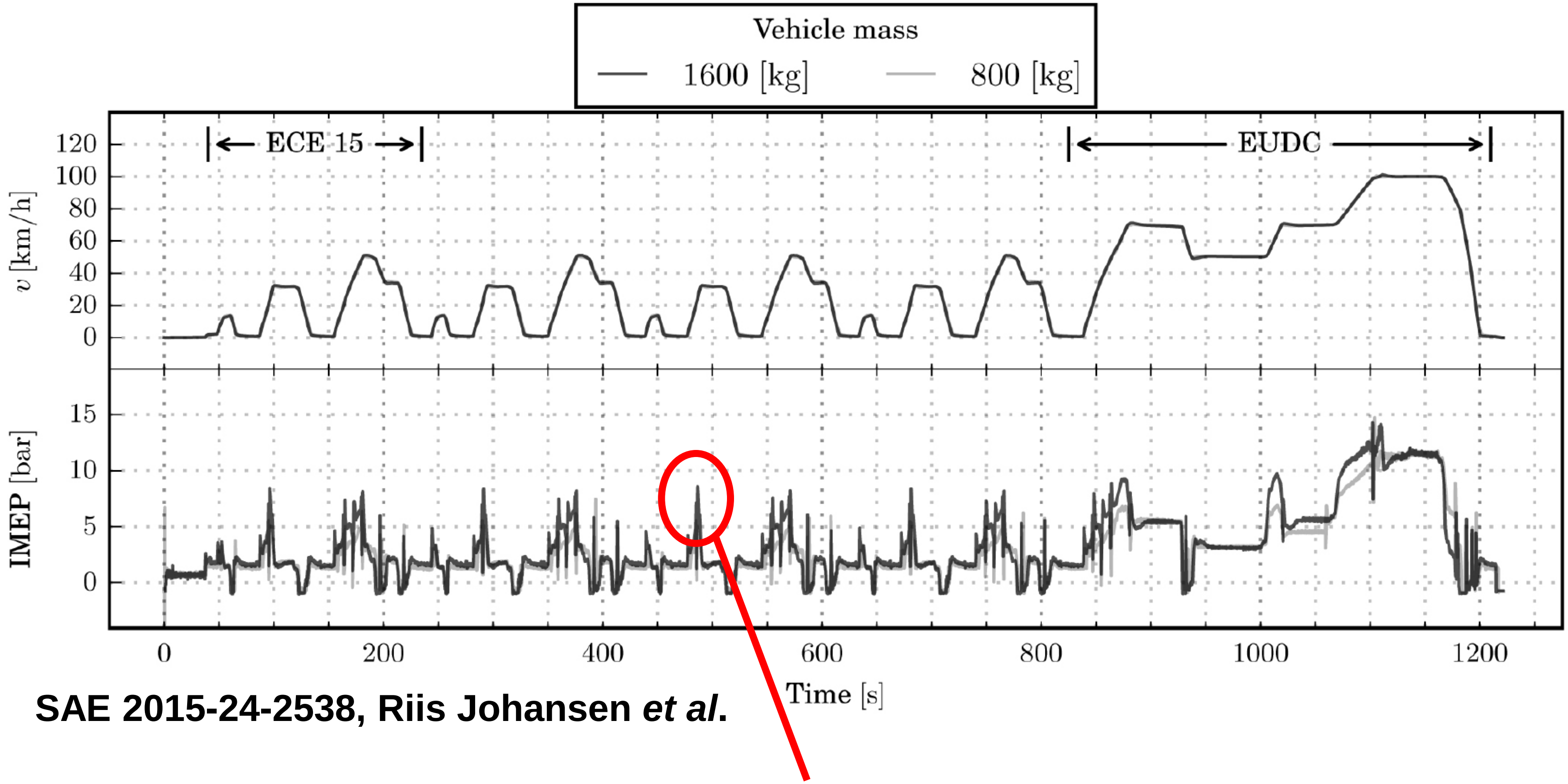
- Here, study eight RON = 98 fuels, and one regular E10 gasoline.
- Octane sensitivity, composition, heat of vaporization, and end-boiling point vary greatly.

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

- PMI varies greatly as well.

Relevance of RON & MON for Transients?

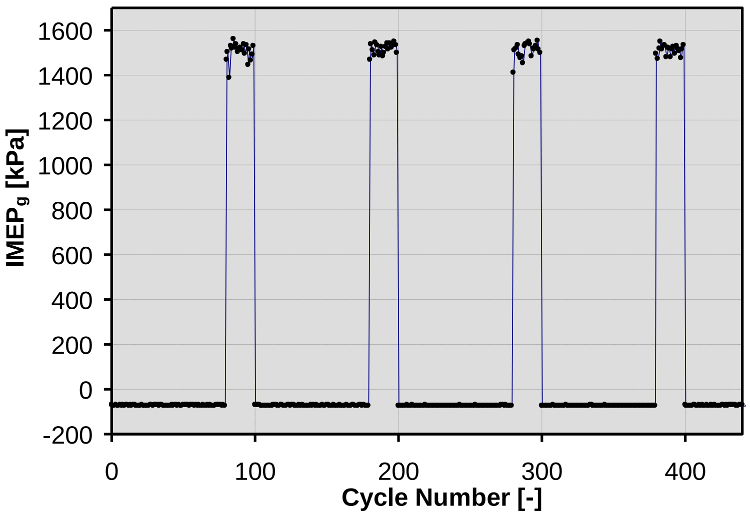
- RON and MON are determined for steady-state conditions.
- Actual vehicle operation is usually not steady-state.

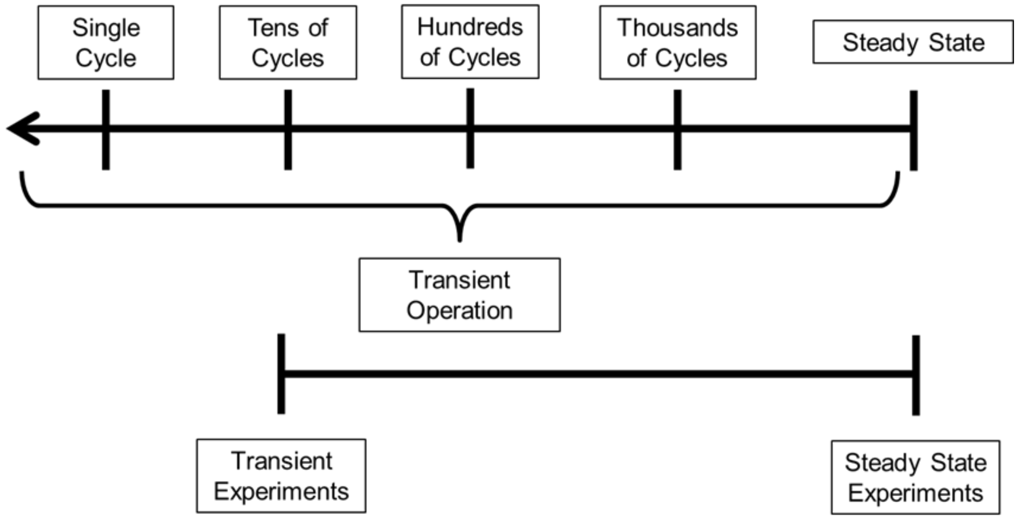


SAE 2015-24-2538, Riis Johansen *et al*.

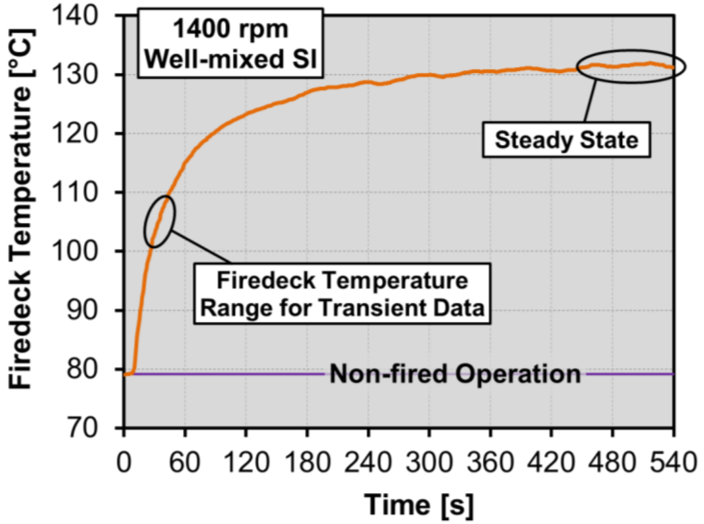
- What is the relevance of RON and MON for load transients?
- How does predictive power of PMI change for transients?

Stoichiometric Test Regimes: Steady State and Transient

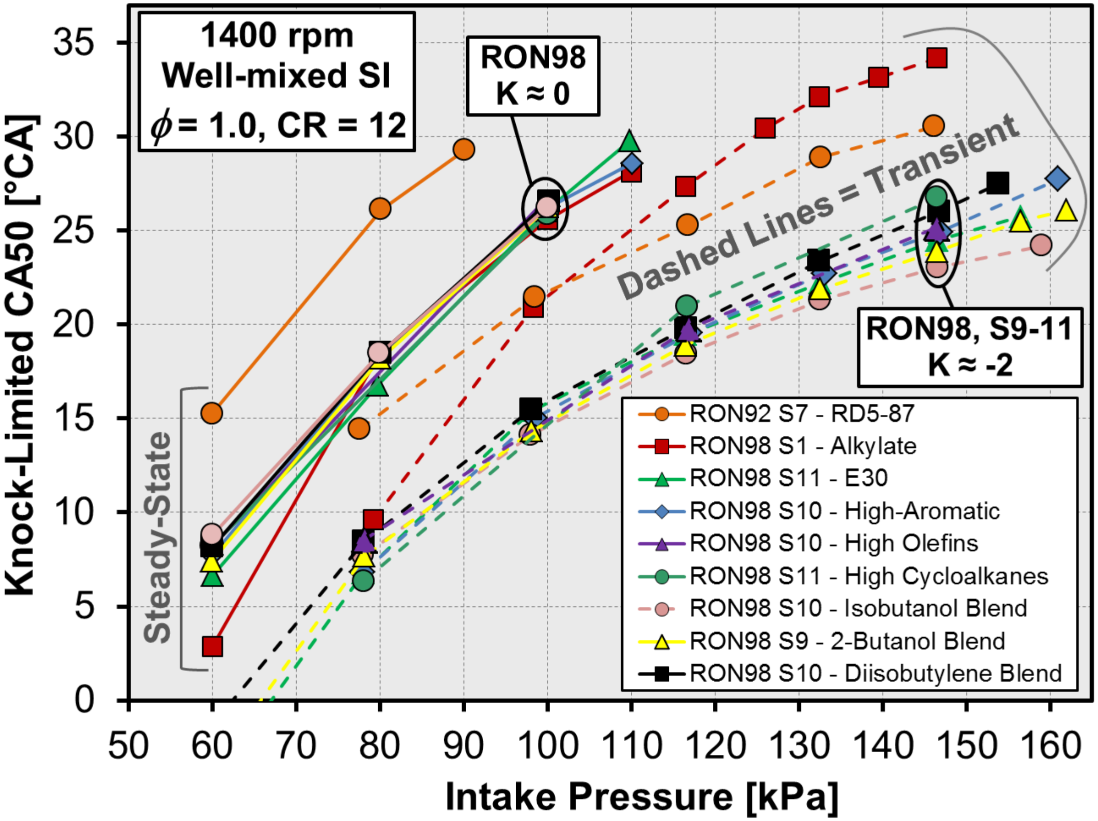




- 20/80 load-transient operation mimics short time scales of vehicle acceleration.
- Lower in-cylinder surface temperatures compared to steady-state.
- Allows testing of knock-limited boosted "beyond RON" conditions.
- See SAE 2017-01-2234 for details on transient testing.



Load-Transient Operation Reveals Benefit of High-S Fuels



- Steady-state: All RON98 fuels provide knock suppression, compared to RON92.
- Load Transient: RON98 high-S fuel provide best boosted performance.
- Identical triple or quadruple injection strategy was used for all fuels, for each type of operation.
  - Allows correlating exhaust smoke with PMI.

