

Catalyst Heating Operation in a DI Diesel Engine: Thermodynamics and Emissions

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Abstract

Bowl geometry study (brief update): a modification to a stepped-lip piston design has been developed based on previous analyses. The purpose of these modifications is to test the hypothesis that if vortex formation can be strengthened, then benefits in thermal efficiency and pollutant emissions can be realized. Initial simulation results predict that the modified piston produces stronger vortex formation for near-TDC main injection timings.

Catalyst heating operation: Future emissions regulations will demand faster catalyst light-off with minimal criteria pollutant emissions. Fundamental understanding of mixture formation, ignition, combustion, and pollutant formation mechanisms during catalyst heating operation is lacking, and the impacts of fuel properties are not well understood. Preliminary studies in Sandia's light-duty diesel engine are directed at understanding how the post/main split ratio and post injection timing impact pollutant emissions, and how various calibration parameters and fuel properties affect the engine's behavior. Injection strategies are developed to test a wide range of loads and combustion phasing values. Analysis of engine results provides data about exhaust temperature and enthalpy, and about pollutant emissions. Thermodynamic analyses indicate that exhaust enthalpy benefits should be greatest when large quantities of fuel are completely burned as late as possible. However, experimental results suggest that retarding post phasing often does not result in improved exhaust enthalpy, as combustion efficiency is degraded as the post injection timing is retarded. It is noted that post injections are observed to decrease unburned hydrocarbon emissions below levels achieved with only a pilot and main injection. Some evidence is provided to suggest that post injections into environments with active heat release may facilitate more complete combustion. The impacts of cetane number and fuel distillation properties on unburned hydrocarbon emissions appear to depend on main injection quantity and post injection timing.



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Outline

Update: piston bowl geometry study

- Testing the piston-cylinder head space hypothesis

Catalyst heating study

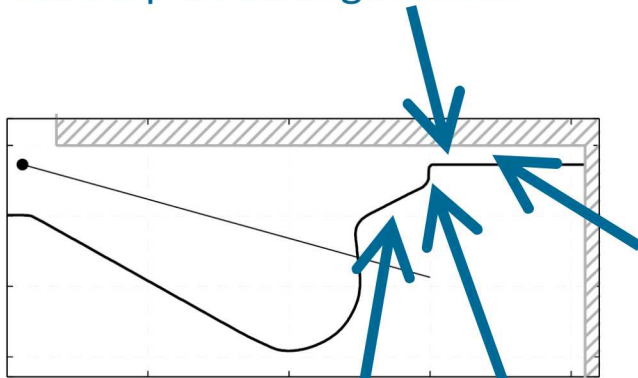
- Motivation/objectives
- Experimental approach
- Expectations based on thermodynamics
- Experimental results and conclusions
- Next steps



Review from August meeting: testing the piston-cylinder head space hypothesis

Hypothesis: increasing the space available for spray-wall separation in the squish region will encourage vortex formation, and thereby improve efficiency and reduce pollutant emissions

Can adverse radial pressure gradients above the step be strengthened?



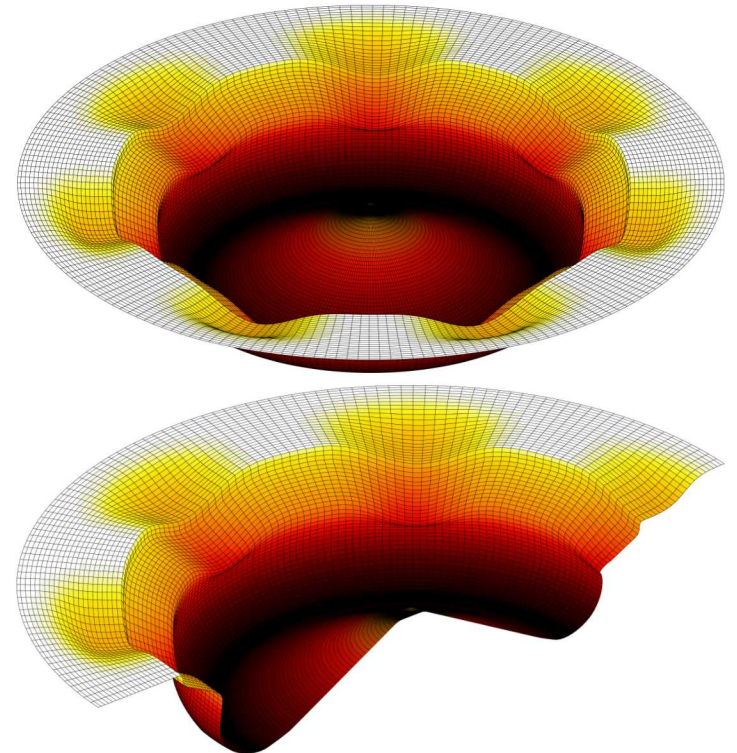
How can this space be expanded...

