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Initial PM/PN Assessment for a DISI Engine Across Wide Ranges of Thermal and Fouling States using a Gasoline and a Simple Surrogate

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Abstract

The role of predictive simulation tools is becoming greater for future engine developments. One goal for CFD is to provide understandings on sources and their significances on perturbation and variations in engine combustion and emissions. For such high-fidelity modeling work, it is crucial for CFD to be able to capture basic trends and order of magnitude differences under conditions that are extremely different. The objective of this study is to provide bookend values of PM/PN from various conditions, and assess significance of fuel effect, thermal state of engine, fouling state of engine, and injection scheme. First, a gasoline (RD5-87) and a simple surrogate fuel (iso-octane) were used to investigate PM/PN emission levels from two extreme thermal state of engine: coldest possible with catalyst heating mode and hottest possible with hot steady-state operation. The result revealed that combinations of thermal state of engine and fuel had effect on PM/PN up to four order of magnitude. This provided a bookend levels of PM/PN that can be utilized for predictive model development in the future. Effect of engine fouling was also probed and provided insights to how large the effect can be on PM/PN. For reliable and repeatable measurement of PM/PN, careful procedure of keeping the cleanliness of engine is required. Lastly, additional experiments with different combinations of thermal state of engine and coolant temperature were conducted to observe the response of PM/PN. It was found that surface temperatures of engine had significantly higher impact on PM/PN than coolant temperature. Also, response of PM/PN to number of split injections differed with surface temperatures despite of the similar coolant temperature. This implies that for future studies with catalyst heating mode, it is necessary to control surface temperatures with certain procedures to mimic the real catalyst heating conditions and devise an optimal injection scheme.

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U.S. DEPARTMENT OF ENERGY

Light Duty Combustion Consortium

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Outline

1. Motivation
2. Effect of fuel and thermal state of engine
3. Effect of fouling state of engine and injector
4. Effect of number of split injections
5. Conclusions

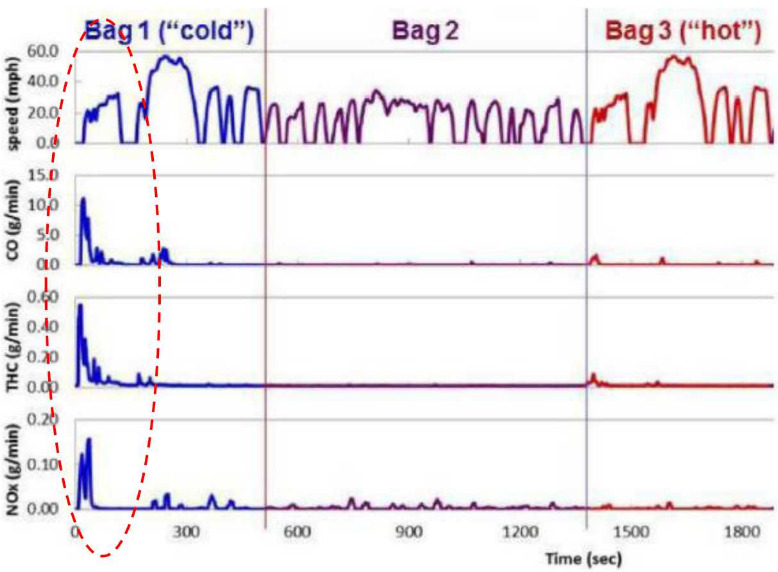
Light-Duty Combustion Consortium

- A majority of the DOE VTO Light-Duty efforts from FY19 are organized as a Light-Duty Combustion Consortium.
- The progress reported here is for the AOP task "**Spray-flow Interactions, Combustion, Soot Formation and Autoignition in an Optical DISI Engine**".
- A majority of this task falls under the "Spray & Films" Team, led by Lyle Pickett and Chris Powell.
- The current efforts support the Purpose "**Emissions Reduction**", particularly the "Cold-Start Thrust", led by Scott Curran.
- In this Purpose, a 5-year goal for the Consortium is to develop predictive CFD capabilities for SI cold-start and warm-restart operation, capable of accurately capturing COV, emissions, and EGT.
- Here, an initial book-end exercise is reported, determining sensitivity and order of magnitude of PM/PN emissions to four major boundary conditions:

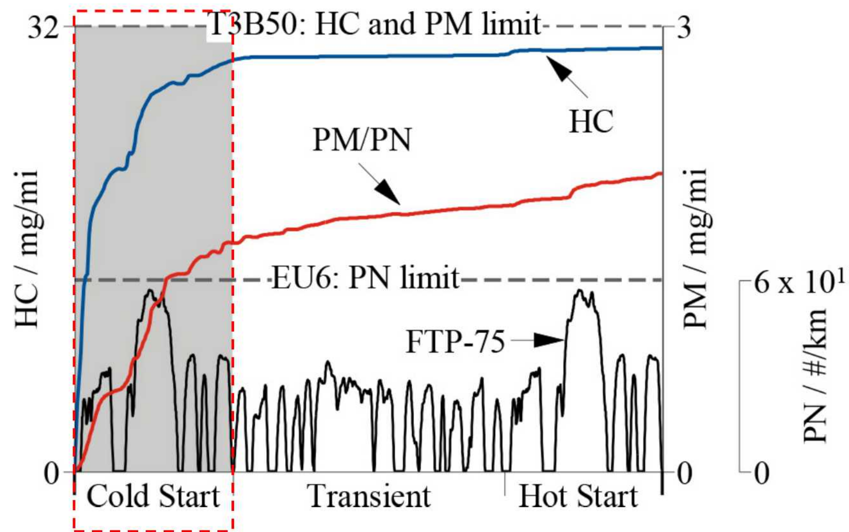
A. Thermal state	**B. Gasoline fuel representation**
C. Engine fouling state	**D. Injection schedule**

Emission Characteristics from Gasoline PV

- Tailpipe emission from gasoline PV is found to be cleaner than Diesel PV owing to three-way catalyst (TWC).
- When TWC is not active (i.e. cold start condition), above statement is no longer true.
- To minimize gaseous emissions from gasoline PV, it is very important to achieve fast light-off of TWC.
- Soot emission also increases when engine is cold.



[Pihl et al., SAE 2018-01-1264]



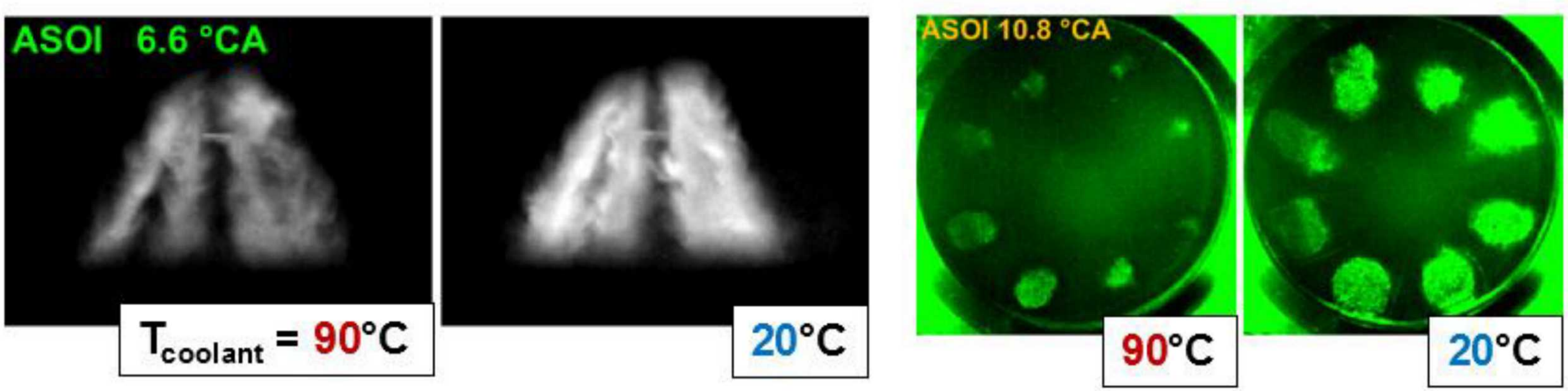
[Rodriguez and Cheng, SAE 2016-01-0827]

Challenges of Fast Light-off of Catalyst

- For expedite light-off of TWC, fast catalyst heating mode is employed in gasoline engines.
- In this operating mode, combustion phasing is retarded as much as possible to achieve higher exhaust enthalpy flux.
- However, since engine is cold, combustion stability is relatively low.
- For combustion with retarded phasing, main combustion event takes place while cylinder volume is expanding. This poses further challenge on achieving good combustion stability.
- High soot emission due to inhomogeneous mixture as well as increased wall-impingement as liquid fuel penetrates and persists longer.

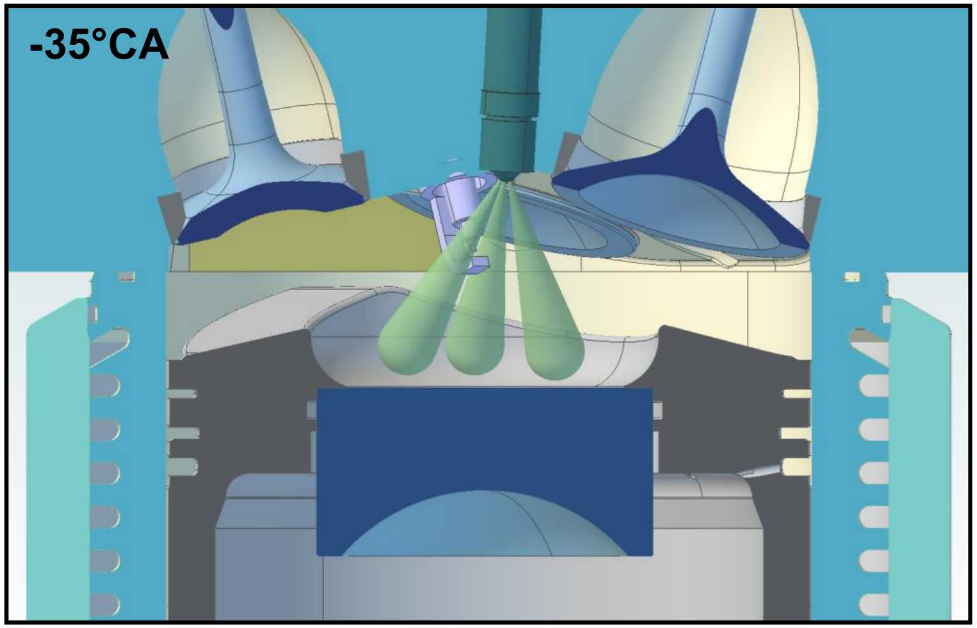
Spray and RIM imaging result from AEC meeting in Jan. 2019

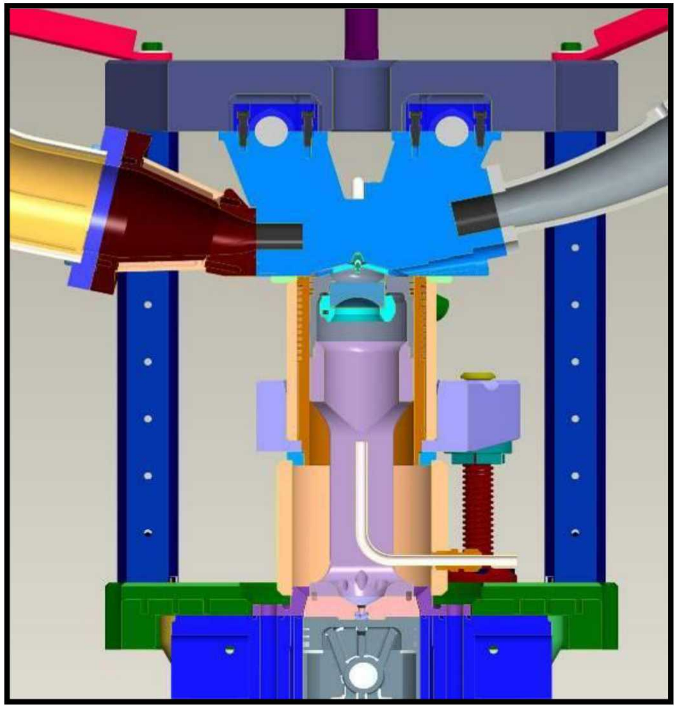
E30, SOI_a = -41°CA, Injection duration = 600 μs

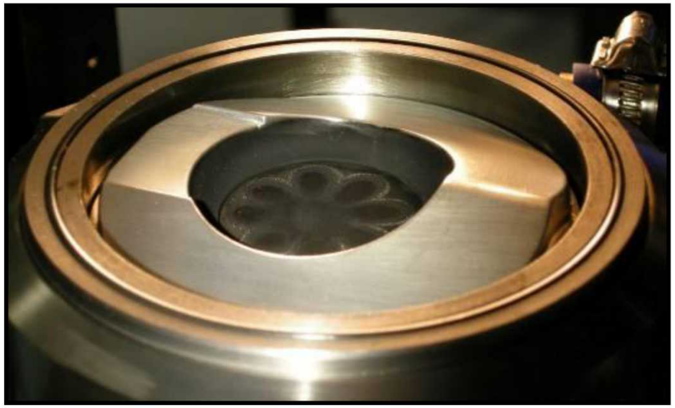


Research Engine

- Designed for spray-guided stratified-charge operation.
- 8-hole injector. 60° included angle. P_{inj} = 120 bar.
- Drop-down single-cylinder engine.
- Automotive size. 0.55 liter swept volume.
- Identical geometry for All-metal and Optical.
- One valve operation for swirl.
- CR = 12.