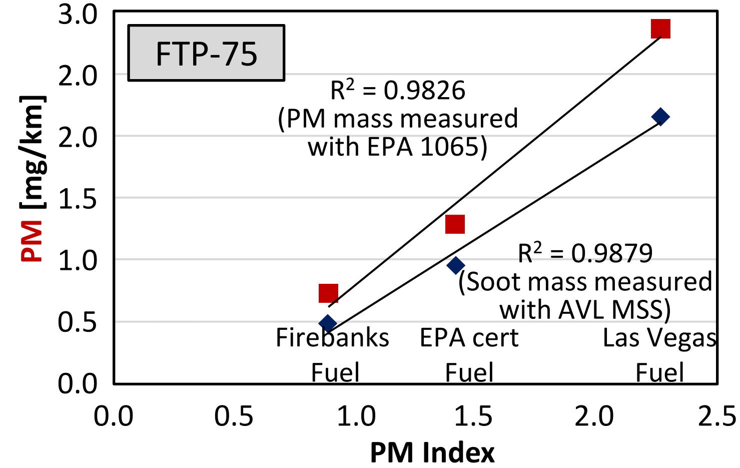
Introduction to Particulate Matter Index (PMI)

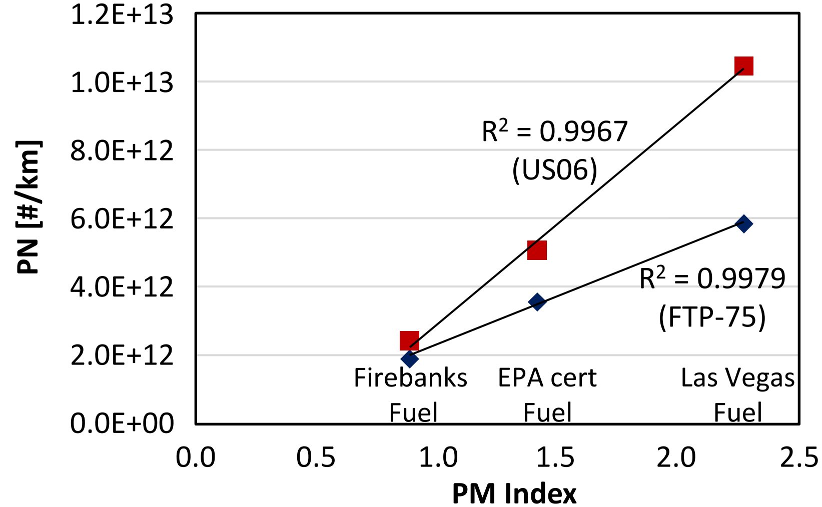
$$PMI = \sum_{i=1}^{n} I_{[443K]} = \sum_{i=1}^{n} \left(\frac{DBE_i + 1}{VP\,(443K)_i} \times Wt_i \right)$$

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

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

- The correlation was initially derived by Honda for PFI engines, and verified with PN measured under NEDC cycle test.
- Validation of the correlation with a GDI engine were also carried out under US06 and FTP-75 cycle test.
- The overall results suggest that the correlation works well for prediction of sooting tendency of given fuel.

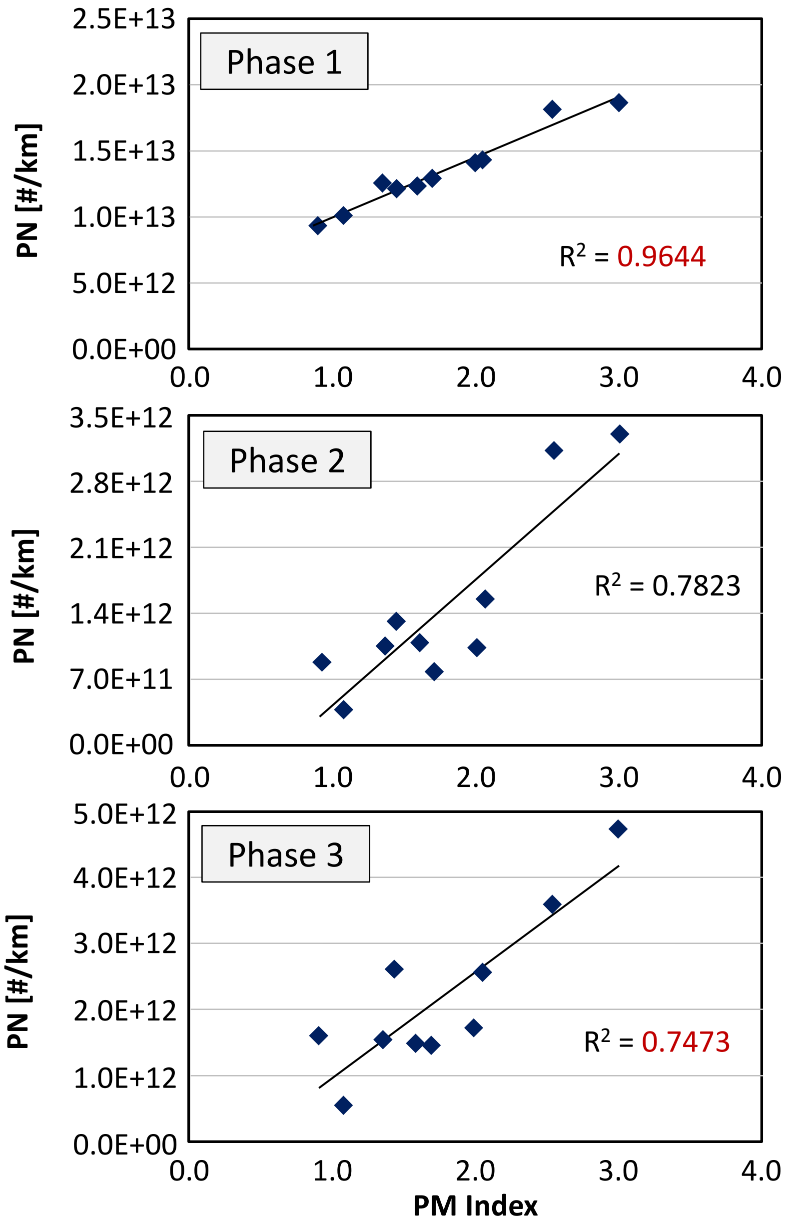




[Graphs redrawn from SAE 2010-01-2115]

PMI Evaluation on FTP-75

- PMI metric was tested more extensively by Honda, using a GDI engine on FTP-75 cycle.
- When the measured PN were separated into three phases of the test cycles, the correlation for phase 2 and 3 were not as high as that of phase 1.
- When PMI was compared with PM, the correlation deteriorated even further.
- There are some conditions where PMI becomes less accurate. (Works well when engine is not fully warmed-up where wall wetting effect becomes pronounced.)



[Graphs redrawn from Aikawa and Jetter, IJER, 2014]

Fuels Used by Honda for PMI Development

- Test fuels for development of PMI correlation were formed by blending indolene and additives below.

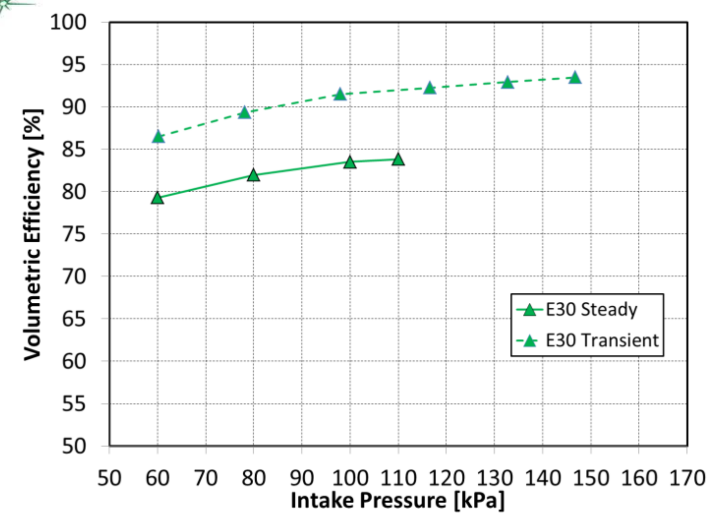
Additive	FBP** [K]	DBE
2,2,4- Trimethylpentane	372	0
Dodecane	489	0
Ethylbenzene	409	4
α-Methylstyrene	436	5
1,2,4-Trimethylbenzene	442	4
Divinylbenzene	468	6
Napthalene	491	7
Indene	455	6
Ethanol	351	0

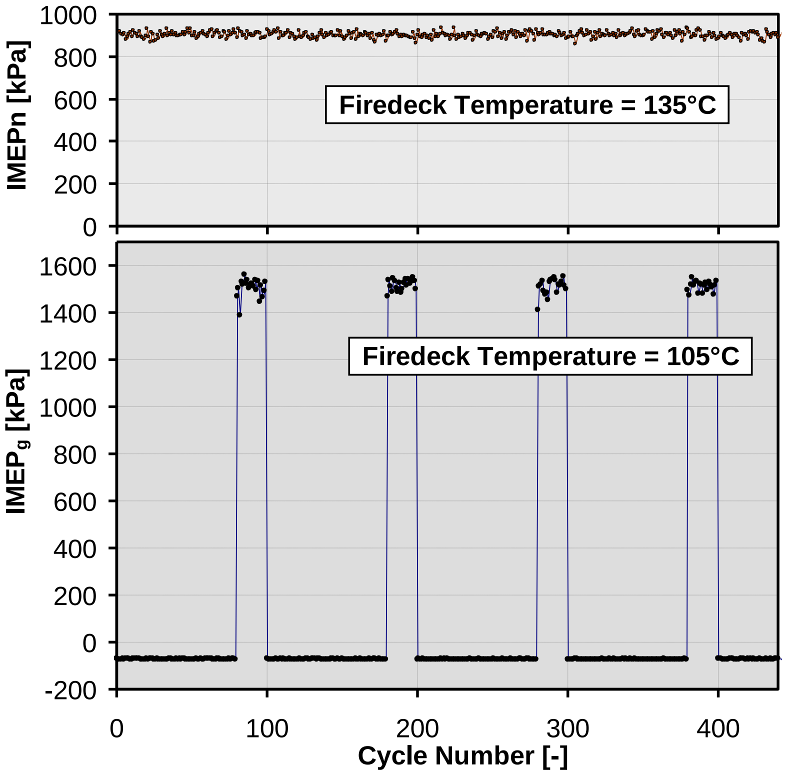
**FBP = final boiling point

- Although validation of PMI correlation was carried out using variety of test fuels, evaluation of PMI correlation for fuel which mainly consist of oxygenated hydrocarbon was not carried out. (E10 max.)

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

Stoichiometric Operating Conditions

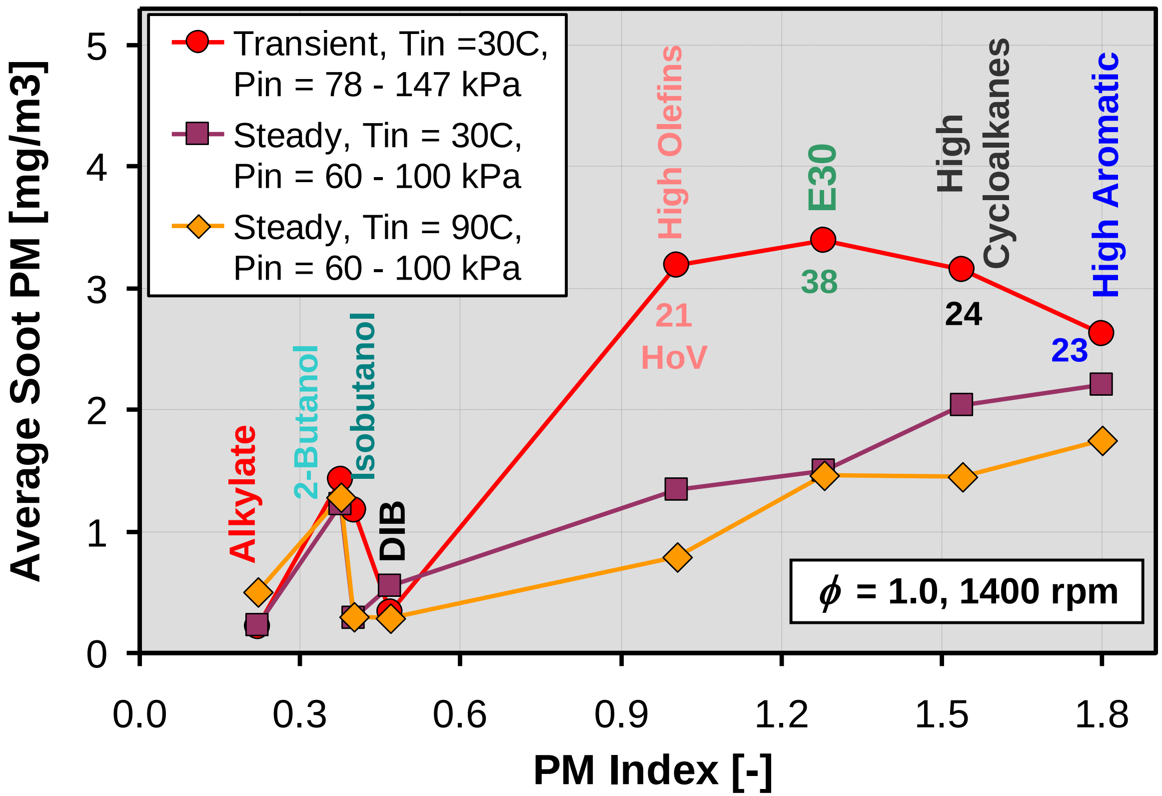




- ϕ = 1.0, 1400 rpm.
- $T_{coolant}$ = 75°C for steady state.
- T_{in} = 30°C and 90°C.
- P_{in} = 60 – 110 kPa.
  - SOI_1 = -310°CA, ΔSOI = 20°CA, triple injections.
- $T_{coolant}$ = 90°C for transient.
- P_{in} = 78 – 147 kPa. T_{in} = 30°C. SOI_1 = -270°CA, ΔSOI = 20°CA, quadruple injections.
- Lower thermal state is evidenced by higher volumetric efficiency.