While preserving this vertical surface?

And the angular relationships of the step?

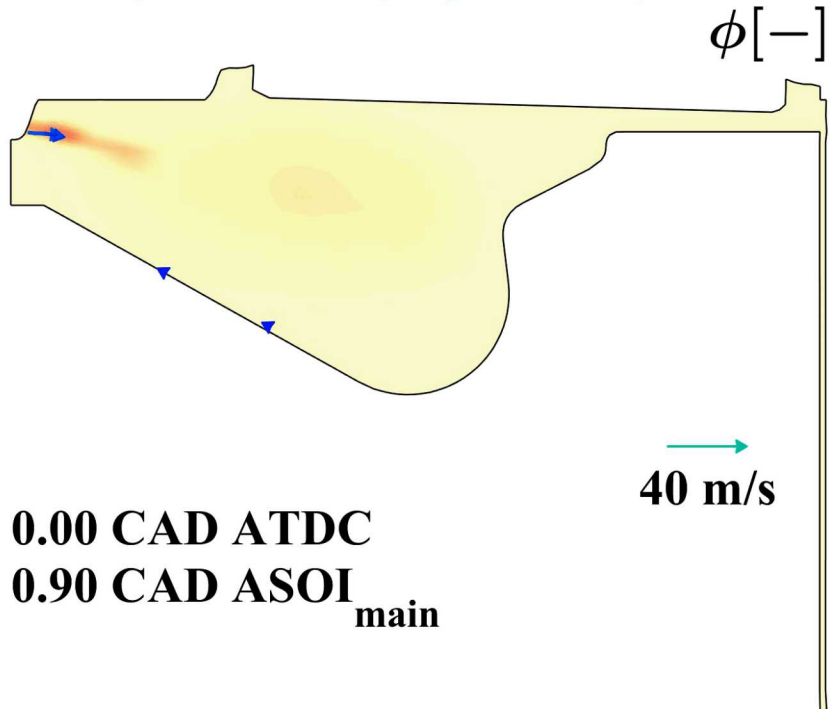


Idea: add dimples shift the step profile downward for each spray

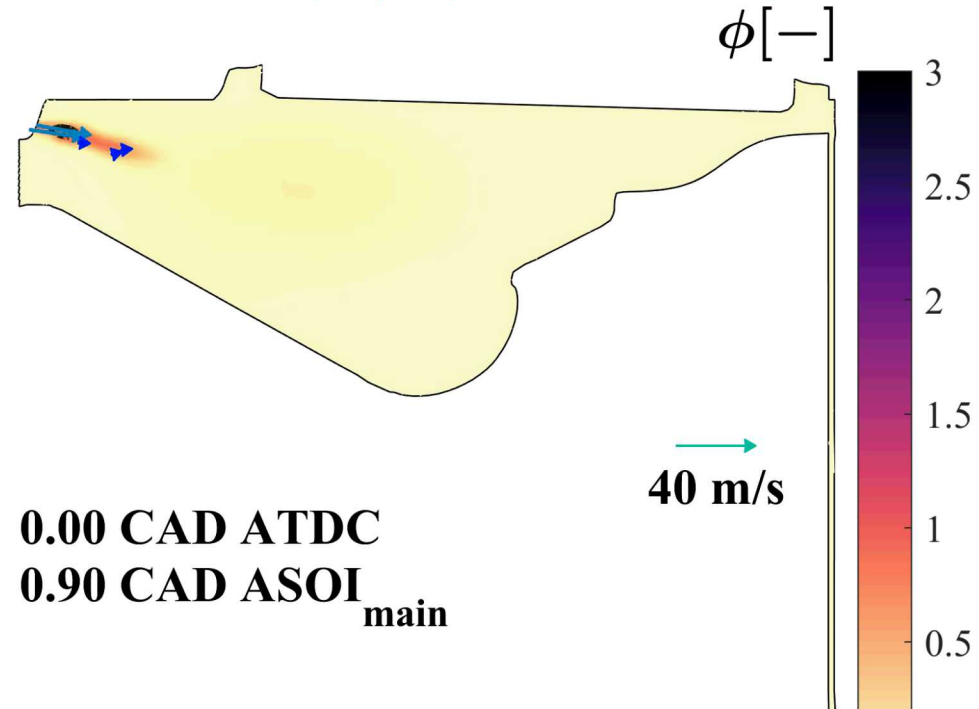


Preliminary predictions indicate that the dimpled modification may enhance vortex formation at near-TDC injection timings

Stepped-lip: little vortex formation results from separation of spray from step



Dimpled stepped-lip: significant vortex formation as spray separates from step



- Preliminary results; details are subject to change
- Ongoing analyses -> publications describing combustion system design parameter effects on flow and vortex evolution in progress



Bowl geometry study - recap

- Rotationally symmetric, dimpled, stepped-lip piston: increases space between the step and the cylinder head, maintains aspects of original step geometry at spray-wall interaction sites
 - The changes made to the stepped-lip design are predicted to strongly influence spray-wall interactions and turbulent flow / vortex evolution
- Objective of ongoing analyses: mechanistic understanding of how this bowl geometry change impacts turbulent flow evolution
- Results will be included in publication(s) documenting the effects of combustion system design parameters on vortex formation