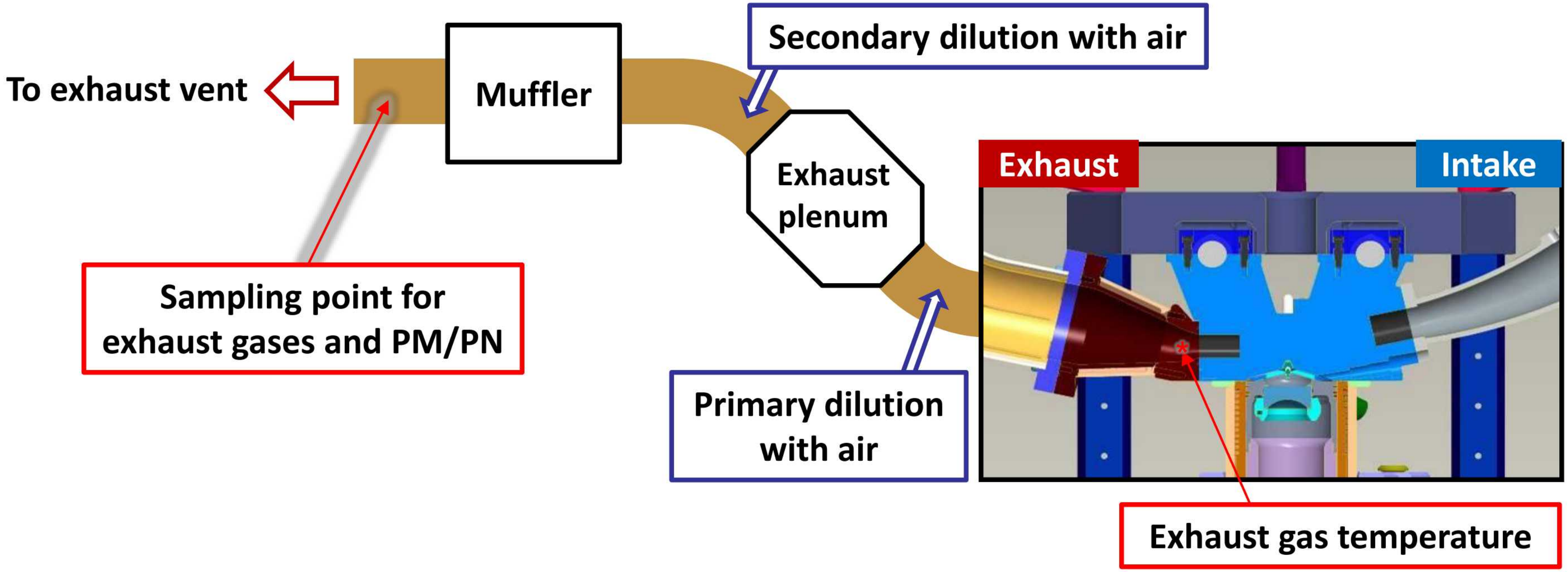






Emission and Temperature Measurements

- Instruments used for exhaust gas compositions and PM/PN measurement
  - Horiba MEXA-584L: UHC, CO, CO_2, and NO
  - CAI instruments: NO/NO_2, CO/CO_2
  - AVL Micro-Soot Sensor: PM / AVL Advanced Particulate Counter: PN
- Exhaust gas was diluted using air to lower dew point and avoid condensation of water vapor in exhaust system and instruments.
- Thermocouple (K-type, ϕ 3.2 mm) for exhaust gas temperature measurement was located ~10 mm downstream of the exhaust port exit.



ACEC Guideline for Catalyst Heating Mode

- Following criteria from AECE guideline were considered for selection of engine operating condition.
- The guideline is for steady-state operation.
- In this study, transient operation was used.

Approach:	LDV/LDT TWC	Unit
Mode:	catalyst heating	
Engine speed	1300	rpm
NMEP	200	kPa
Coolant temperature (coolant out of engine)	20	°C
Intake air temperature (ambient)	20	°C
Lambda	1.00	
Exhaust temperature	> 450	°C
Heat Flux	3~10	kW/liter of disp.
Combustion stability (SDIMEP)	<0.45	bar
COV_IMEP	<20	percent

Selection of Intake Air Flowrate

- Needed a intake air flowrate which allows
  - to achieve sufficient exhaust enthalpy flux for catalyst heating mode
  - hot steady-state operation of engine without severe knock at reasonable combustion phasing

⇨ **Tested air flowrate of 3.06 g/s which resulted in ~52 kPa intake pressure at 1300 rpm.**

- Computation of exhaust enthalpy flux was done following the ACEC guideline:
  - Exhaust heat flux in kW/liter = mass_flow*Cp*delta T/disp

  where:

  mass_flow = fuel flow + air flow

  Cp = f(T) but we will assume fixed @ 1000K = 1.25 kJ/kg/K, (source: Figure 4-17, Heywood)

  delta_T = measured_exhaust_T – 20°C reference

  disp = engine displacement in liters

- Following the equations above, exhaust enthalpy flux is estimated to be ~4.3 kW/liter for catalyst heating mode while satisfying criteria of average $IMEP_n$, CoV of $IMEP_n$, and coolant temperature closely.
- Even for hot steady-state operation, AKI-87 gasoline used in this study was knock-free at CA50 = 15°CA. This fuel was knock-limited at higher intake pressure.

⇨ **Thus, the intake air flowrate of 3.06 g/s was considered a good compromise.**

Experimental Conditions

- RD5-87 : representative of market E10 gasoline of AKI 87
- Iso-octane : “simplest” surrogate fuel
- Two extreme thermal state: catalyst heating (coldest), hot-steady (hottest)
- CA50 = 15°CA to avoid knock at hot steady-state operation. Used this phasing for all operations except for catalyst heating mode.

Parameter	Value	Unit
Fuel	RD5-87, Iso-octane	
Engine speed	1300	rpm
Coolant temperature (**entering engine**)	20 (Catalyst warm-up), 75 (steady)	°C
Intake air temperature	20 (Catalyst warm-up), 30 (steady)	°C
Intake air flow rate	3.06	g/s
Intake pressure**	~ 52	kPa
Lambda	1.00	
Injection pressure	120	bar
Injection strategy	Double injection	
Split ratio (Based on electric command)	50/50	
Injection duration/pulse	823 (RD5-87), 783 (Iso-octane)	μs
Injection timing	-310	°CA
CA50 for steady-state operation	15	°CA

**varied with thermal state of engine/intake temperature

All CA are referenced to aTDC firing.

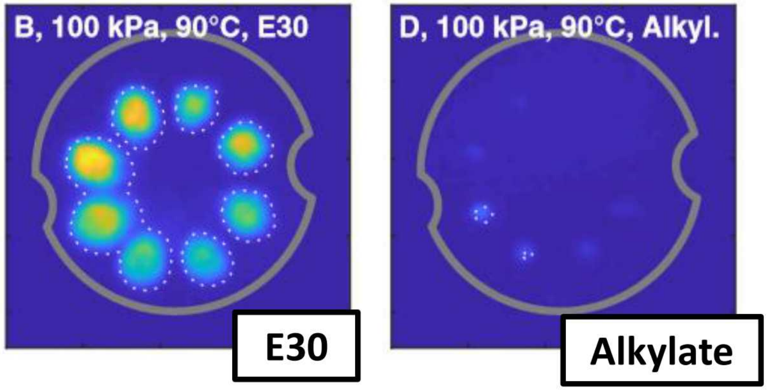
Key Fuel Properties

- Iso-octane has lower boiling point than RD5-87.
- Large difference of PMI between RD5-87 and iso-octane.

	E10 RD5-87	Iso-octane	E30	Alkylate	High Olefin
RON	92.1	100.0	97.9	98.0	98.3
MON	84.8	100.0	87.1	96.7	87.9
Octane Sensitivity	7.3	0.0	10.8	1.3	10.4
Oxygenates [vol.%]	10.6	0.0	30.6	0.0	0.0
Aromatics [vol.%]	20.9	0.0	13.8	0.7	13.4
Alkanes [vol.%]	49.4	100.0	40.5	98.1	56.4
Cycloalkanes [vol.%]	11.3	0.0	7.0	0.0	2.9
Olefins [vol.%]	4.9	0.0	5.6	0.1	26.5
T10 [°C]	57	-	61	93	77
T50 [°C]	98	-	74	100	104
T90 [°C]	156	-	155	106	136
Boiling point [°C]	-	99	-	-	-
Net Heat of Combustion [MJ/kg]	41.9	44.3	38.2	44.5	44.1
Heat of Vaporization [kJ/kg]	412	271	532	308	333
AFR Stoichiometric	14.1	15.1	12.9	15.1	14.8
HoV [kJ/kg stoichiometric charge]	27.3	16.8	38.4	19.1	21.1
Particulate Matter Index	1.68	0.19	1.28	0.22	1.00

Fuel Effects on Wall-Wetting

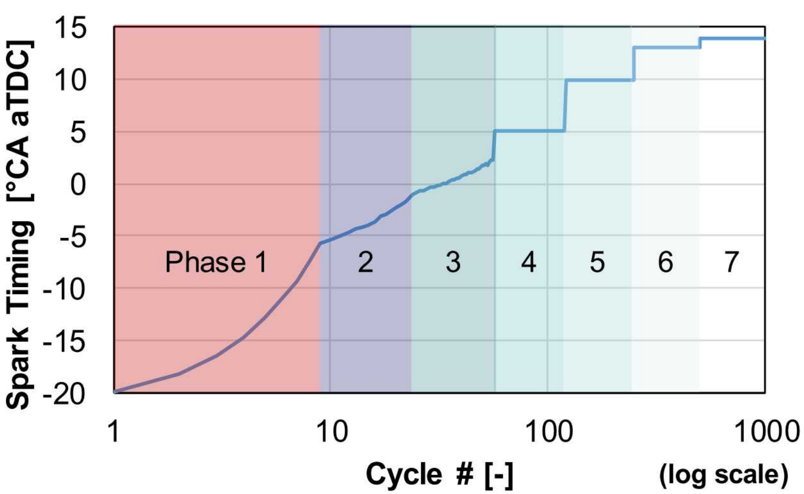
- Volatility of fuel has significant effect on wall-wetting.
  - Late injection, $T_{coolant}$ = 90°C

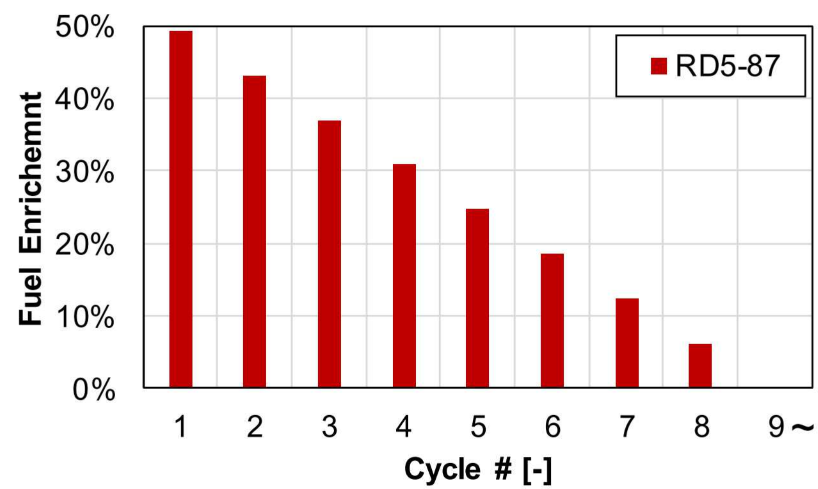


Details about Catalyst Heating Mode

- To mimic catalyst heating mode of a cold engine, engine was soaked at 20°C and operated with transient manner.
- To maintain average $IMEP_n$ ~ 200 kPa and avoid misfiring cycles during transient operation at cold start condition, fuel enrichment and spark timings were varied based on pre-programmed script.
- Fuel enrichment was applied only for the first 8 cycles.