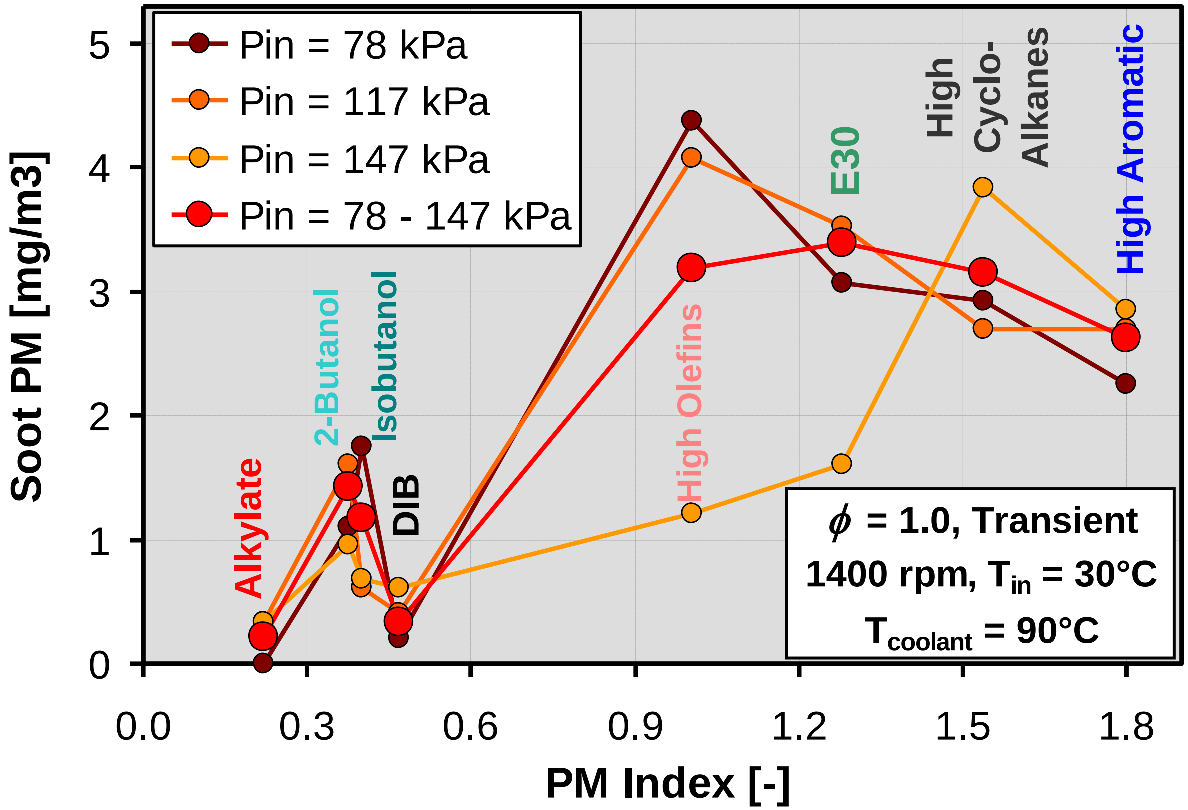
Exhaust Soot vs. PMI

- Steady-state well-mixed stoichiometric PM scales nearly monotonically with PMI.
  - 2-butanol and isobutanol are exceptions. Why?
  - Higher T_{in} reduces soot PM some. Consistent with faster vaporization.
- For cooler transient operation, High-Olefin, E30, High-Cycloalkane fuels break the monotonic trend.
- Wall-wetting issues?
- AVL Smoke Meter 415S
  - Measures filter blackening.
  - Meter converts filter blackening to soot concentration [mg/m³].



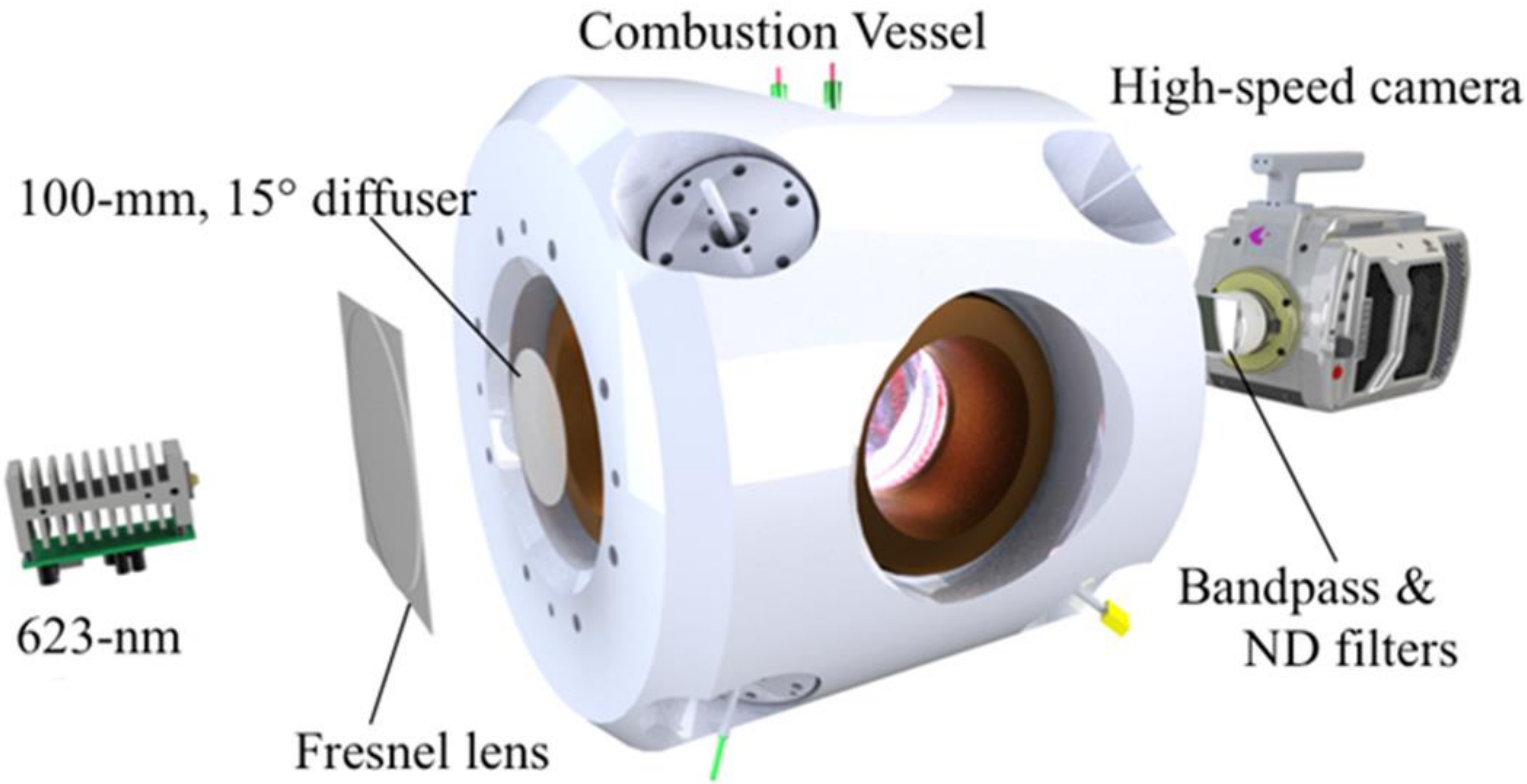
Transient Exhaust Soot vs. PMI

- For cooler transient operation, soot PM is highly dependent on the intake pressure.
- Especially for High-Olefin and E30 fuels.
- Why are the trends so complex?
- Direct injection, so spray variability can contribute to soot trends.



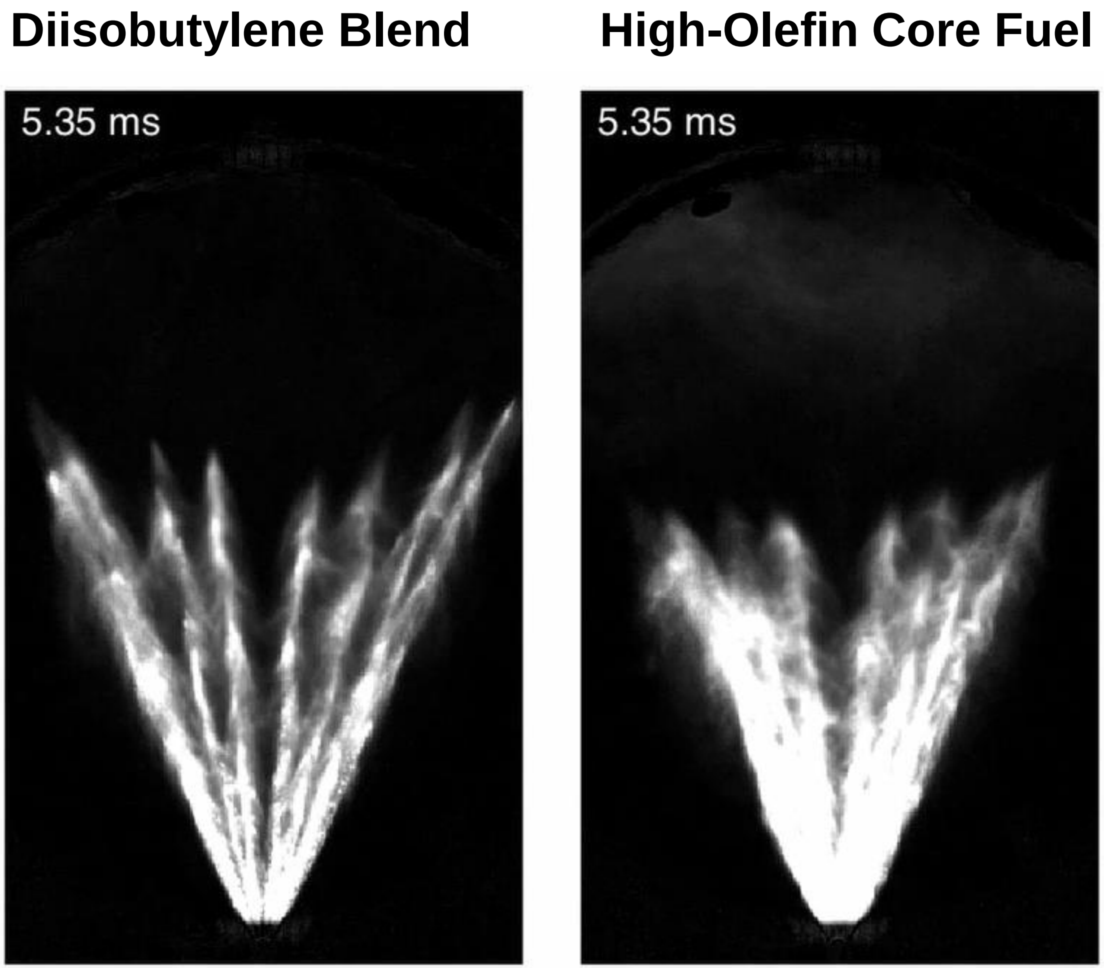
Spray Visualization Setup

- Constant volume spray vessel.
- Diffuse background illumination.
- Light-extinction technique to visualize fuel droplets.



Spray Visualization

- T_{gas} = 188°C, P = 100 kPa, P_{inj} = 120 bar.
- 3x 1.0 ms injections, 2.38 ms between SOIs (ΔSOI = 20°CA @ 1400 rpm.)
- Longer penetration for surrogate fuel (wall wetting issues.)



- Lingering droplet clouds for full boiling range High-Olefin fuel (bulk-gas soot).
- Fuel effects on spray development contributes to reduce predictive quality of PMI.

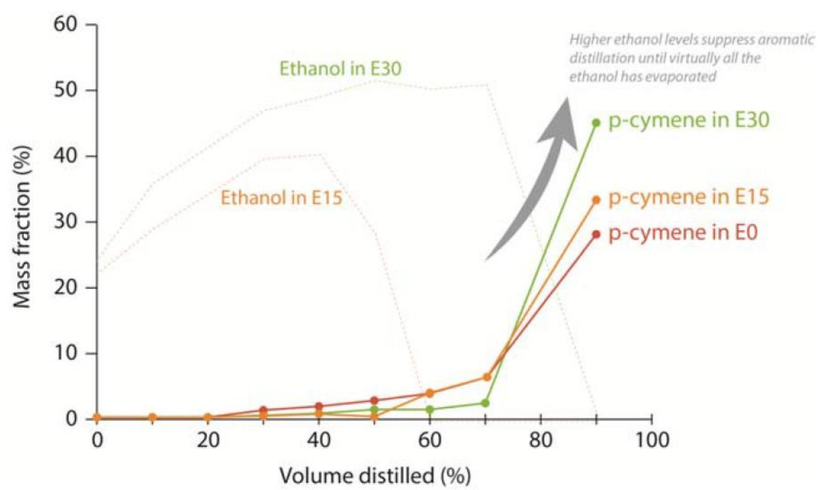
Interactions of Fuel Components

- NREL results show that ethanol possibly can exacerbate PM issues.
- This may happen for other alcohols as well, like 2-butanol and isobutanol.
- Such interactions are not captured by PMI, reducing its predictive power.