- Combusting simulations underway to predict:
 - Heat release rate
 - Soot formation / oxidation



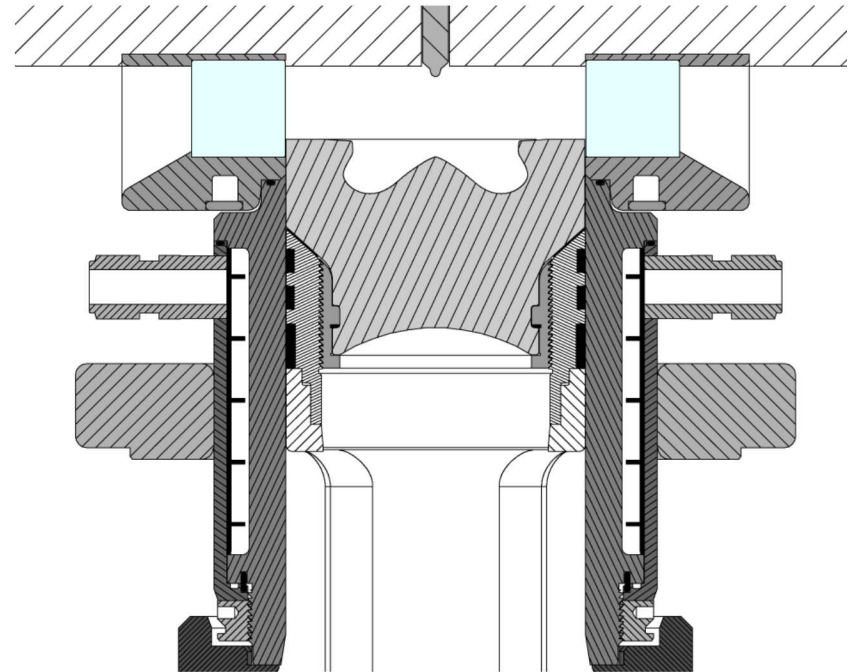
Motivation/objectives of catalyst heating study

- Motivation for catalyst heating operation
 - Future emissions regulations demand faster, cleaner catalyst light-off operation
 - Create exhaust with a high temperature and enthalpy flux to achieve rapid light-off of exhaust aftertreatment catalysts
 - Minimize untreated criteria pollutant emissions and fuel consumption
- Long-term project objectives
 - Provide thermodynamic, emissions, and optical data for a range of catalyst light-off operation
 - Develop mechanistic understanding of mixture formation, ignition, combustion, and pollutant formation with post injections in catalyst heating operation
 - Develop understanding of fuel property impacts on catalyst heating information
- Approach for initial study (last use of Sandia LD diesel engine)
 - Fix pilot and main timing, focus on post mass, timing, and split ratio
 - Thermodynamic and emissions measurements for parametric variations, including:
 - Cetane number
 - Binary fuel blend vs. full boiling range fuel
 - 1 post vs. 2 posts
 - Optical measurements