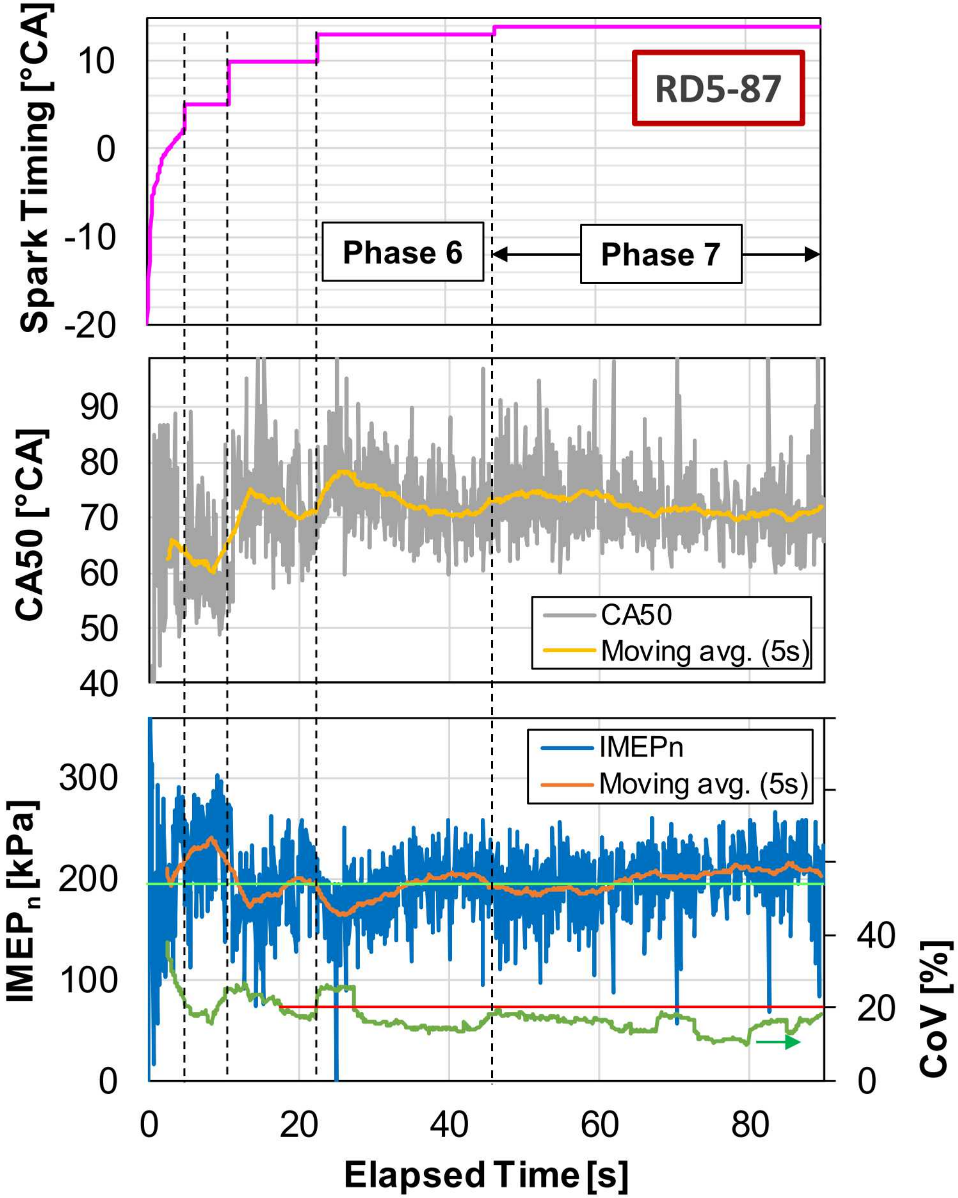
Phase	Spark timing	Δ(spark timing)/cycle	# of cycles per phase	Fuel enrichment
1	-20	1.8	8	**Yes**
2	-5.6	0.3	16	**No**
3	-0.8	0.1	32	
4	5	0	64	
5	10		128	
6	13		256	
7	14		500~	



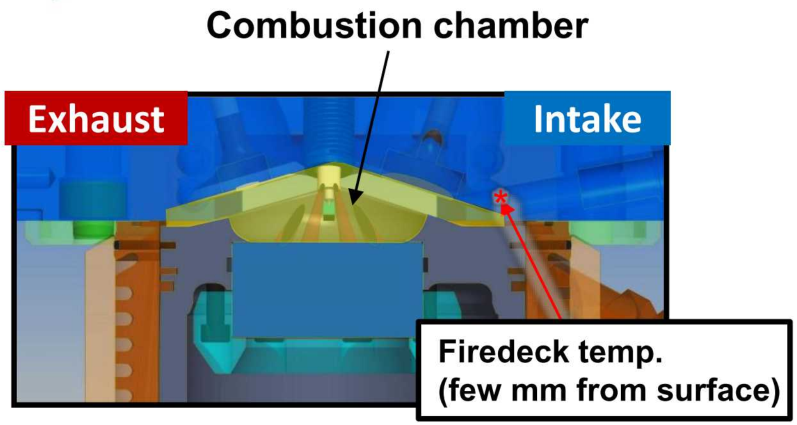


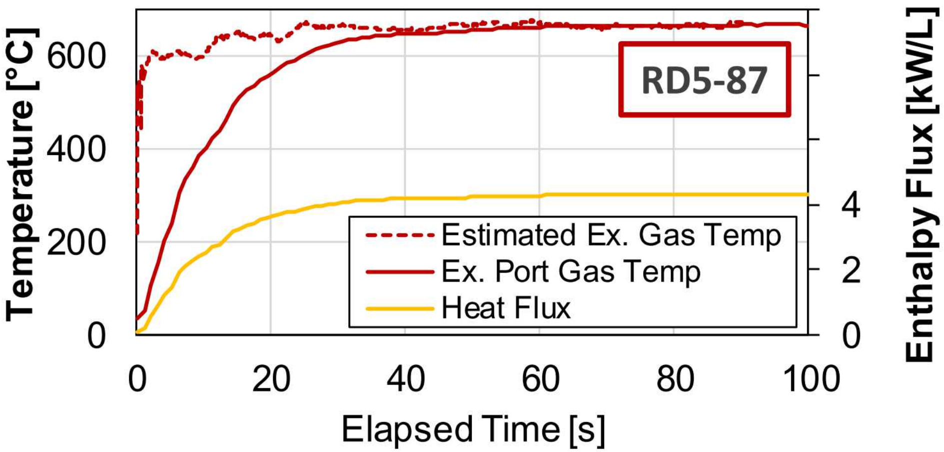
Details about Catalyst Heating Mode

- Fuel: RD5-87
- Within each phase of spark timing schedule, CA50 keeps advancing due to change in thermal state of the engine.
- Small change in CA50 leads to relatively large change in $IMEP_n$.
    - Adds difficulty to designing the transient spark timing schedule.
- Using the prescribed spark timing schedule, $IMEP_n$ can be maintained close to the target value of 200 kPa.
- Spark timing schedule can be improved further.

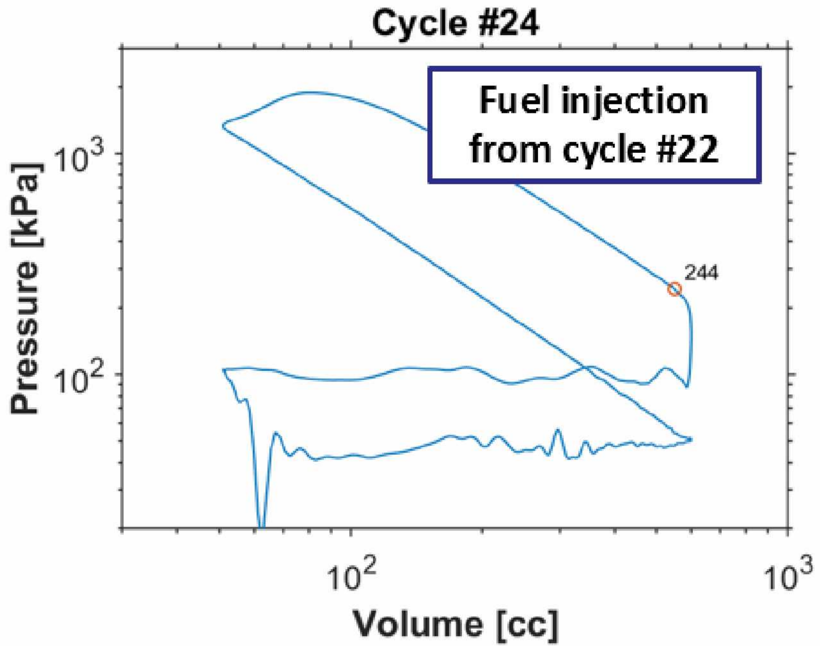


Details about Catalyst Heating Mode





- Slow response time of exhaust gas temperature measurement is attributed to
  - finite time needed for convective heat transfer from exhaust gas to thermocouple
  - heat loss from exhaust gas to cold exhaust port