Co-Optimization of Fuels & Engines

JULY FY16 HIGHLIGHT

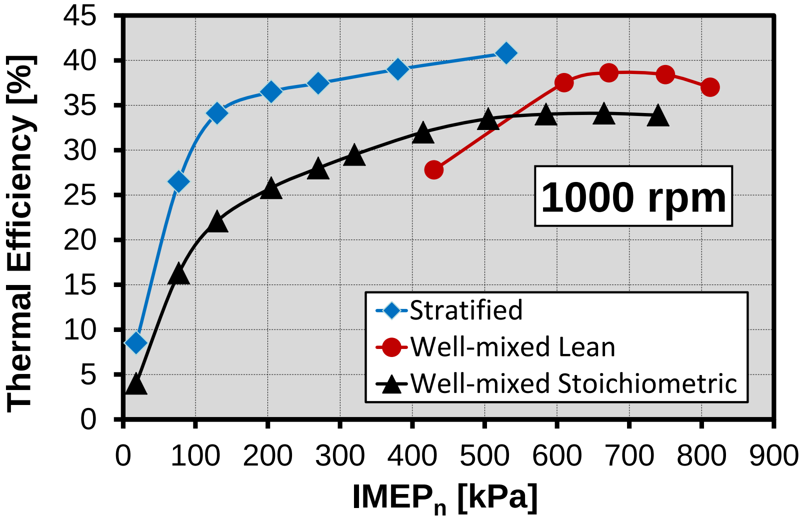
Ethanol's Suppression of Aromatic Distillation May Increase Likelihood of Particulate Matter Formation

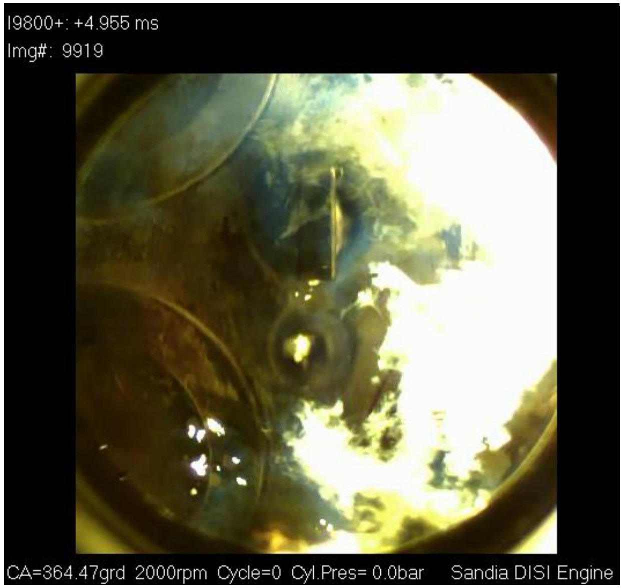


Distillate composition results for 10 volume percent blends of p-cymene in E0, E15, and E30. The mass fractions of ethanol and p-cymene in collected distillate fractions, as functions of percent fuel distilled are shown. Similar results were obtained from two other fuel sets prepared using cumene 4-t-butyltoluene.

Stratified-Charge Potential and Concerns

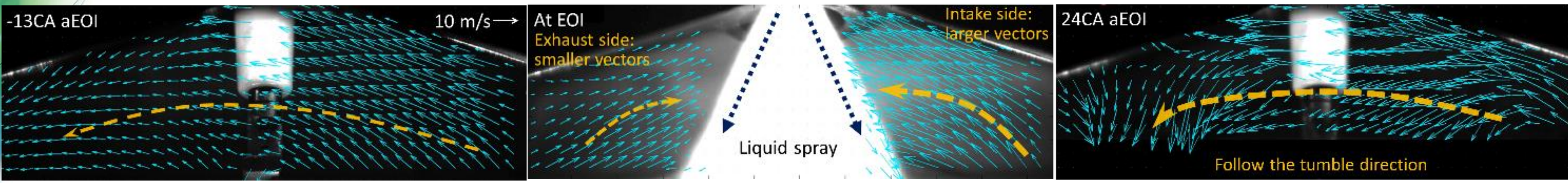
- Lean operation may well be required for SI engines to meet CO_2 requirements.
- Stratified-charge operation has a strong efficiency potential.
- A new fuel should be compatible with stratified-charge SI operation.
- A specific concern is the sooting propensity.

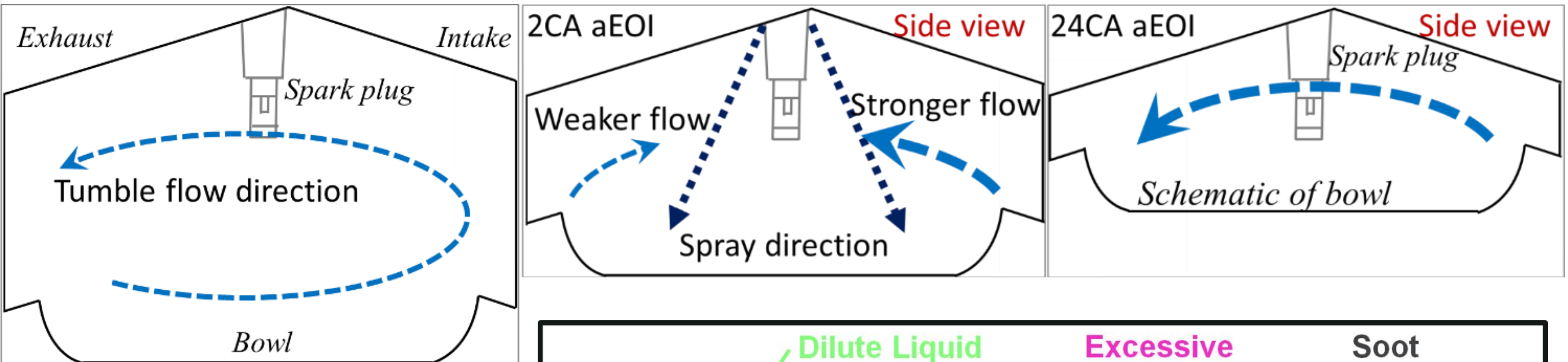


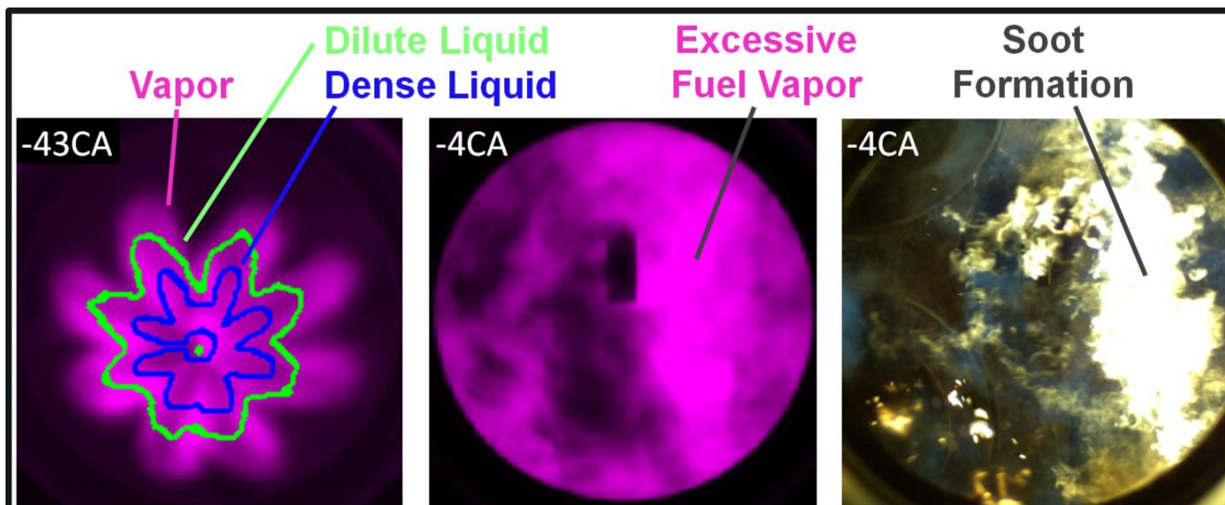


Certification Gasoline, 2000 rpm

Tumble Effect on Vapor Spread at 2000 rpm



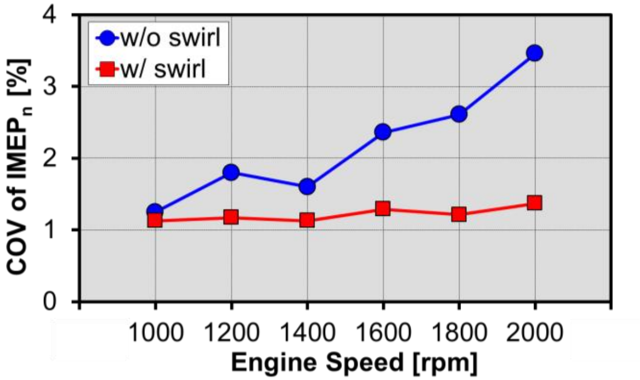




W. Zeng, M. Sjöberg, D.L. Reuss, Z. Hu, Proceedings of the Combustion Institute, 2017.

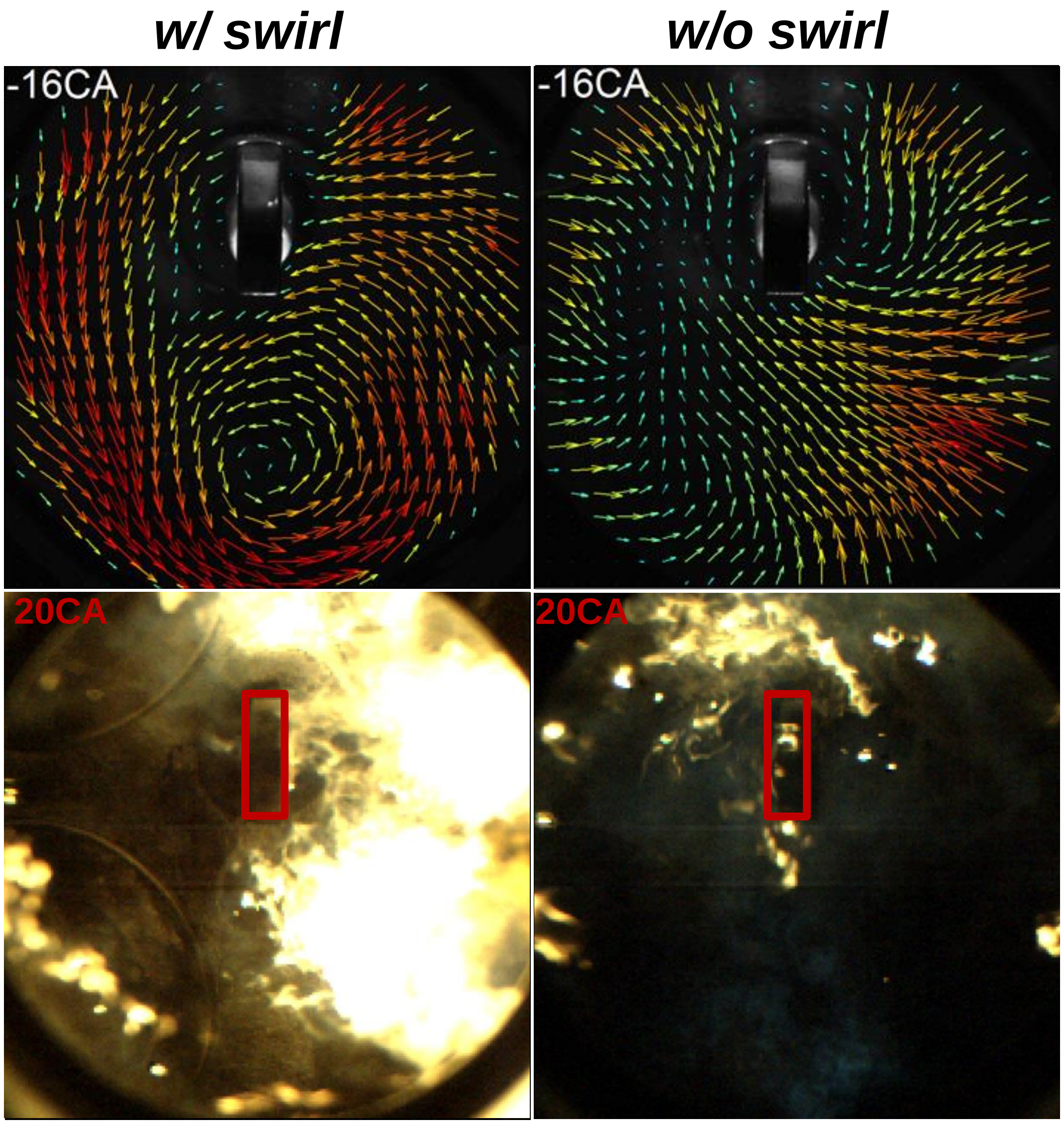
Swirl Flow Stabilizes Combustion

- Intake-generated swirl is required to stabilize stratified combustion at higher speeds.
  - Spray-swirl interaction creates a repeatable vortex.
  - Effective flame propagation.