Baseline engine operation

	0% EGR	30% EGR
Bore x stroke	82 mm x 90.4 mm	
Piston bowl	Re-entrant, no valve cutouts	
Swirl ratio	2.2	
Nozzle holes	7 x 139 μm 149° opening angle $k_s = 1.5$	
EVO	0.1 mm @ 130 CAD ATDC	
Engine speed	1500 rpm	
Intake mass flow rate	8.51 g/s	
Intake composition (mole fractions)	O2: 21% N2: 79% CO2: 0%	O2: 18.7% N2: 79.36% CO2: 1.94%
Intake temperature	31 °C	49 °C
Coolant temperature	30 °C	
TDC density (est.)	21.2 kg/m ³	
Injection pressure	500 bar	
Start of Pilot Injection	15 CAD BTDC	
Pilot quantity	2 mg	
Start of Main Injection	0 CAD ATDC	
Main quantity	3, 5, 7 mg	
SOI first post	10-30 CAD ATDC	
First post quantity	2, 4, 6 mg	
SOI second post	15-43 CAD ATDC	
Second Post quantity	2, 4, 6 mg	



- Skip-fired operation
 - Emissions corrected for dilution
 - Thermodynamic data reported as average of 50 consecutive skip-fired cycles

Injection strategy / hydraulic bench calibrations

- Injection strategies
 - Pilot quantity and timing fixed
 - Main timing fixed (SOI near TDC)
 - Three main quantities
 - Three post1 quantities
- Injection quantities depend on other injection quantities and dwells
 - Each calibration has been developed with the hydraulic injection rate/quantity meter with a fixed backpressure
- Total injected fuel mass is estimated from emissions measurements where possible
 - This carbon-balance estimated fuel mass is used to compute emissions indices, etc.

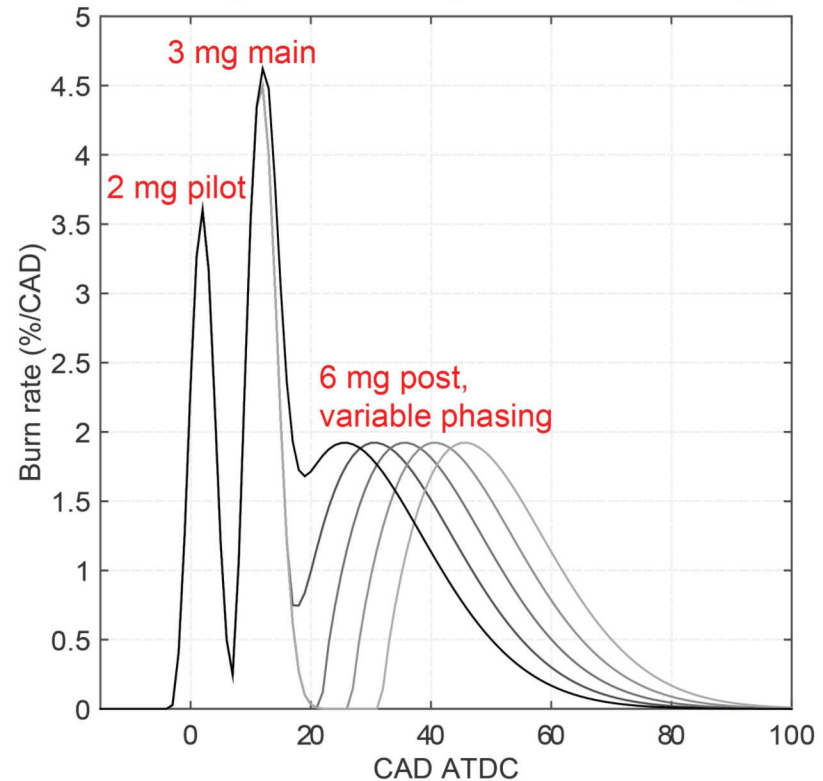
Injected Mass (mg)					Hydraulic start of injection (CAD ATDC)			
Total	Pilot	Main	Post1	Post2	Pilot	Main	Post1	Post2
5	2	3			-15	TDC		
7	2	3	<-2->				10,14,18,22,26,30	
9	2	3	<-4->					
11	2	3	<-6->				10	15,20,25,30,35,40
13	2	3	2	<-6->			18	23,28,33,38,43
7	2	5			-15	TDC		
9	2	5	<-2->				10,14,18,22,26,30	
11	2	5	<-4->					
13	2	5	<-6->				10	15,20,25,30,35,40
13	2	5	2	<-4->			18	23,28,33,38,43
9	2	7			-15	TDC		
11	2	7	<-2->				10,14,18,22,26,30	
13	2	7	<-4->					
13	2	7	2	<-2->			10	15,20,25,30,35,40
							18	23,28,33,38,43