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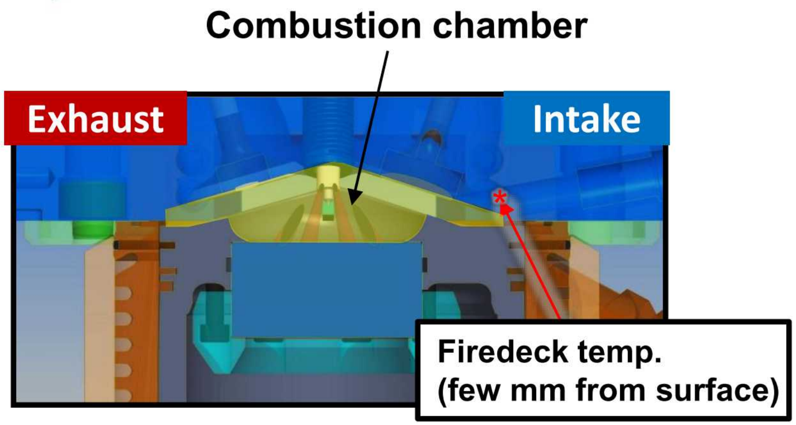
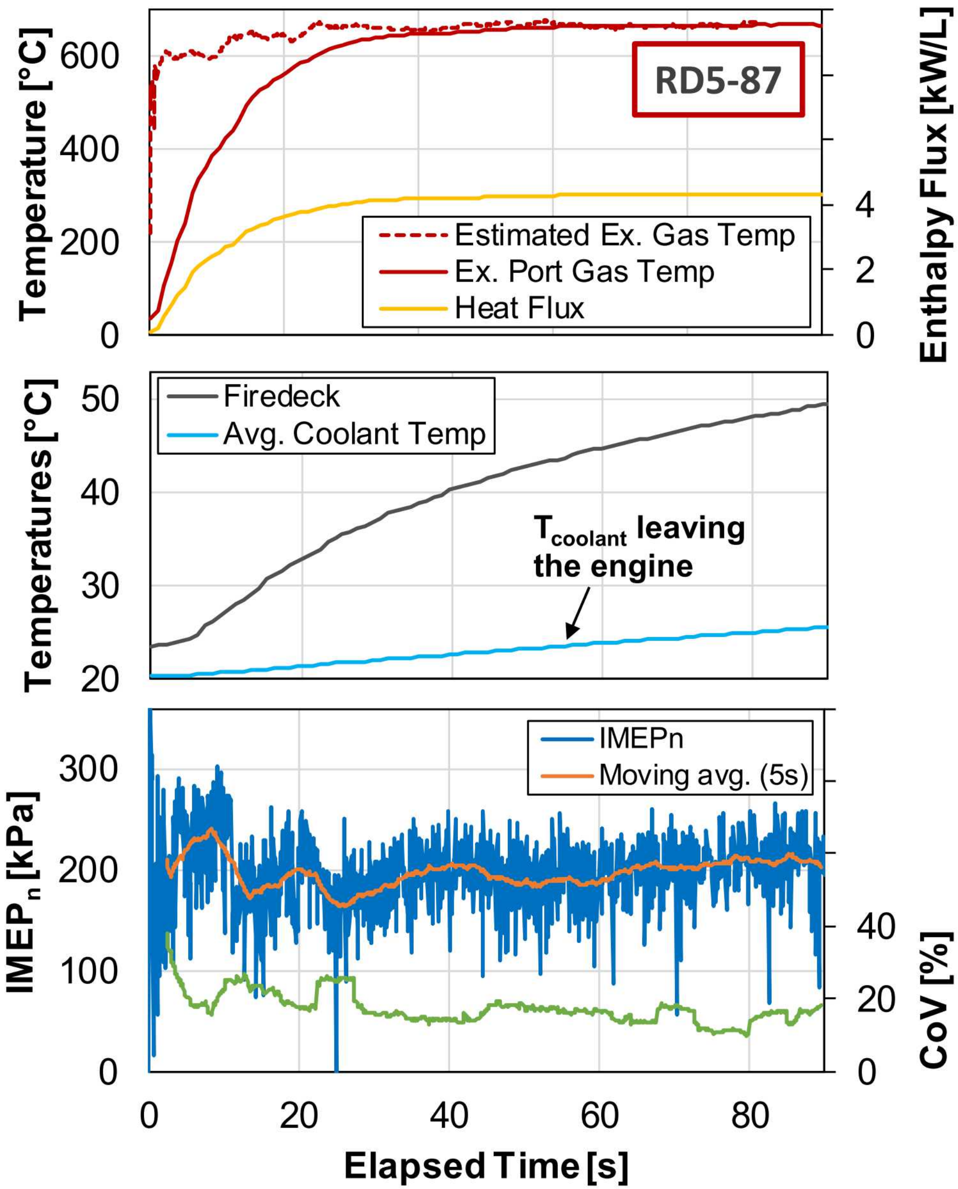


- Slow response time of exhaust gas temperature measurement is attributed to
  - finite time needed for convective heat transfer from exhaust gas to thermocouple
  - heat loss from exhaust gas to cold exhaust port
- Firedeck temperature deviates from initial temperature as more cycles with combustion progresses.
- The average coolant temperature also keeps increasing due to insufficient cooling of coolant.

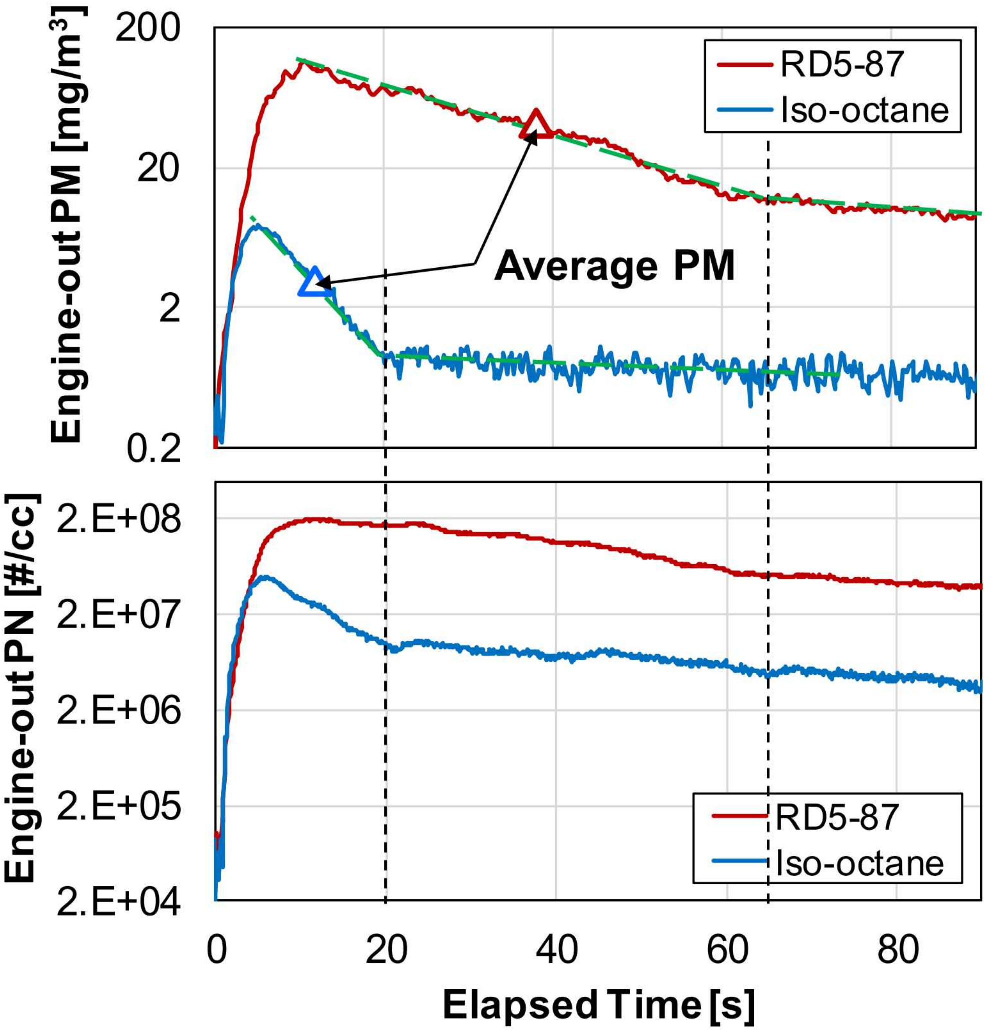


PM/PN Emission from Catalyst Heating Mode

Catalyst heating mode
$T_{coolant}$ ~ 25°C, $T_{firedeck}$ ~50°C
CA50 ≈ 70°CA, $IMEP_n$ ≈ 200 kPa

- Close to one order of magnitude lower PM/PN for iso-octane than RD5-87.
- Transient emission overshoots initially and keeps falling at certain rate.
- At a certain time, the rate of reduction in PM and PN changes.
  - Possible indication of change in soot formation mechanism.
  - Surface temperature could be high enough to reduce fuel film significantly.
- Transient emissions from iso-octane reached a semi-steady-state values quicker.
  - Could be due to lower boiling point of iso-octane than RD5-87.

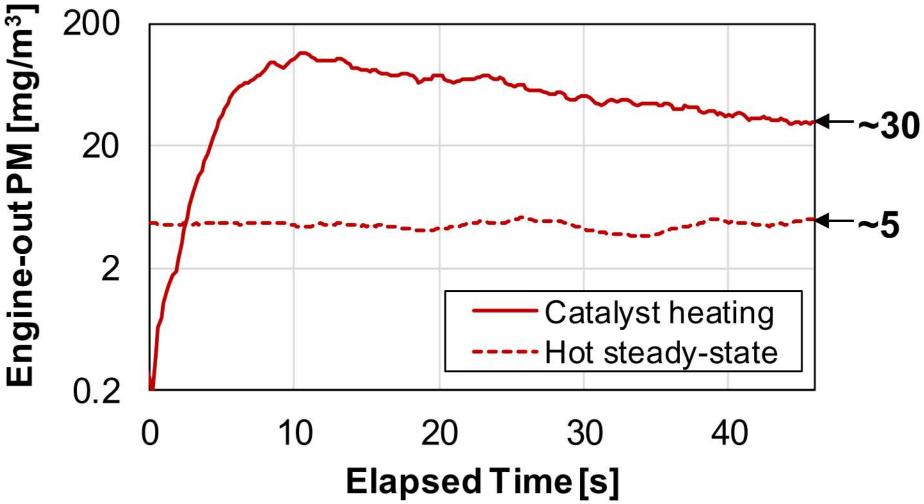
	E10 RD5-87	Iso-octane
T90 [°C]	156	-
Boiling point [°C]	-	99



PM/PN Emission from Steady State Operation

Hot steady-state operation
$T_{coolant}$ ≈ 75°C, $T_{firedeck}$ ≈ 110°C
CA50 ≈ 15°CA, $IMEP_n$ ≈ 550 kPa

- Close to order of magnitude difference in PM with change in engine thermal state for RD5-87.



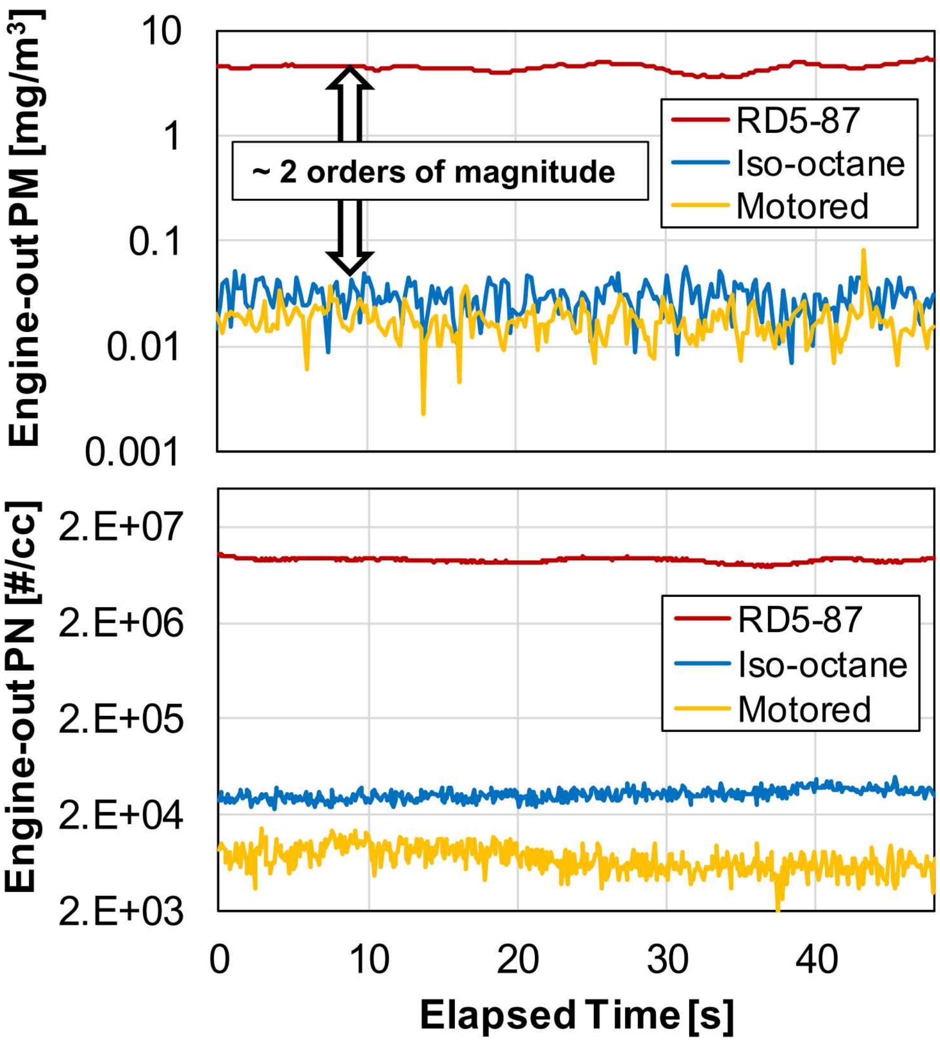
PM/PN Emission from Steady State Operation