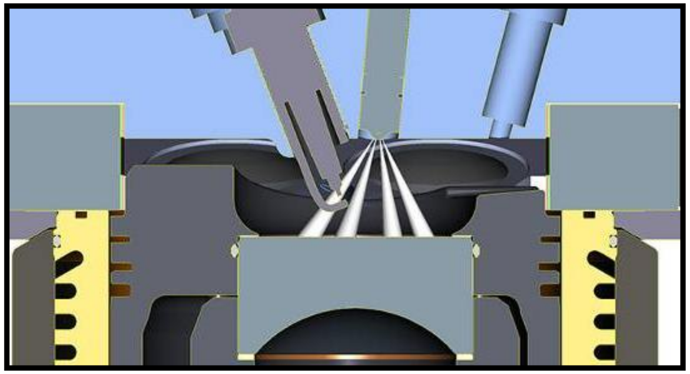
- Swirl generated by inactivating one intake valve.
  - Increases tumble as well, which can induce elevated soot emissions.

W. Zeng, M. Sjöberg, D.L. Reuss, and Z. Hu, Combustion and Flame, June 2016.



High-Speed Spray Visualization

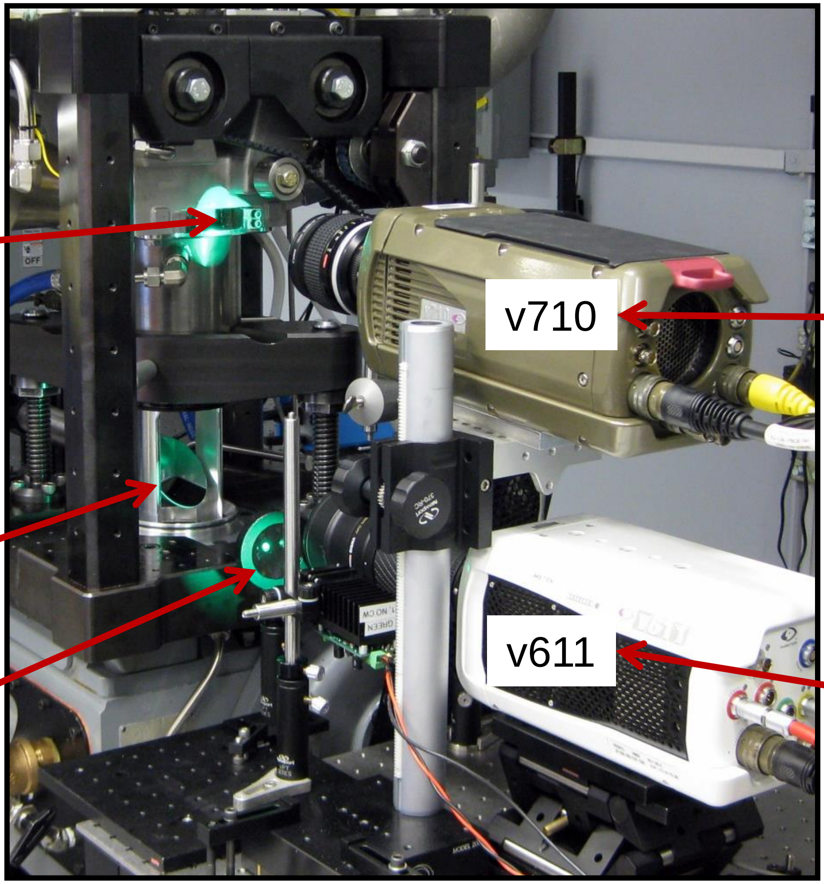
- 60 kHz = 0.1°CA resolution @ 1000 rpm.
- Dual cameras for side and bottom views.



Pent-roof side window and LED 2

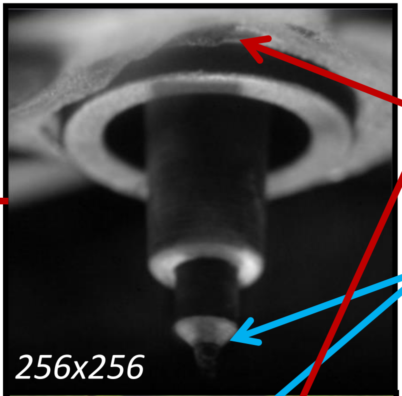
45° Bowditch Mirror

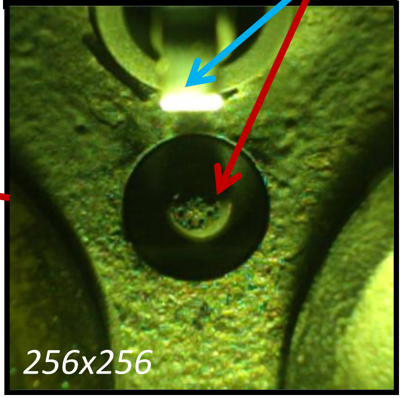
Focusing lens for LED 1



Injector tip

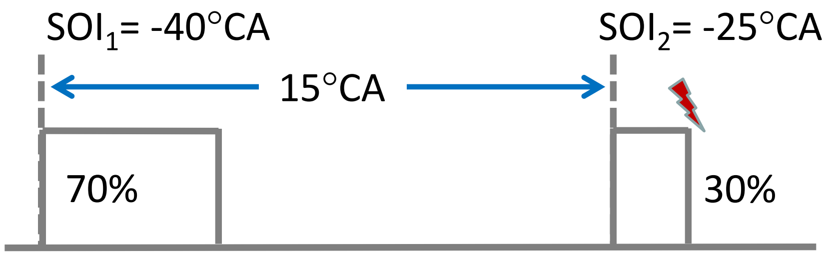
Spark plug

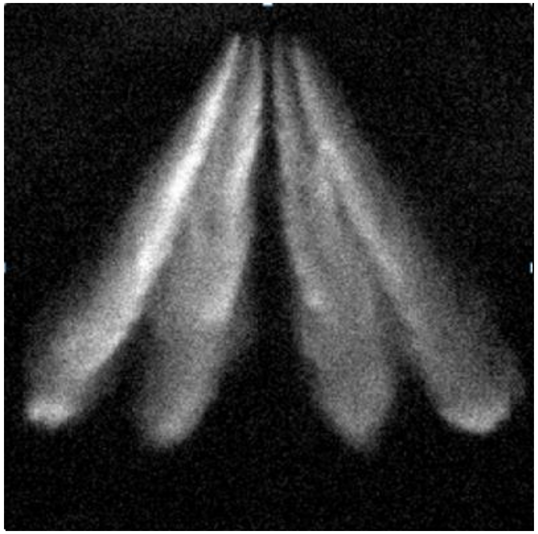




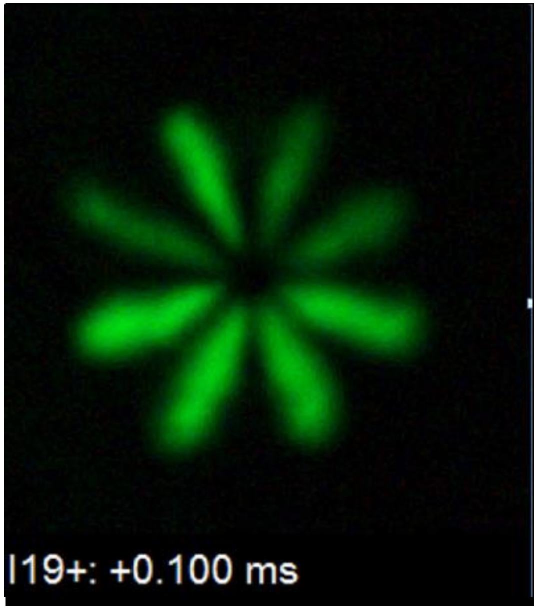
High-Speed Spray Visualization

- This study uses 70/30 split ratio.





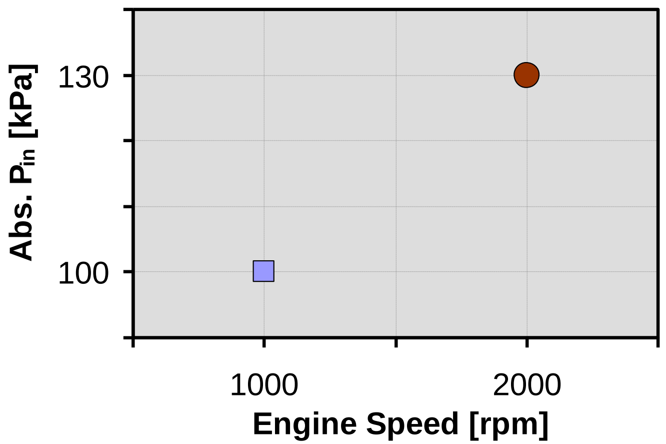
- Tail ignition.



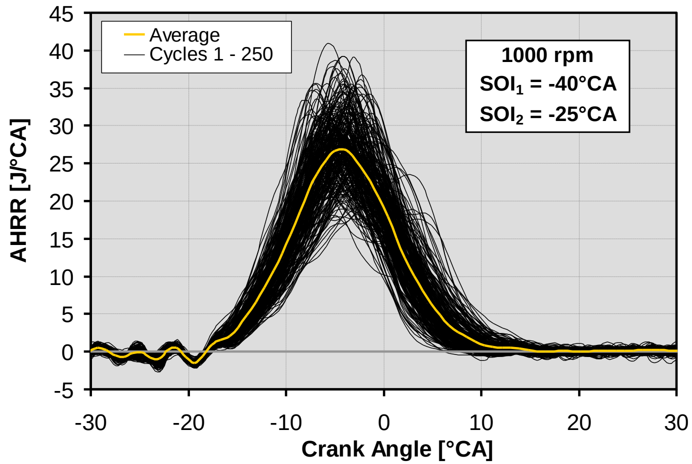
- Injection pressure = 170 bar.
- Near vertical injector orientation.
- 60° included angle.

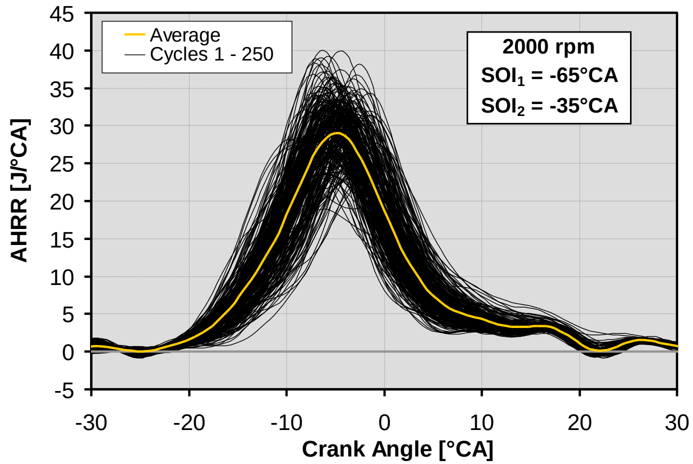
Stratified Operating Conditions

- Low and moderate speed.
- Higher intake pressure at 2000 rpm to mimic turbocharger.
- Use N_2 dilution to simulate $[O_2]$ – reducing effect of cooled EGR.
- $\phi_m = 0.33$.
- $T_{in} = 30°C$, $T_{coolant} = 75°C$.
- SOI adjusted to maintain combustion phasing.