Simple thermodynamic modeling

- Simple GT-POWER simulations are performed to better understand thermodynamic effects
- Simulated heat release profiles
 - Wiebe profiles defined for pilot, main, and post heat release
 - Heat release duration scales with fuel quantity, but not phasing
 - Assume 100% combustion efficiency
- Specific heat ratio computed as a function of temperature and composition
- Modified Woschni heat transfer model
- Thermodynamic quantities are computed from the closed portion of the cycle
 - Work, heat loss, change in internal energy
 - Exhaust temperature
 - Exhaust enthalpy flux

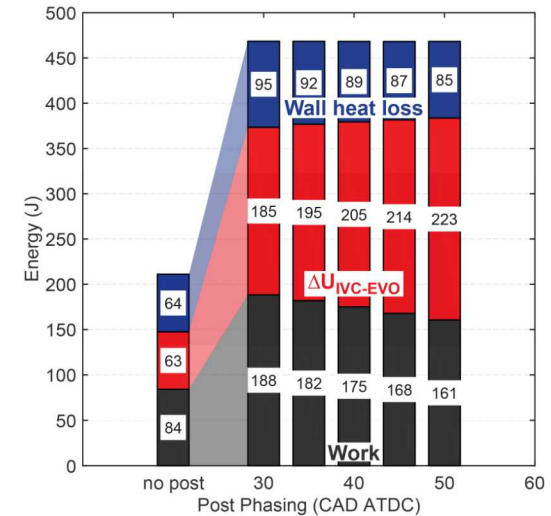
Sample heat release profiles:
2-3-6 (pilot-main-post mass in mg)



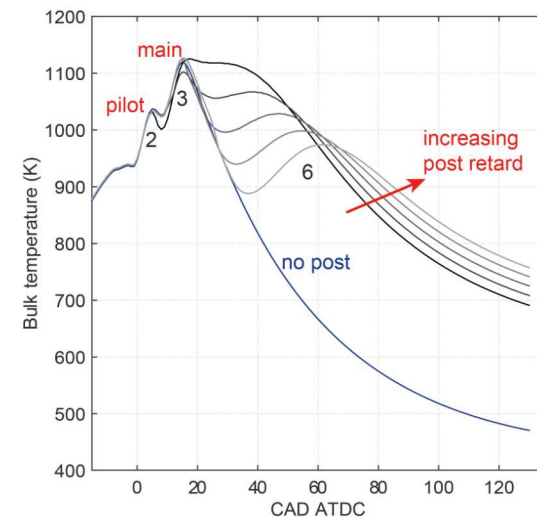
Thermodynamic simulation results: post phasing effects

- Energy balance: work, **internal energy change**, and **wall heat loss**
 - Adding a post injection increases work output; retarding the post injection decreases it
 - **The post injection effectively increases available exhaust energy**
 - **Retarding the post combustion phasing increases available exhaust energy**
 - Later post combustion phasing may reduce wall heat loss
- Bulk gas temperature
 - Retarding post timing tends to increase bulk gas temperatures later in the cycle
- Objective of catalyst light-off strategies: achieve complete combustion as late as possible

Energy balance for 2-3-6 case



Bulk gas temperature for 2-3-6 case



Results: simulated exhaust temperatures/heat flux

- Exhaust temperature computed assuming isentropic expansion from bulk gas temperature at EVO
 - Method also applied to experimental results