Hot steady-state operation
$T_{coolant}$ ≈ 75°C, $T_{firedeck}$ ≈ 110°C
CA50 ≈ 15°CA, $IMEP_n$ ≈ 550 kPa

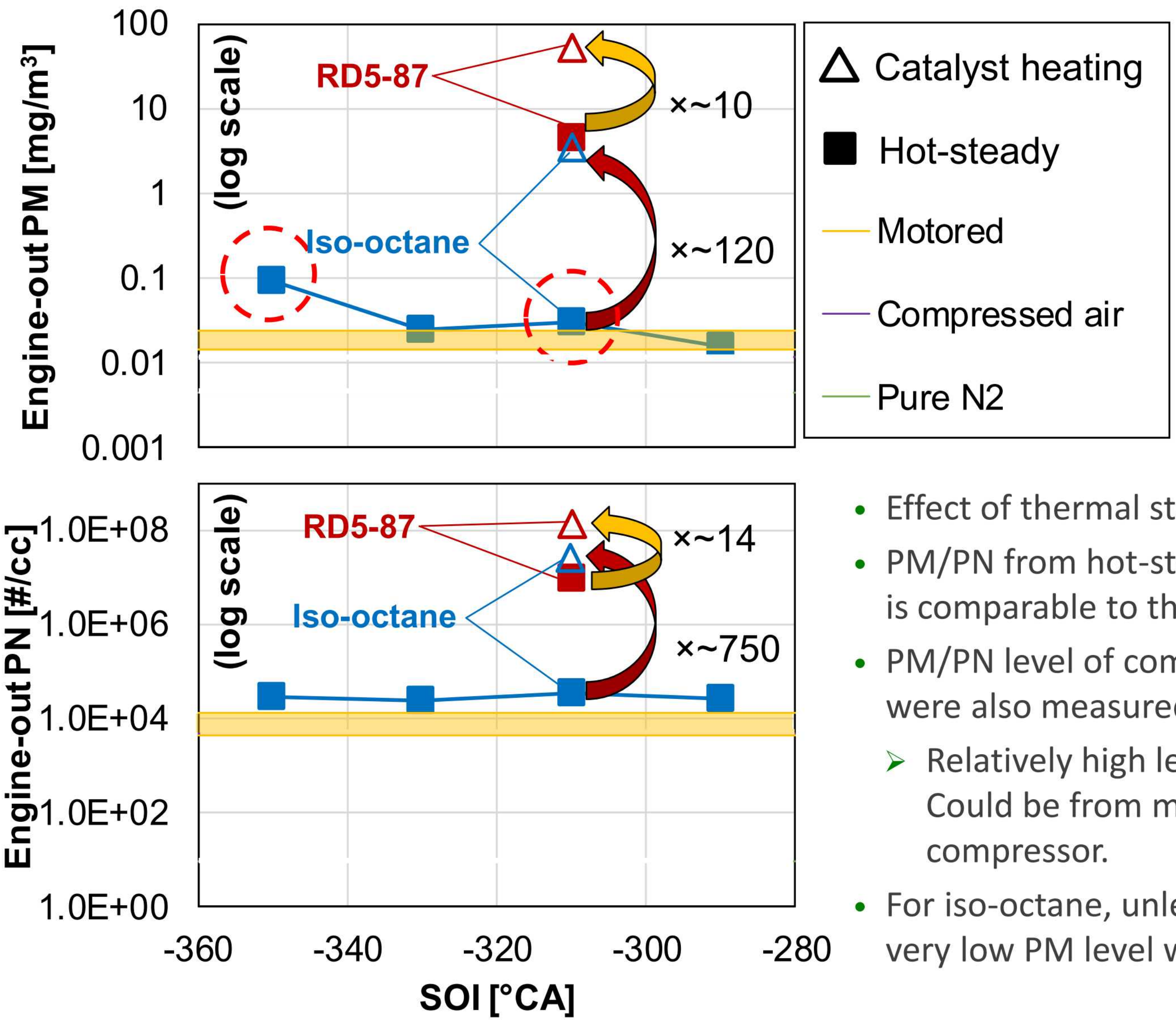
- Close to order of magnitude difference in PM with change in engine thermal state for RD5-87.
- Differences between PM/PN levels of two fuels are even greater.
  - PMI: 1.68 vs 0.19
- PM and PN levels show some degree of variation even at the steady-state operation.

	PM [mg/m³]		PN [#/cc]	
Fuel	RD5-87	Iso-octane	RD5-87	Iso-octane
Avg	4.53	0.03	7.68E+06	3.26E+04
CoV	8.0%	33.2%	5.0%	13.3%

- CoV of PM and PN for iso-octane was much higher due to overall low values.
  - Average PM level is similar to that from motored engine.

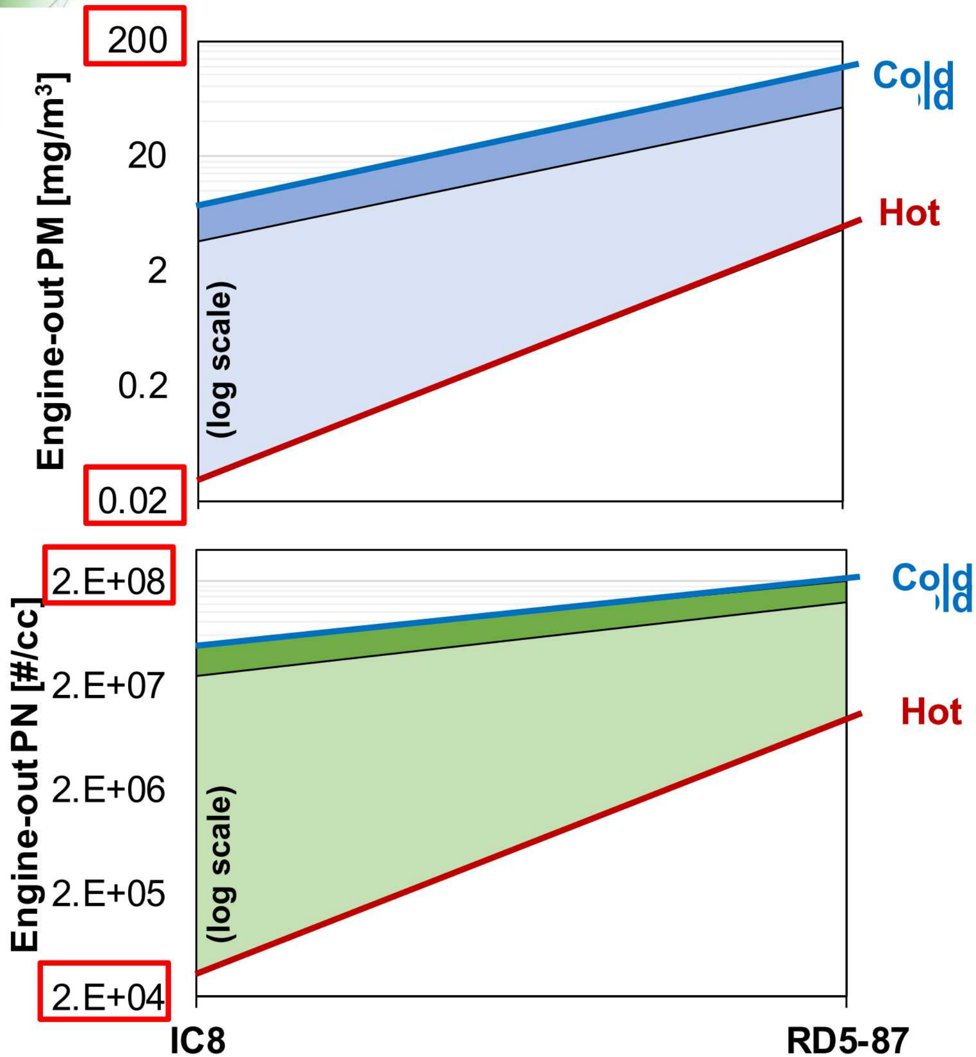


Average PM/PN Emission

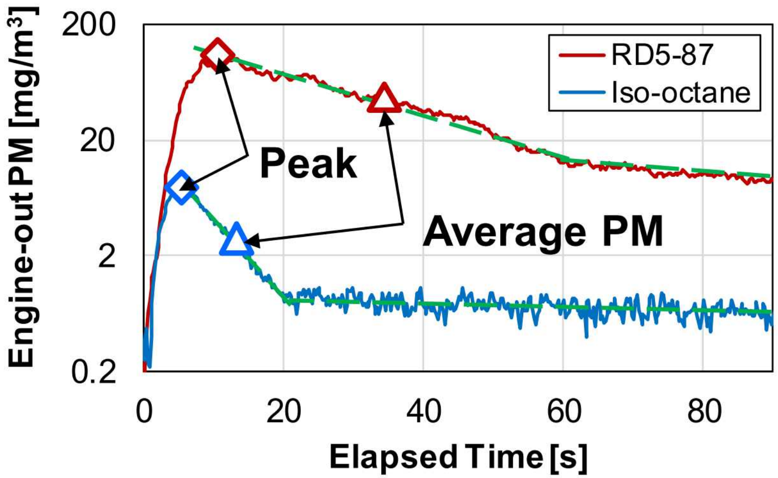


- Effect of thermal state on PM/PN varies with fuel.
- PM/PN from hot-steady operation using iso-octane is comparable to that from motored condition.
- PM/PN level of compressed air and pure nitrogen were also measured.
  - Relatively high level of PN for compressed air. Could be from moisture and/or lubricant from compressor.
- For iso-octane, unless SOI is extremely advanced, very low PM level was maintained.

Average PM/PN Emission



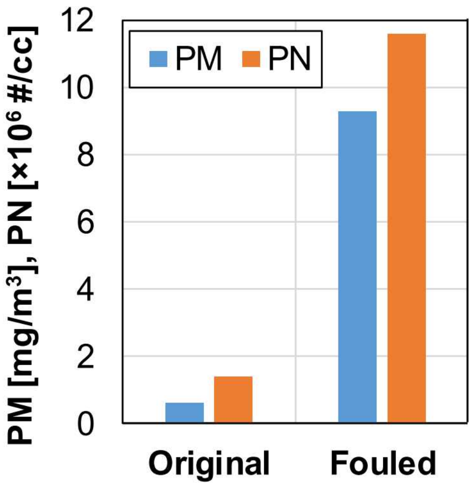
PMI: 0.19 **1.68**



- Most extreme difference in PM/PN from RD5-87 (full-boiling point gasoline) and iso-octane (simplest surrogate fuel) can be as large as **4 orders of magnitude**.
- CFD needs to be able to capture strong effect of thermal states and fuels on PM/PN.