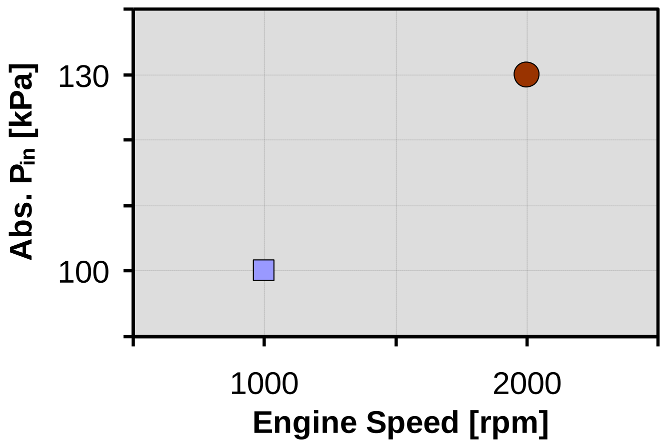
$$\phi_m \equiv \frac{\left(F/C\right)_{Actual}}{\left(F/A\right)_{Stoichiometric}}$$

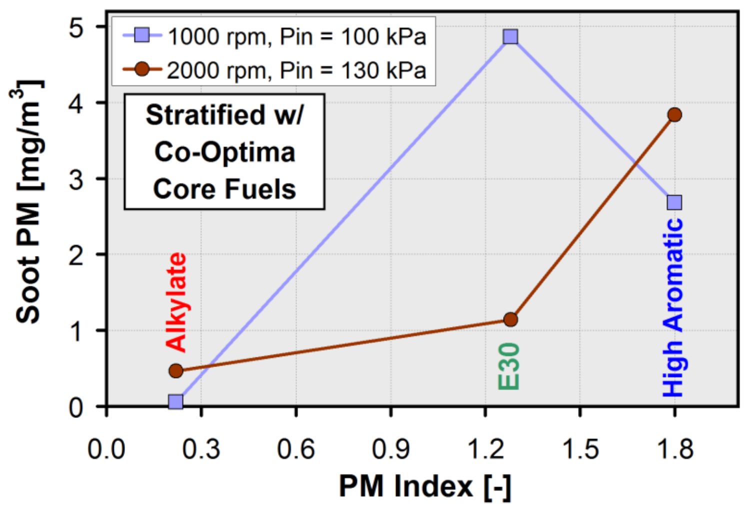




Relate Exhaust Soot to Fuel Properties - PMI

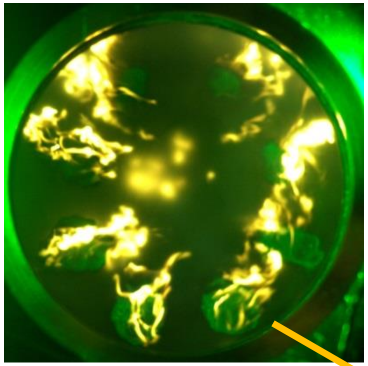
- Exhaust soot increases monotonically with PMI for higher-speed boosted operation.
  - Bulk-gas soot is a major pathway.
- PMI is a poor predictor for non-boosted operation.



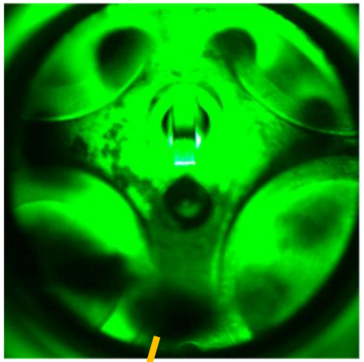


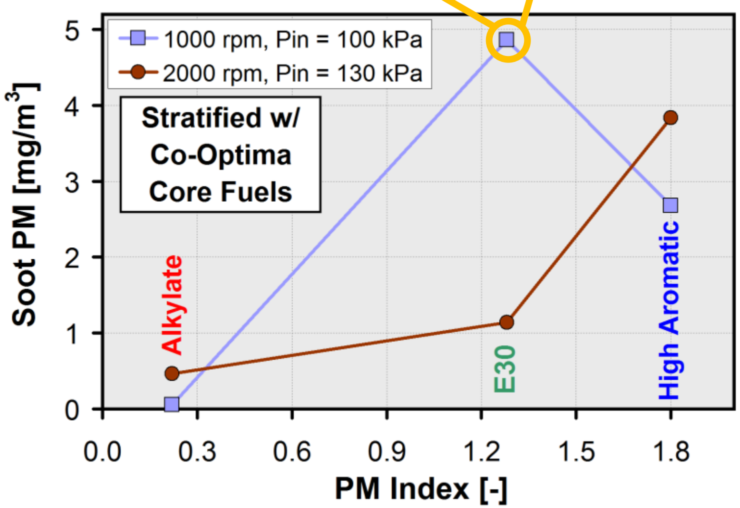
Exhaust Soot vs. PMI

Fuel Films & Pool Fires

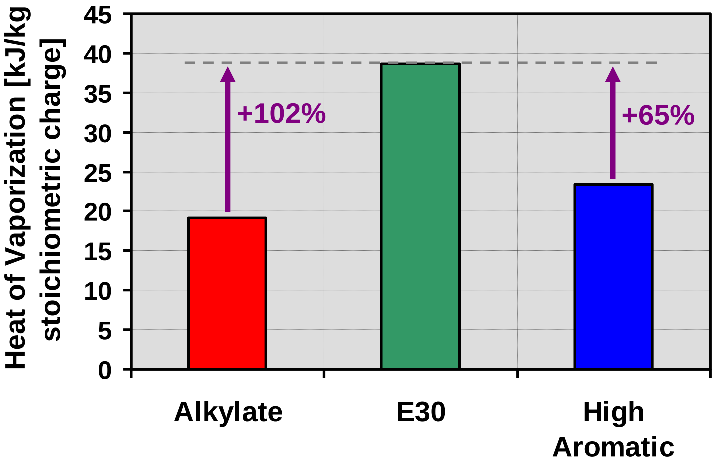


Soot Deposit Detection



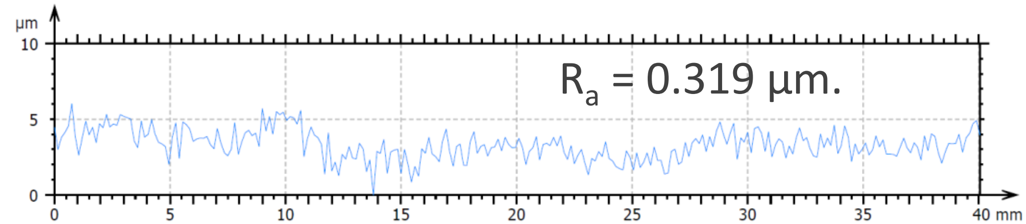


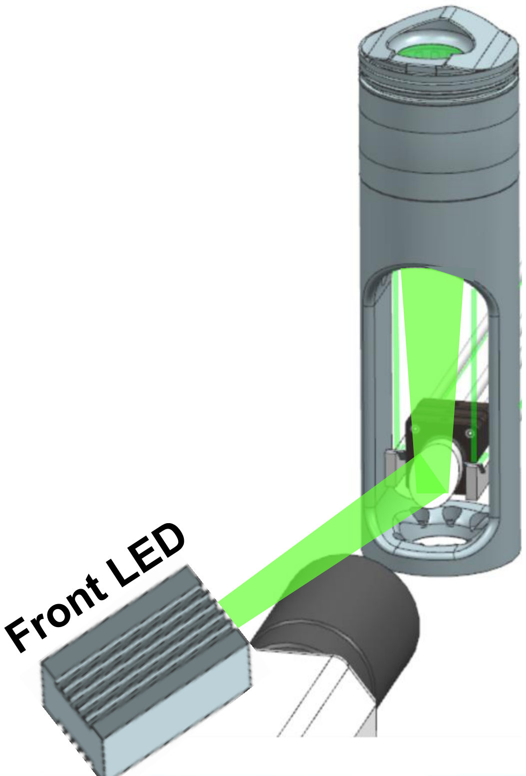
- E30 does not follow PMI for non-boosted stratified.
- Wall-wetting issues.
  - Higher HoV and lower AFR.

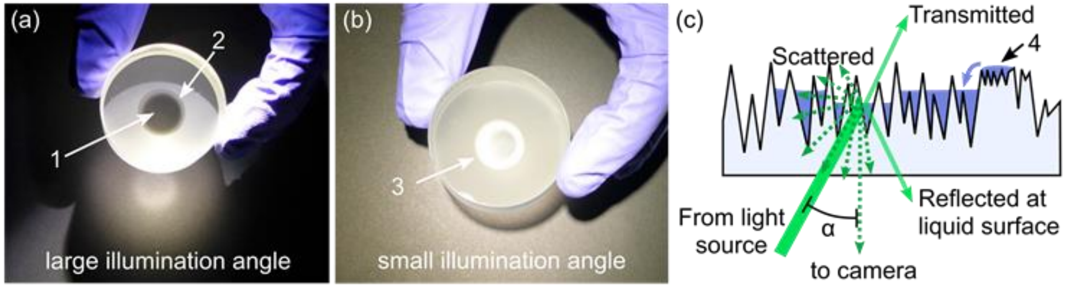


Development of Wall-Wetting and Pool-Fire Diagnostics

- Use Refractive Index Matching (RIM) to detect fuel films, following Fansler, Drake et al. (e.g. SAE Paper 2003-01-0547.)
- Front illumination is easy to implement, and provides quantification of fuel-film area.
- Ground-surface window reduces depth of focus.

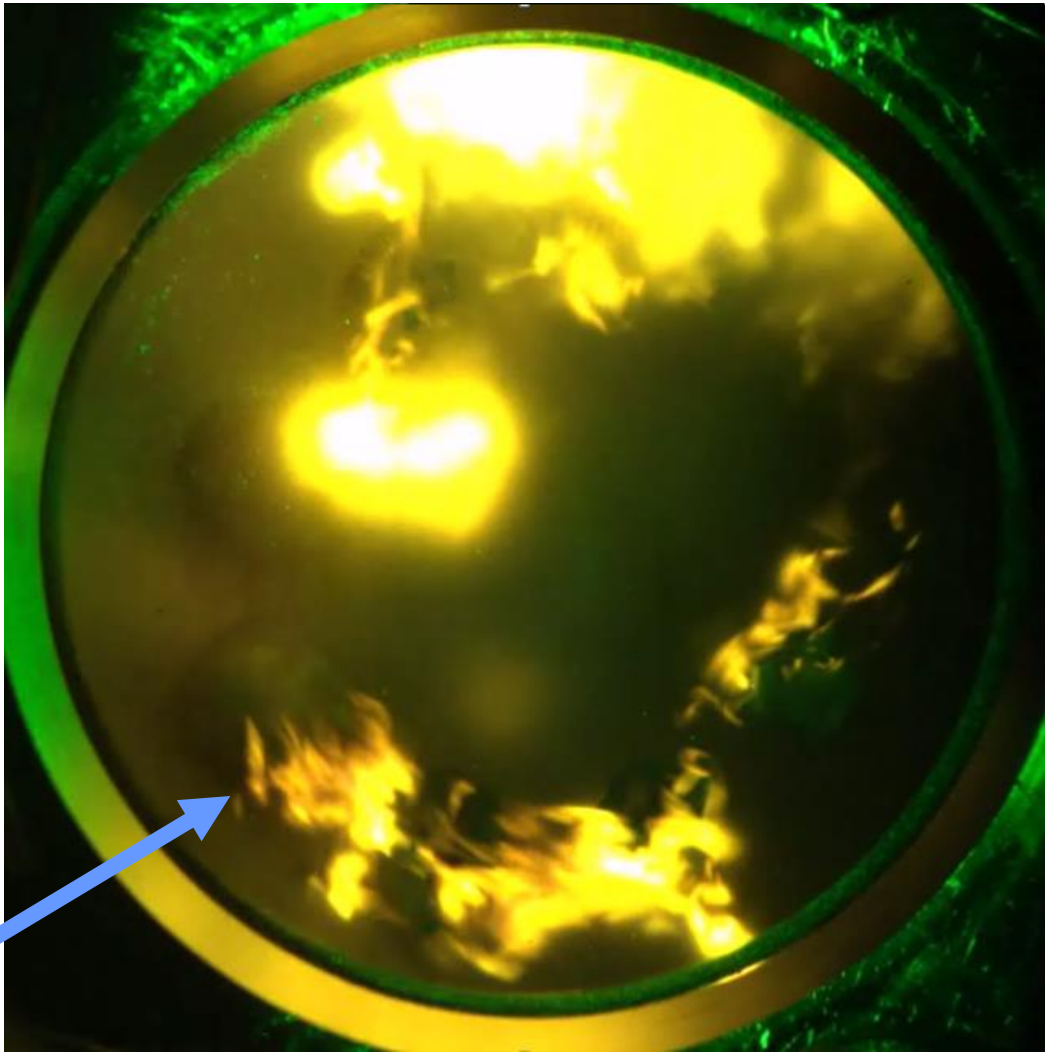






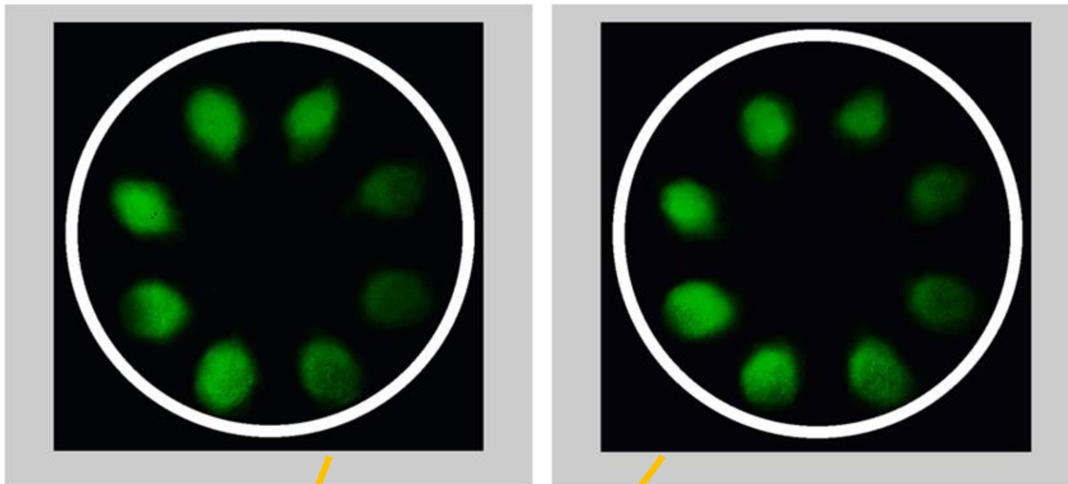
Flame Imaging with Ground-Surface Window