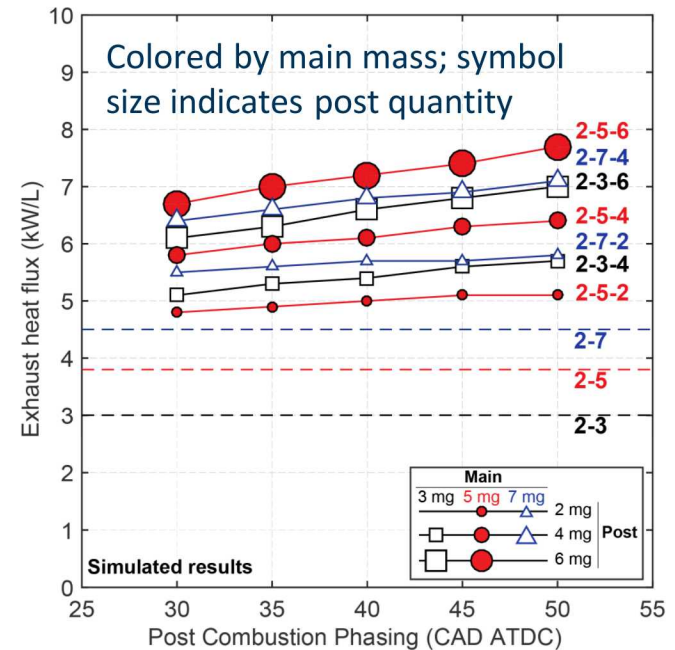
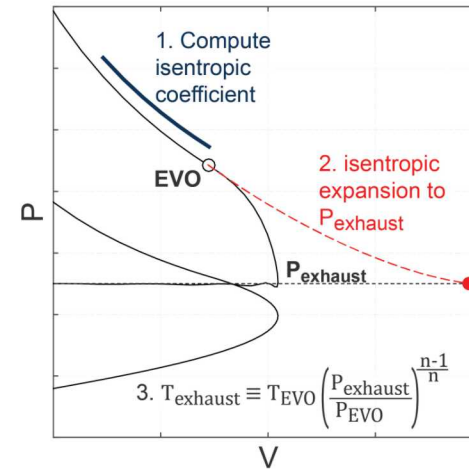
- Exhaust heat flux calculation: ACEC guidelines

$$\Phi_{ex} = \frac{(\dot{m}_{air+fuel})(c_{p,exhaust})(T_{ex}-20^{\circ}C)}{V_d} \left[\frac{kW}{L} \right]$$