Effect of Fouling of Combustion Chamber Surface

- When testing repeatability of PM/PN measurement, significant change in emission level was found.
  - Original state: several days of lean mixed-mode operation using clean fuels (i.e. Alkylate, PRF, and other surrogate fuels)
  - Signs of fouling detected after several hours of operation with lower thermal state of engine.



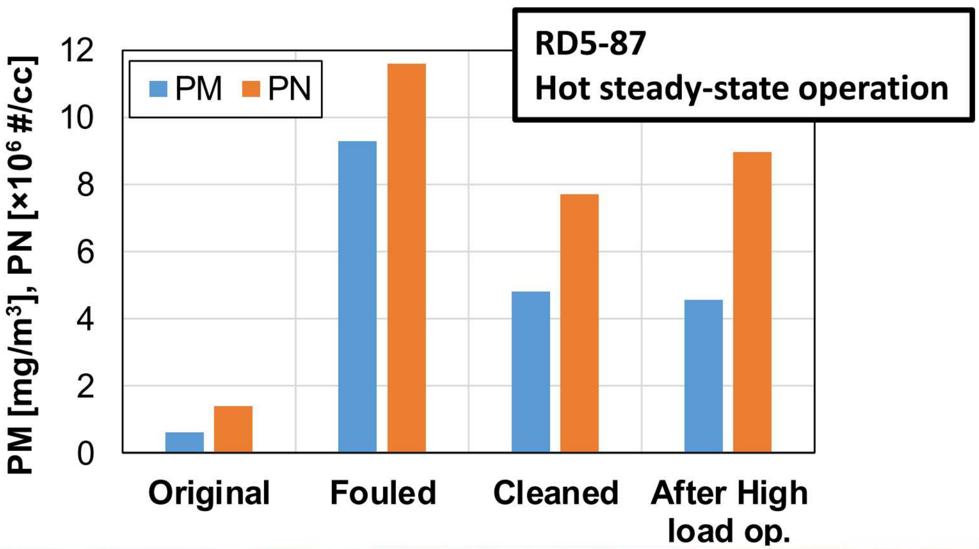
RD5-87
Hot steady-state operation

Firedeck (before cleaning)

Piston (before cleaning)

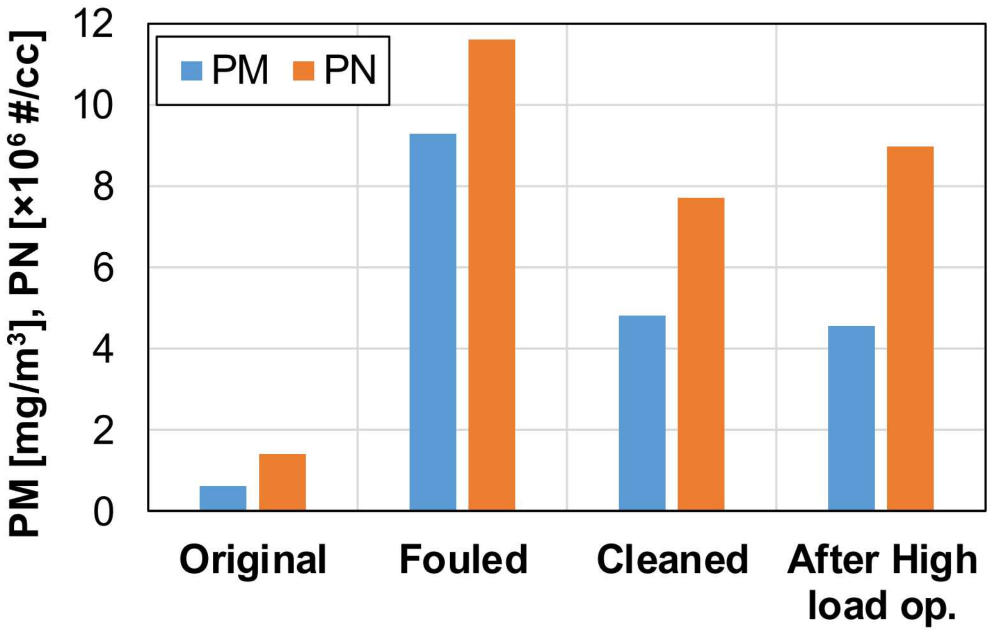
Effect of Fouling of Combustion Chamber Surface

- When testing repeatability of PM/PN measurement, significant change in emission level was found.
  - Original state: several days of lean mixed-mode operation using clean fuels (i.e. Alkylate, PRF, and other surrogate fuels)
  - Signs of fouling detected after several hours of operation with lower thermal state of engine.
- Removing deposits from the piston and side window surfaces helped to reduce PM/PN level by some degree.
  - Injector tip was not cleaned.
  - Effect of injector tip fouling will be discussed later.
- High load operation to increase surface temperature to burn off deposits did not further reduce PM/PN.



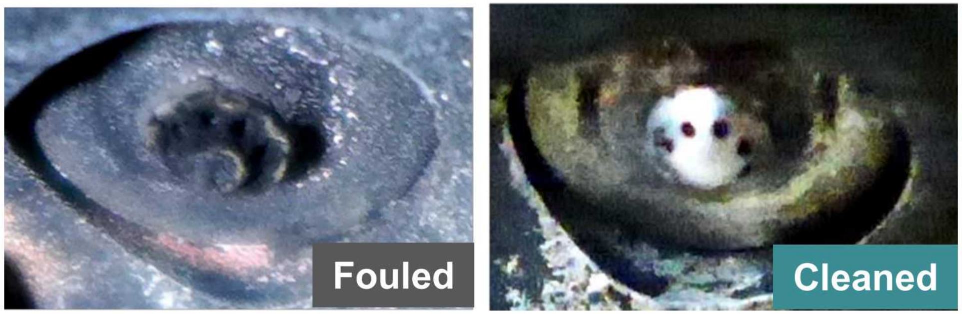
Effect of Fouling of Combustion Chamber Surface

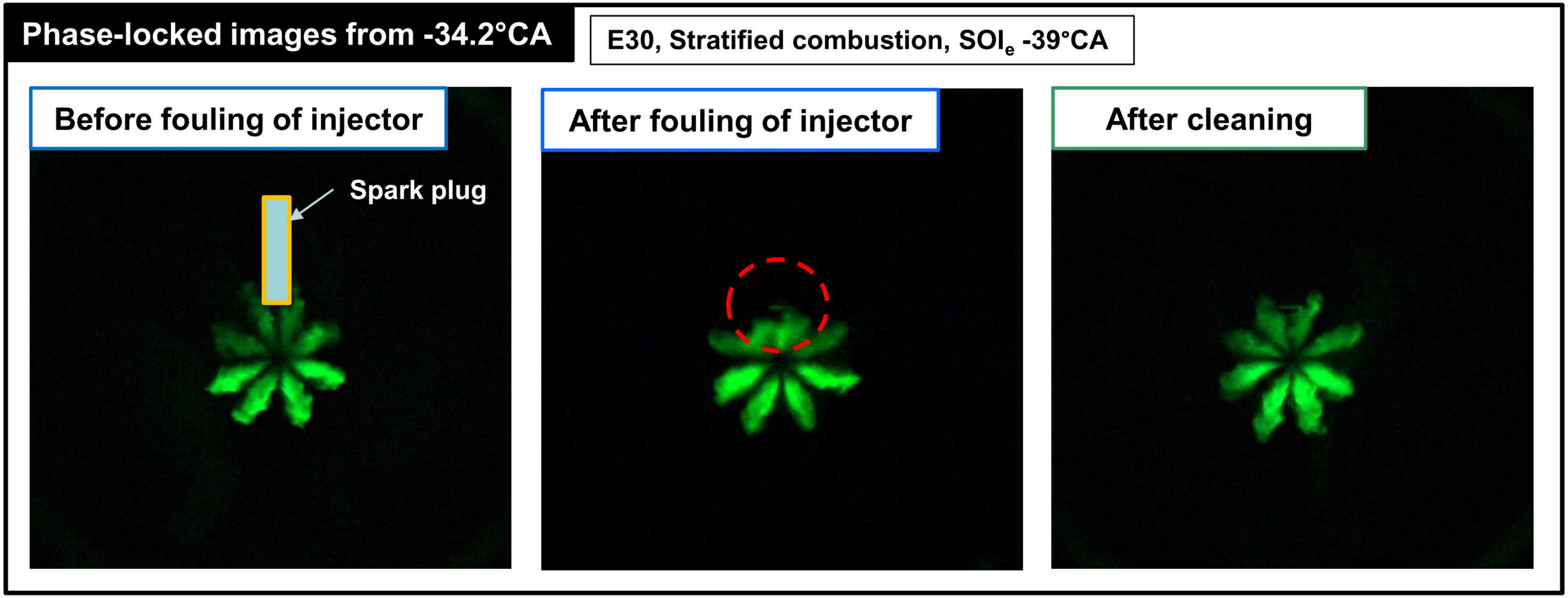
- Implication to experimentalist:
  - Careful procedure of experiment needed for repeatable and reliable PM/PN measurement.
- Implication to modelers:
  - Needs capability to incorporate the effect of fouling of surfaces for better predictability of PM/PN from CFD.



Effect of Injector Fouling on Spray Characteristics

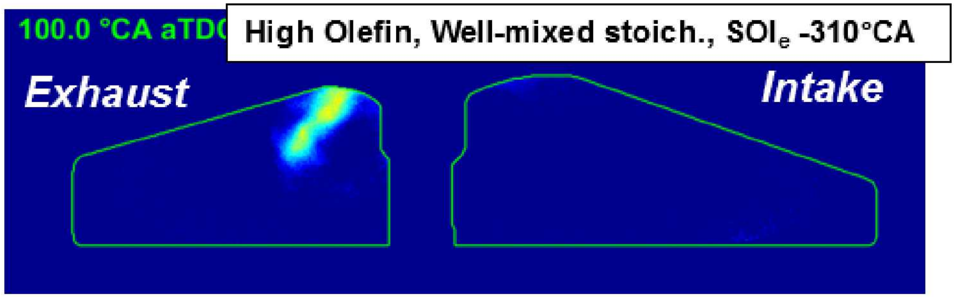
- High-speed images of spray from late injection for stratified combustion was recorded.
- Spray from fouled injector showed that two plumes straddling spark plug are behaving differently than others.
- Cleaning the injector tip helped to bring back the spray characteristics close to original one.