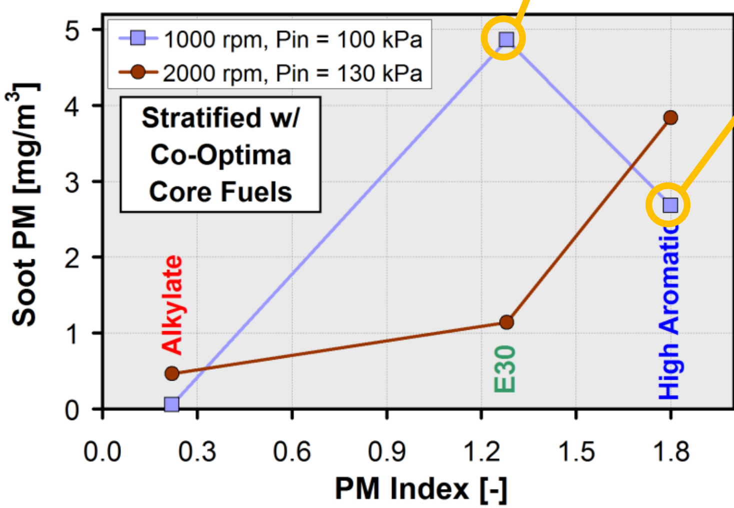
1000 rpm, P_{in} = 100 kPa,
Single injection, SOI = -31°CA,
Spark Timing = -24°CA
E30 fuel

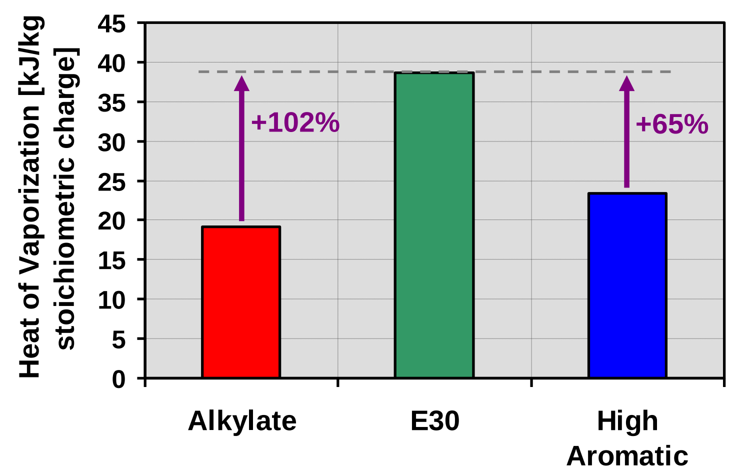


Flames with sharp features are close to the window surface. It is clear from movies that these flames are attached to the surface, indicating pool-fires.

Wall-wetting for E30 and HA

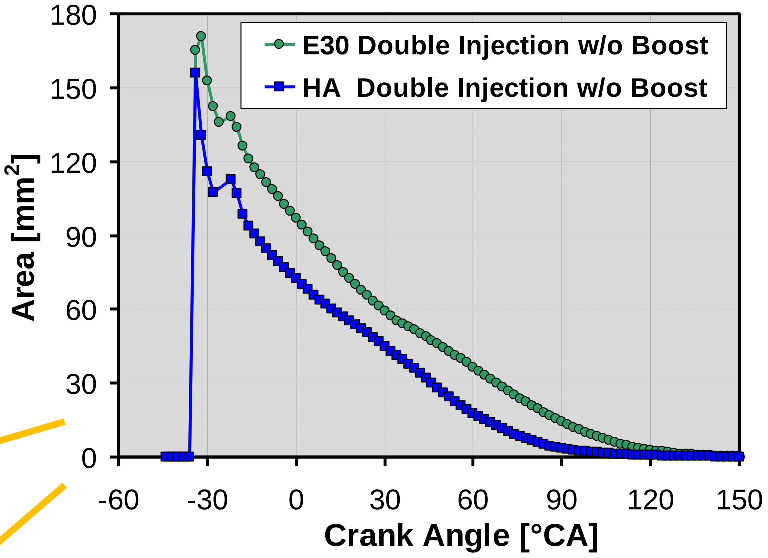


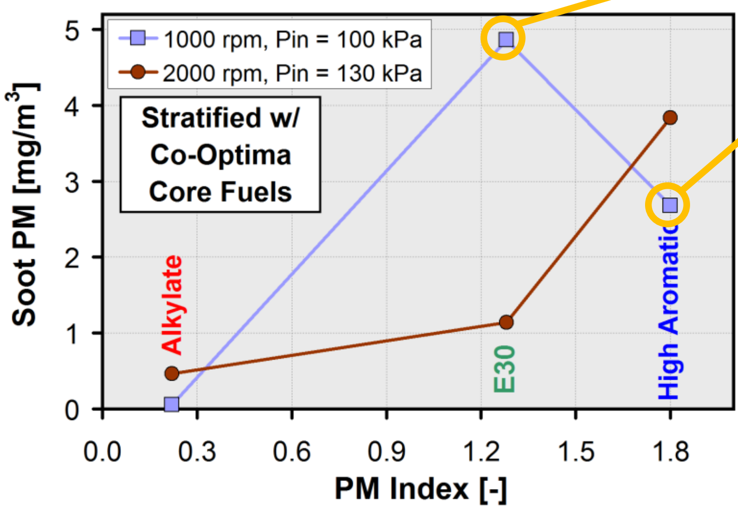


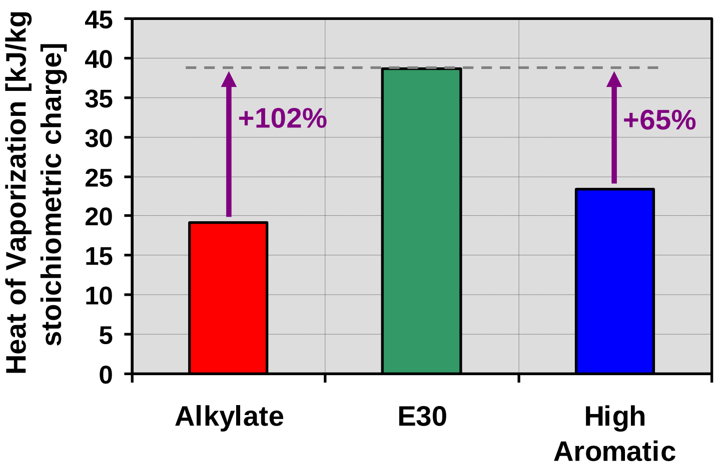


Wall-wetting Area for E30 and HA

- Wall-wetting issues.
  - Higher HoV and lower AFR.
- Wetted area is not much greater for E30.
  - Motivates efforts to quantify fuel-film thickness.

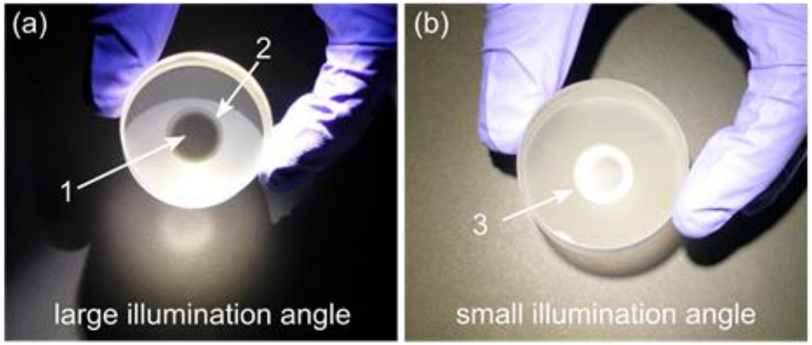


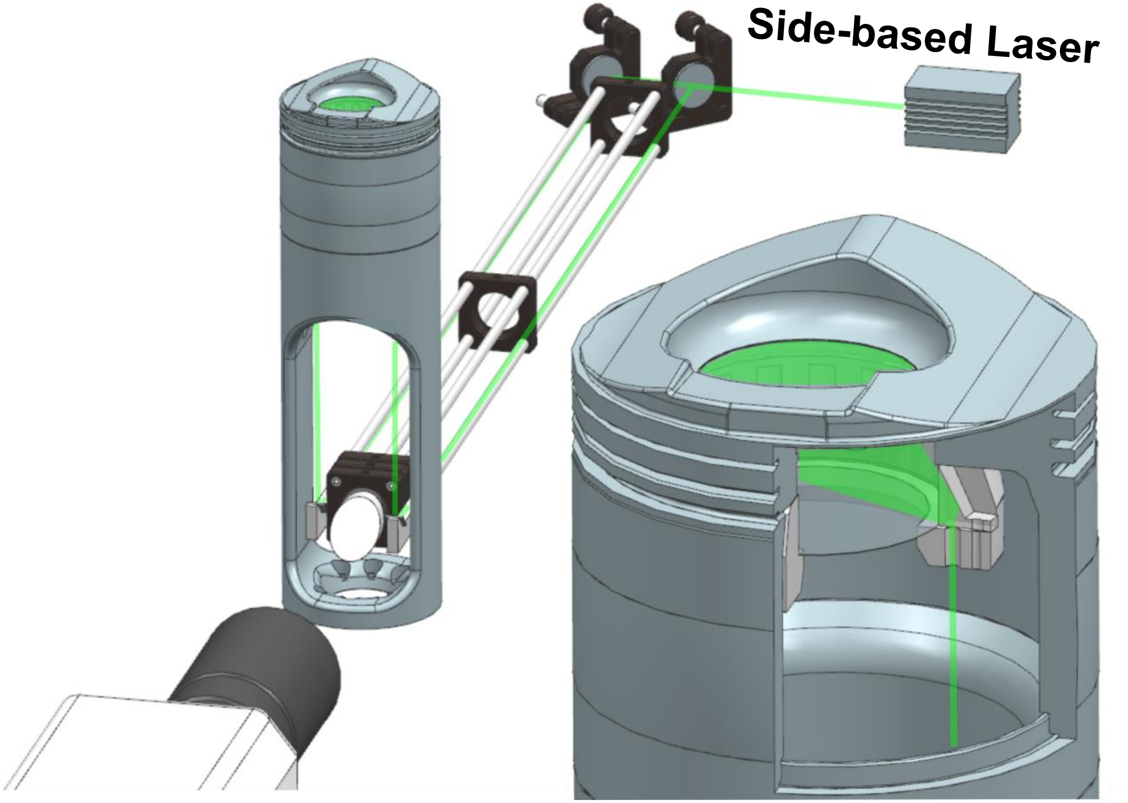


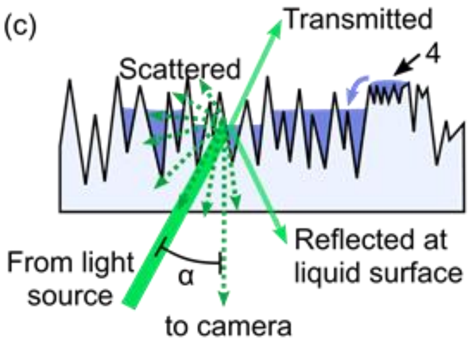


Development of Wall-Wetting Diagnostics

- Side illumination provides both area quantification, and semi-quantitative thickness.