$$c_{p,exhaust} = 1.25 \frac{kJ}{kg K}$$

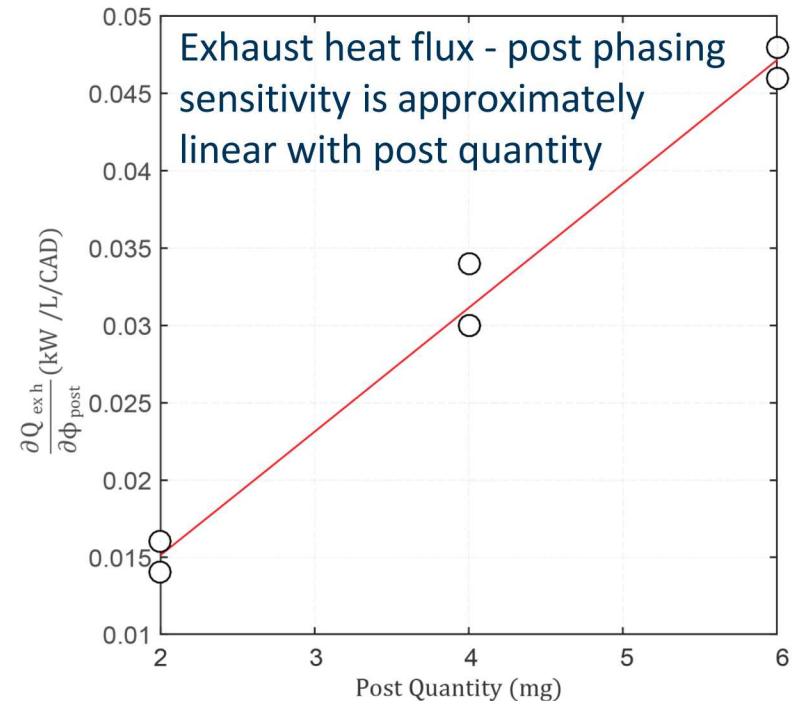
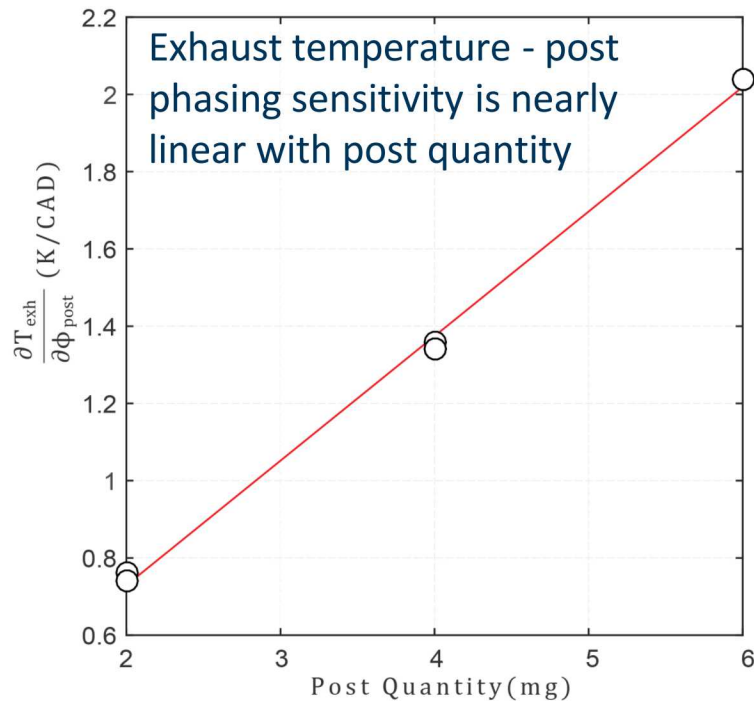
- Ways to increase exhaust heat flux for fixed pilot and main quantities
 - Increase post mass
 - Retard post combustion phasing

- The sensitivity of exhaust temperature/heat flux to post retard seems to depend on post quantity...



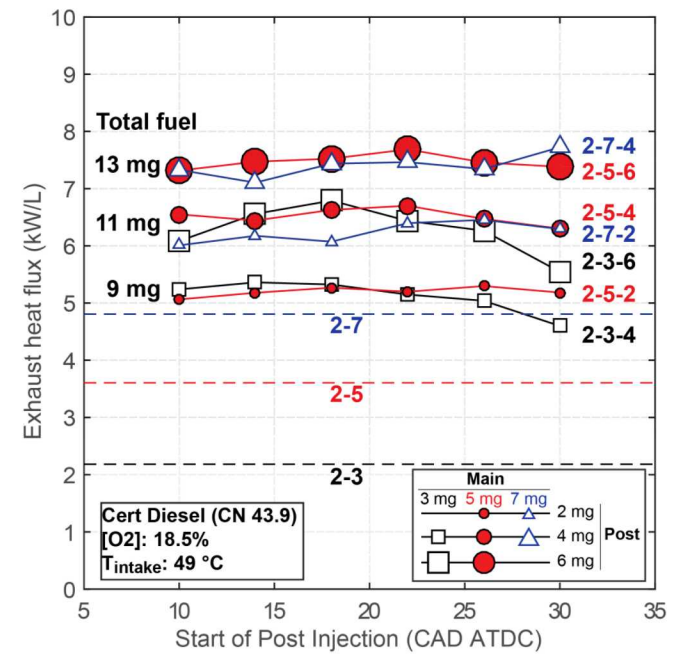
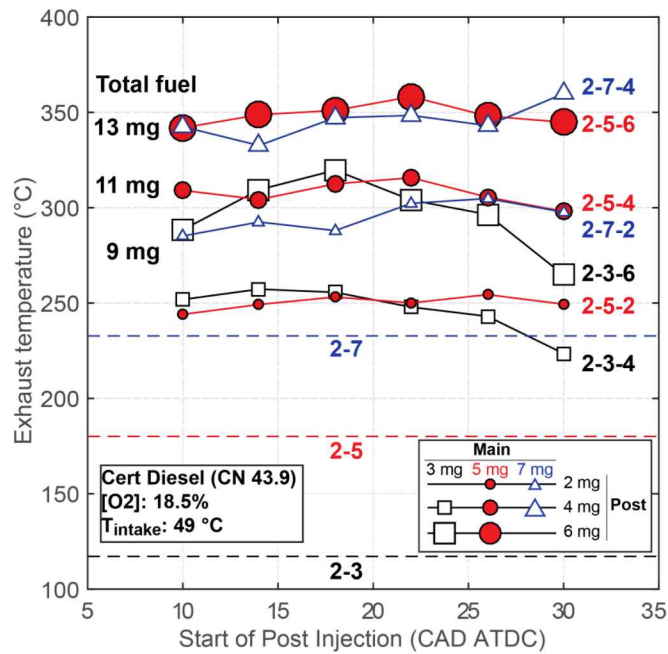
Results: sensitivity of exhaust temperature/heat flux to post phasing