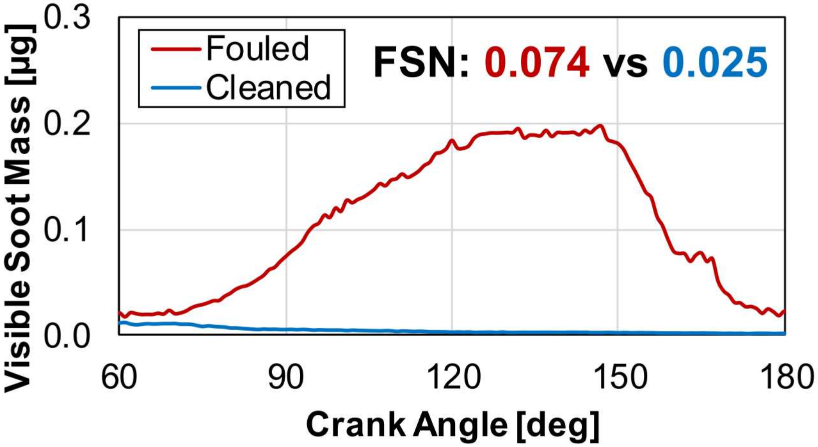


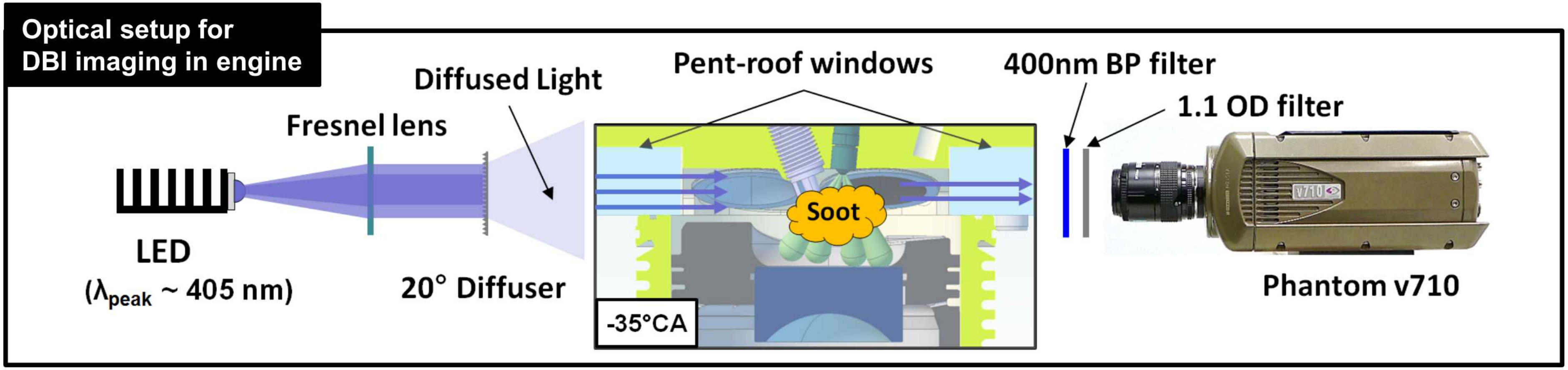


Effect of Injector Fouling on Soot Emission

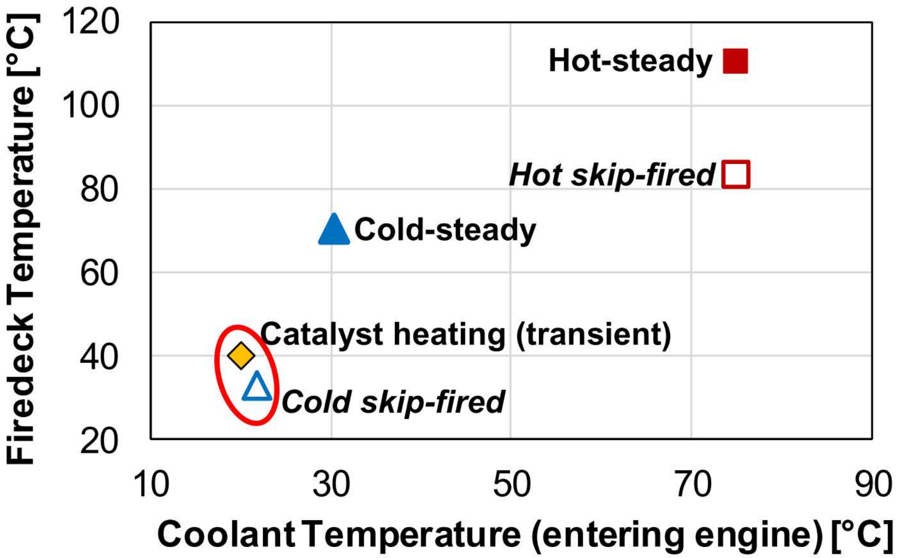
- Using diffused back-illumination technique, in-cylinder soot formation was diagnosed.
- After combustion, a puff of soot from injector was observed. Also confirmed with natural luminosity imaging.
- Such phenomenon disappeared after cleaning injector tip.

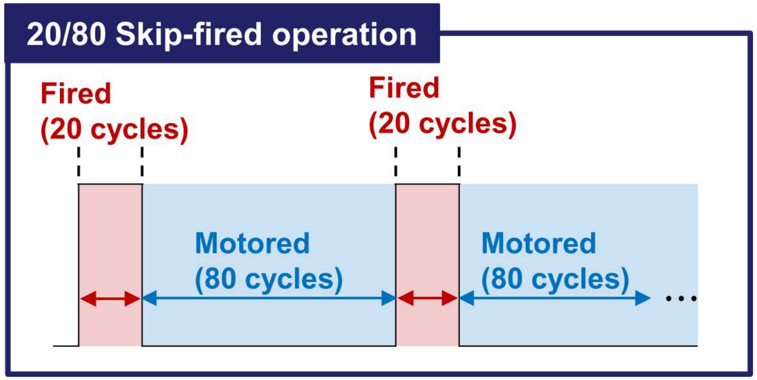






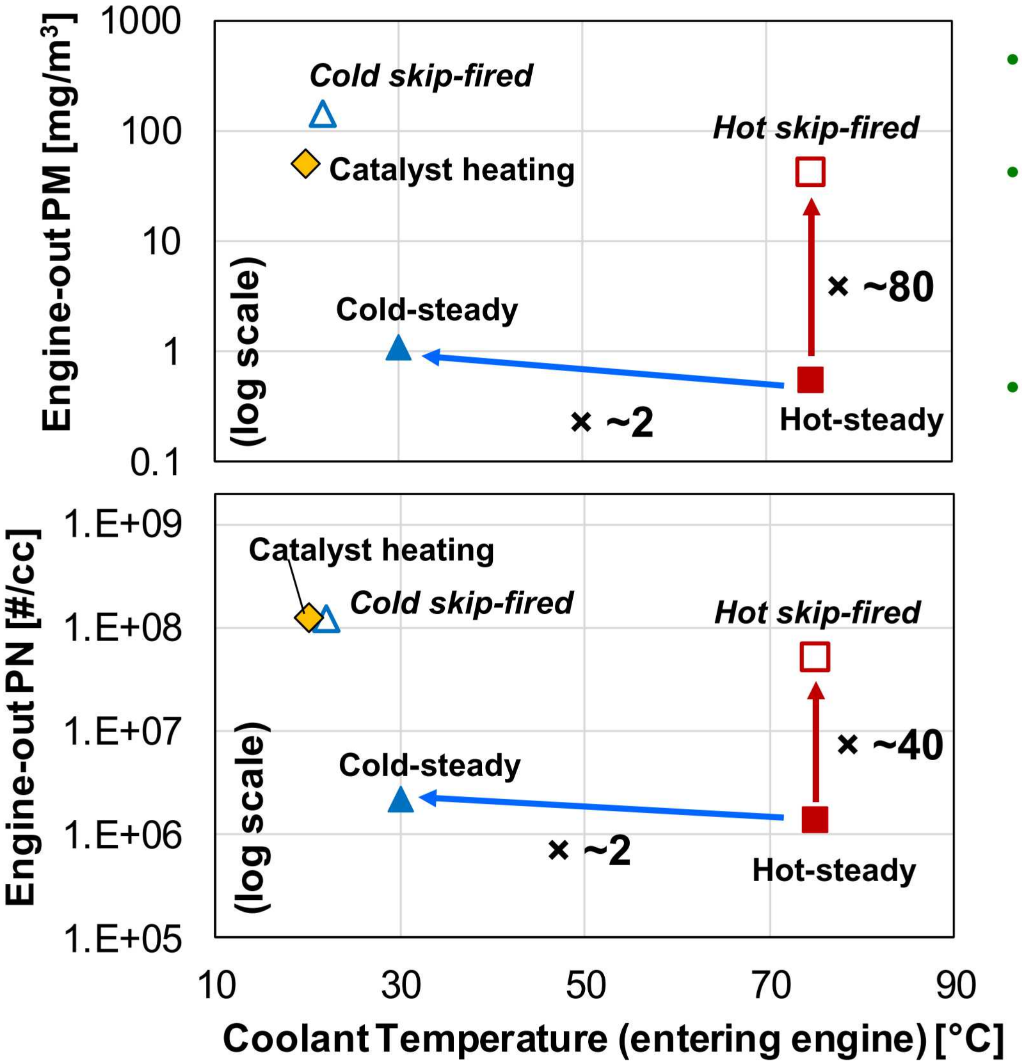
Additional Experimental Conditions





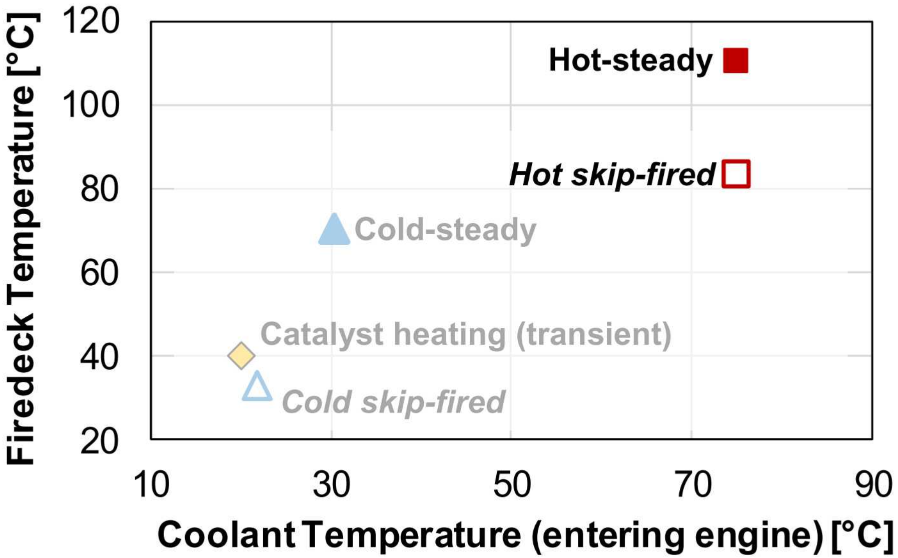
- Cold steady-state operation with ~30°C coolant temperature entering the engine.
- 20/80 skip-fired operation
  - Duty ratio of fired cycle is reduced to 20% from 100 % to maintain the boundary temperatures lower.
  - Helps to probe the effect of boundary temperatures on soot emission.
  - Cold skip-fired operation achieved similar thermal state of engine to that of transient operation of catalyst heating mode.
  - Hot-skip fired represents warm-restart conditions, commonly encountered by engines in today's electrified powertrains.
    1. Engines with stop-start technology.
    2. Hybrid powertrains.

Effect of Thermal State of Engine on PM/PN

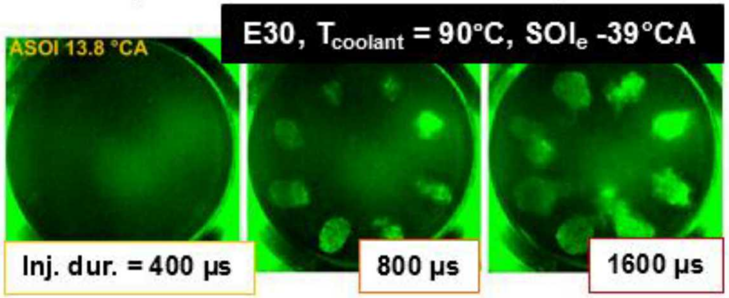


- Data points in figures were acquired prior to detection of fouling of engine.
- Use of lower coolant temperature at steady-state operation had weaker impact on PM/PN than reducing surface temperatures with 20/80 skip-firing operation.
- With cold steady-state operation following the ACEC guideline, PM/PN from catalyst heating mode cannot be replicated due to different surface temperatures of engine components.

Additional Experimental Conditions

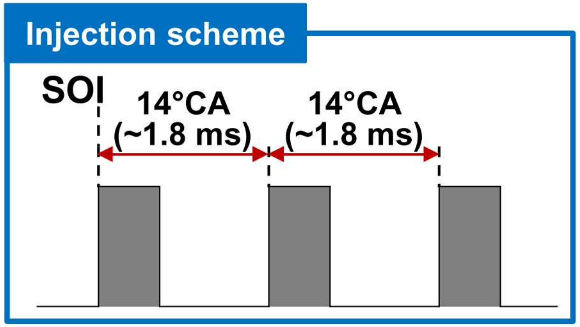


- Effect of # of split injection observed at two different heat loading conditions.
- Holding the average fuel flowrate near constant, number of split injections was increased up to 4.
  - ➢ Having larger number of split injections helps reduce injection duration for each pulse.