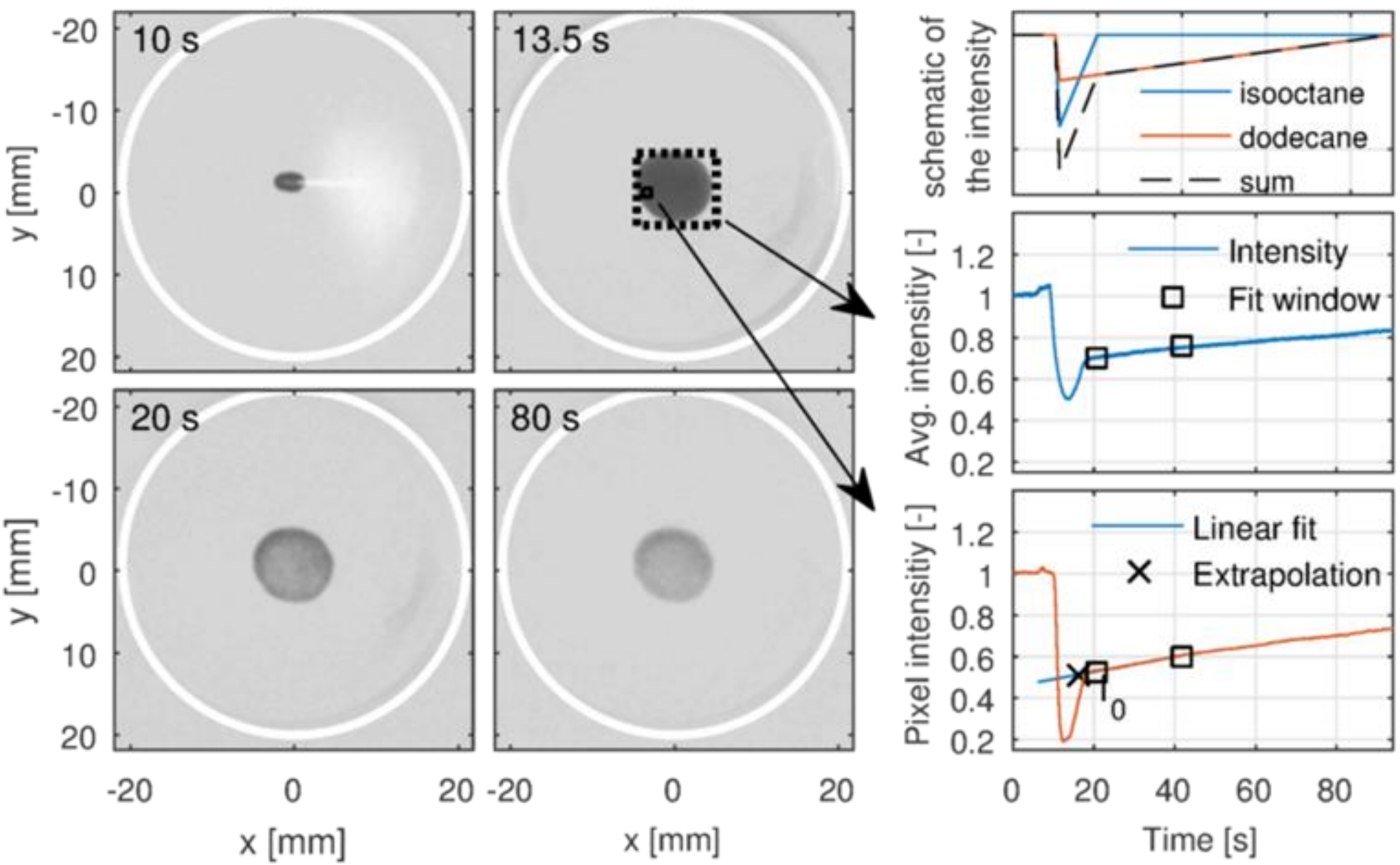




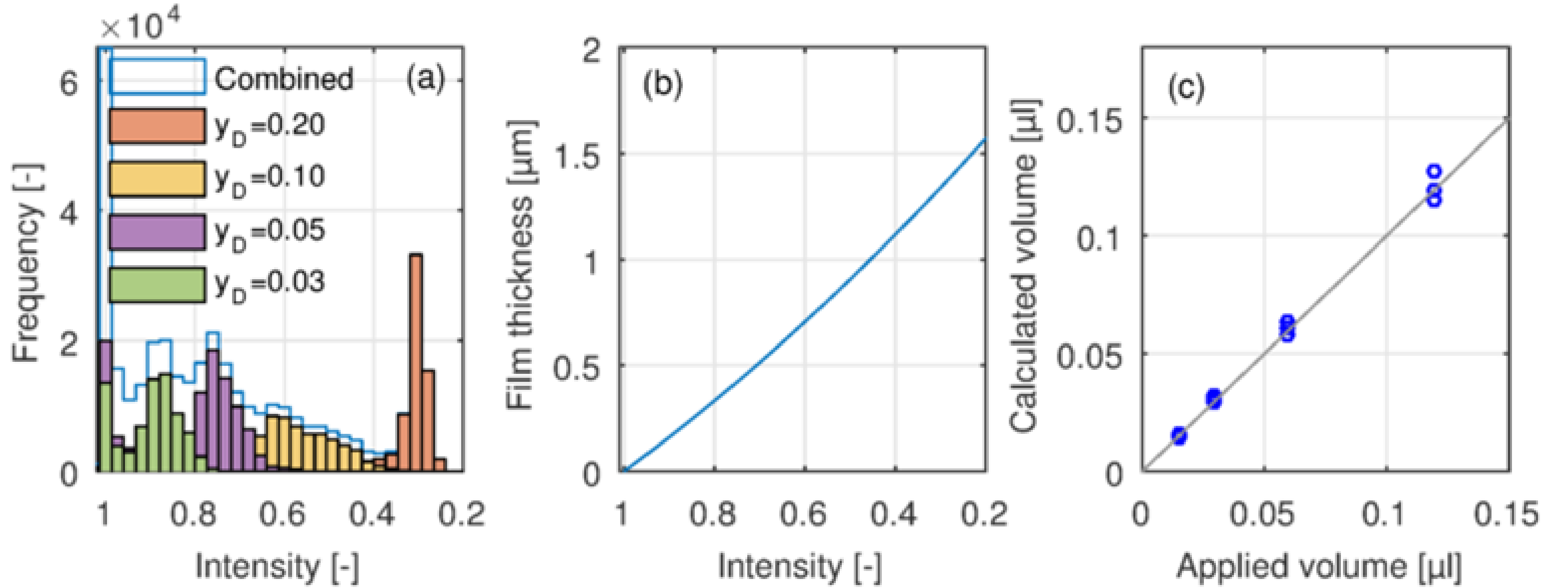


Calibration Procedure

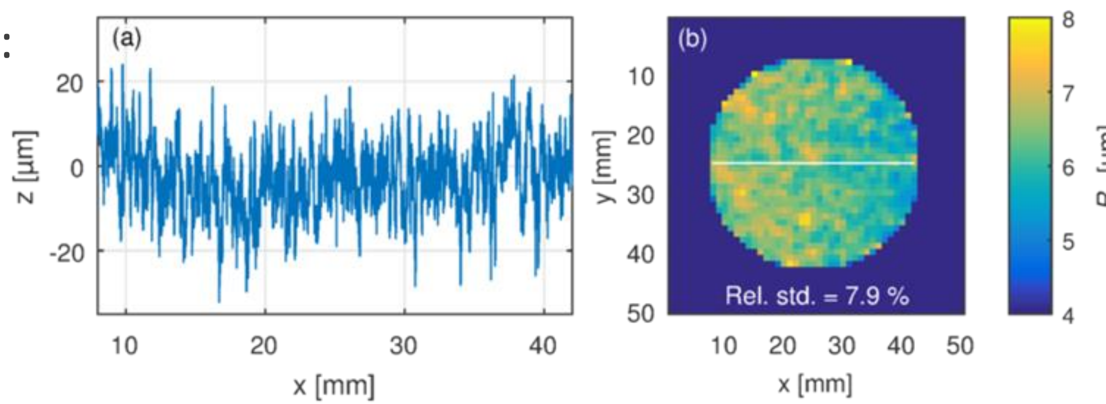
- Mixtures of iso-octane and dodecane were applied with a syringe.



Calibration Procedure

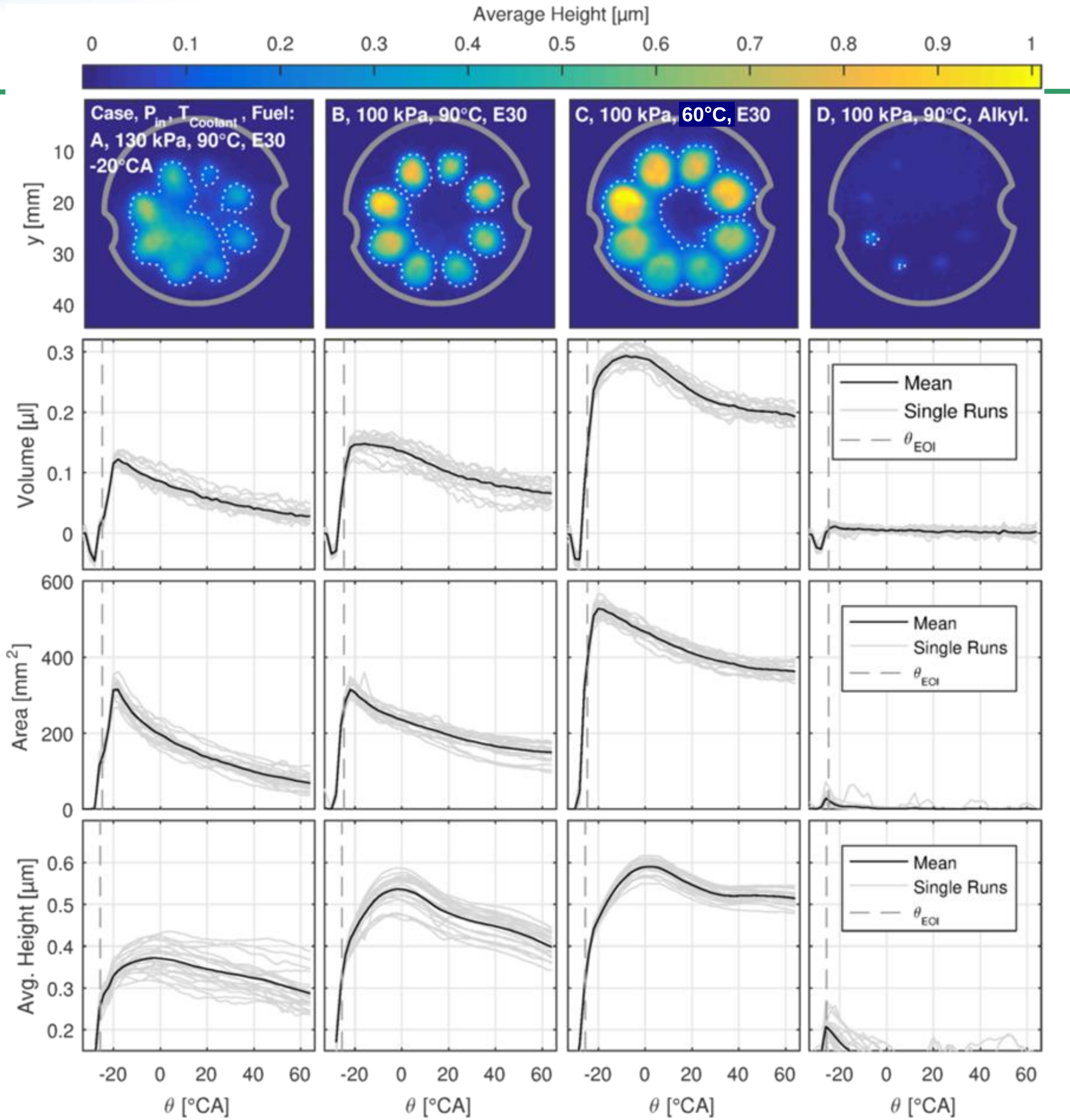


- Various mixtures of iso-octane and dodecane were used.
  - 3, 5, 10, & 20% by volume dodecane.
- Spans the useful dynamic range: 0 – 1.3 µm.
- R_a = 6.3 µm (coarser than front-illumination RIM).



Results

- Wall-wetting reduces with:
  - Higher coolant temperature.
  - More volatile fuel.
  - Higher boost pressure.
- RIM will be an important diagnostics tool for examining other combinations of fuels and operating conditions.



Summary and Conclusions

- Fuel effects on exhaust PM can be very strong for both "well-mixed" stoichiometric and stratified-charge SI operation.
- This needs to be carefully addressed when a new fuel is developed for market introduction, especially with new non-conventional feedstocks / molecules.
- PMI was developed for PFI engines to capture total PN & PM over a drive cycle.
  - Only low levels of oxygenates (ethanol) were considered.
- For current limited test ranges of a DISI engine, PMI is a reasonable predictor of relative exhaust PM level for:
  - Steady-state "well-mixed" stoichiometric operation.
  - Steady-state moderately boosted stratified operation at 2000 rpm.
- PMI is a poor predictor of relative exhaust PM level for:
  - Cooler transient "well-mixed" stoichiometric operation.
  - Steady-state naturally aspirated stratified operation at 1000 rpm.
- Elevated soot PM for fuels with ethanol, iso-butanol and 2-butanol points to the importance of vaporization and co-vaporization properties for soot formation associated with wall wetting.
- The developed RIM wall-wetting diagnostics is one tool that will be used to probe this further.

Acknowledgements

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