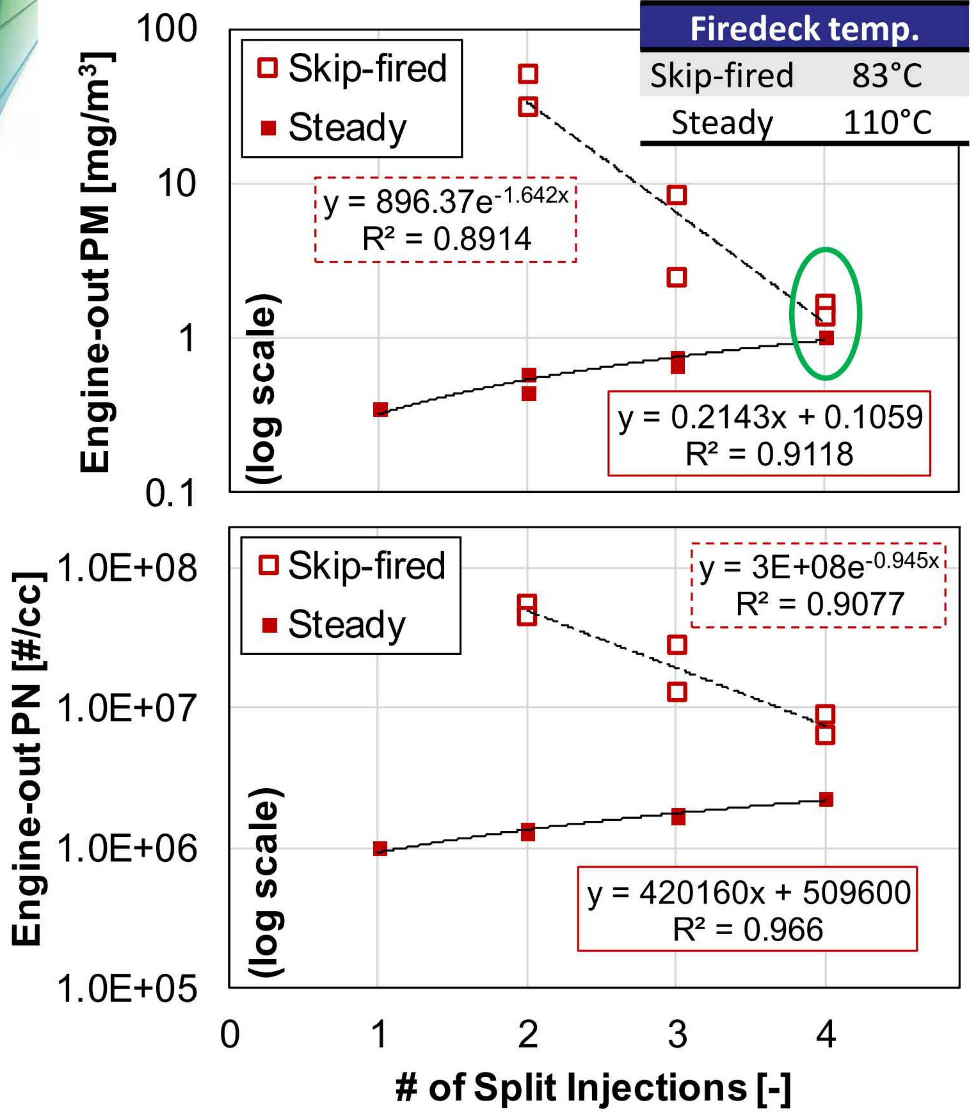
  - ➢ SOI for steady-state operations were selected which minimize PM/PN and CoV of IMEP.

	Steady	20/80 Skip-fired
Injection timings [°CA] (# of injections)	**-310 (2)** -295 (1) -330 (3,4)	**-310 (2)** -290 (2,3,4) -270 (3,4)



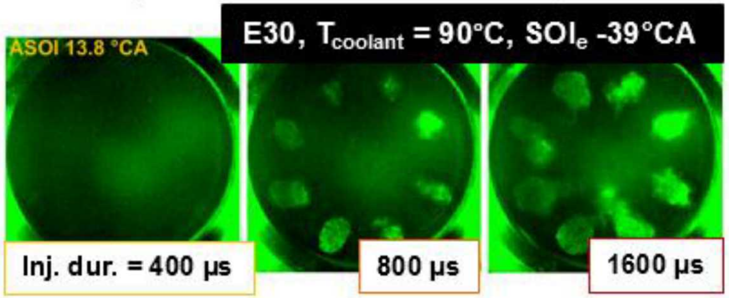
Effect of # of Split Injection on PM/PN

Coolant temperature = 75°C, RD5-87



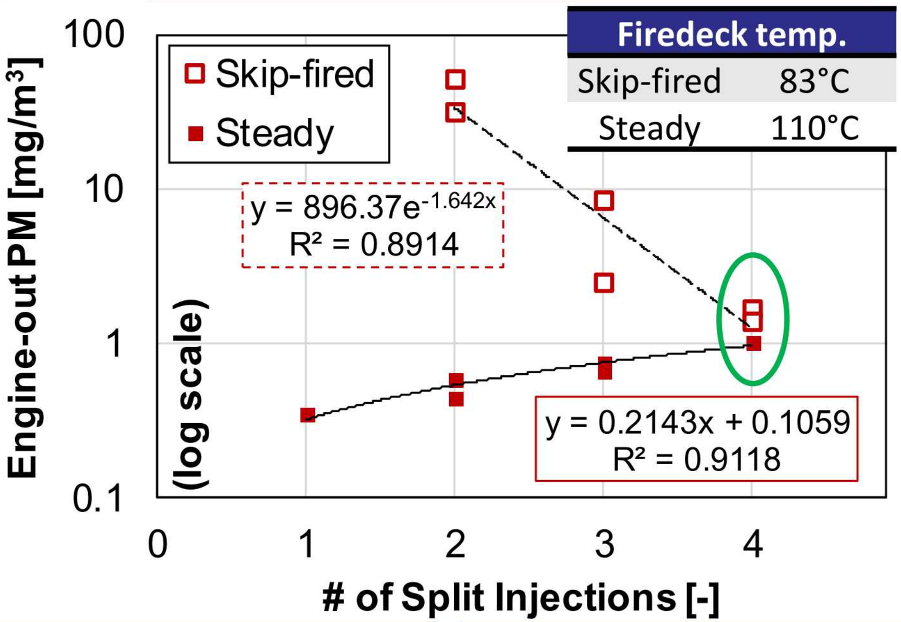
Firedeck temp.	
Skip-fired	83°C
Steady	110°C

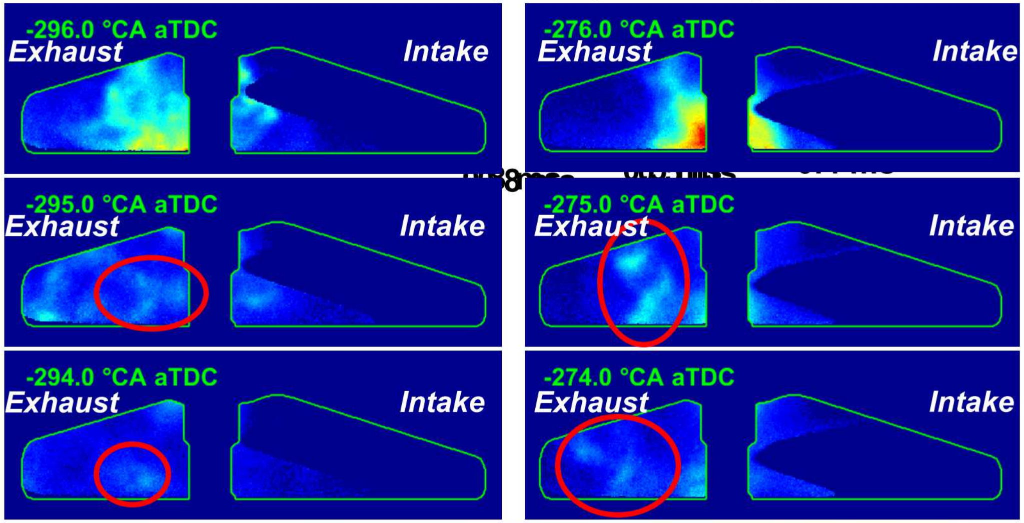
- Response of PM/PN levels to # of split injections were different depending on operating mode.
  - Indicative of different soot formation mechanism for two operating modes.
- Major source of soot emission for skip-fired operation attributable to wall-wetting.



Effect of # of Split Injection on PM/PN

Coolant temperature = 75°C, RD5-87





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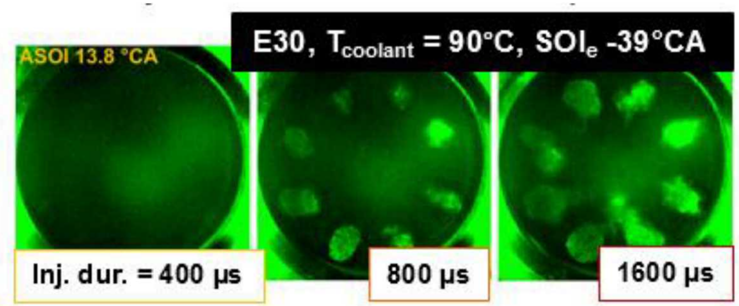
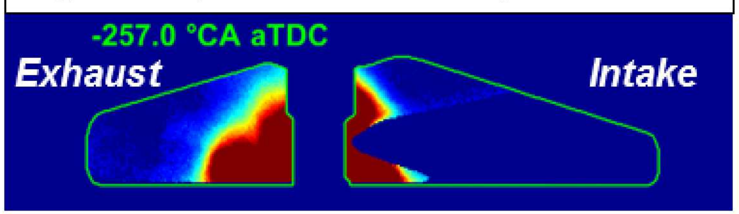


- Signs of large droplets seen near the end of injections.

High Olefin, Well-mixed stoich., SOI -310°CA



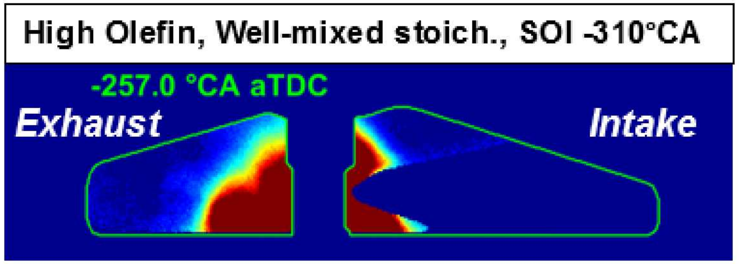
- This is considered to be a primary source of soot emission for steady-state operation.

Conclusions

- Several orders of magnitude differences in PM/PN emission from RD5-87 and iso-octane were observed.
  - PM/PN from iso-octane can be comparable to those from motored engine.
  - Indicates importance of modeling characteristics of fuels to resemble soot emissions from gasoline fuels.
- Fouling of combustion chamber surfaces and injector tip had significant effects in PM/PN.
  - Fouling of injector tip alters not only spray characteristics but also post-combustion soot formation.
  - Need to establish a procedure in terms of keeping similar cleanliness of engine components for repeatable PM/PN measurement.
- Effect of coolant temperature on PM/PN was weaker than effect of surface temperature of engine.
  - Coolant temperature did not fully represent thermal state of engine as it does not reflect surface temperatures.
- With higher # of split injections, it is possible to reduce PM/PN from “cold” engine close to those from “hot” engine.

Future Work

- Repeat the experiments using multi-component surrogate of RD5-87.
- Find optimal injection strategy for low PM/PN and stable combustion for catalyst heating mode.
- Assess effect of in-cylinder flow.
  - Activate the other intake valve to realize 2-valve operation (tumble only).



- Optical diagnostics for certain conditions.
  - Spray, wall-wetting, soot formation
- Measure surface temperatures to help understand PM/PN trends.

Thank you for your kind attention!

Acknowledgements

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