- Simulated exhaust temperature (left) and heat flux (right) become more sensitive to post phasing as post quantity increases
- **Large amounts of fuel burning as late as possible are desirable for catalyst heating operation**



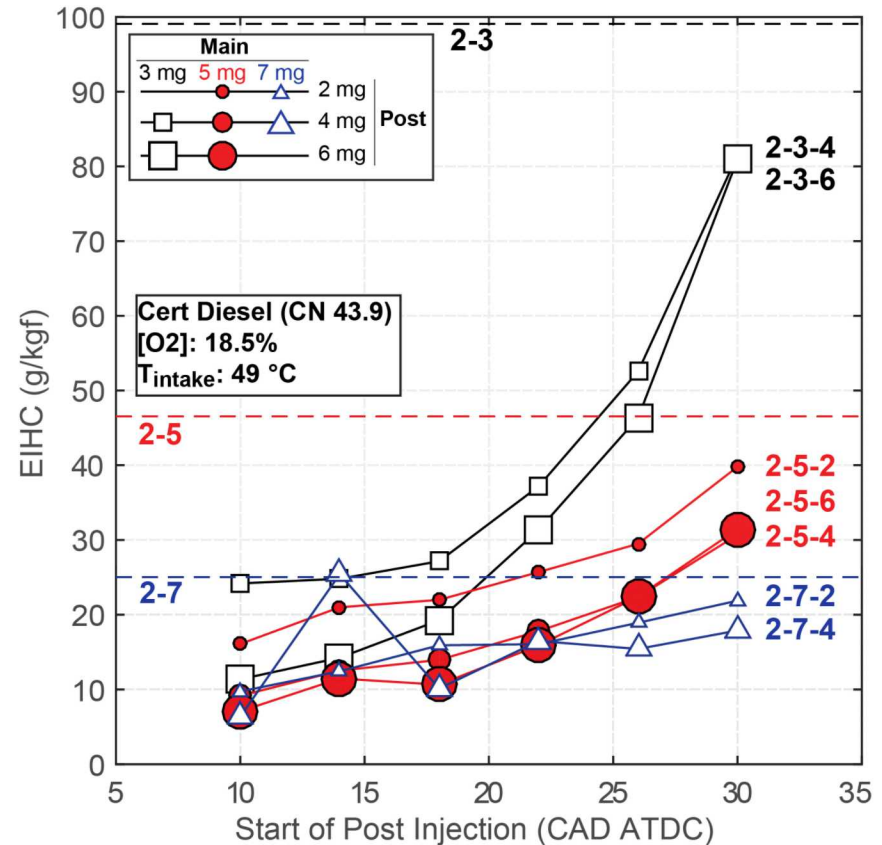
Experimental results: exhaust temperature and heat flux

- Exhaust temperature and heat flux depend most strongly on total fuel quantity
- For a given total amount of fuel, the post-main split affects exhaust enthalpy and temperature to different degrees
 - No clear, monotonic trends are observed
- Exhaust temperature and heat flux often decrease for late post injections
 - Incomplete combustion or increased wall heat loss?



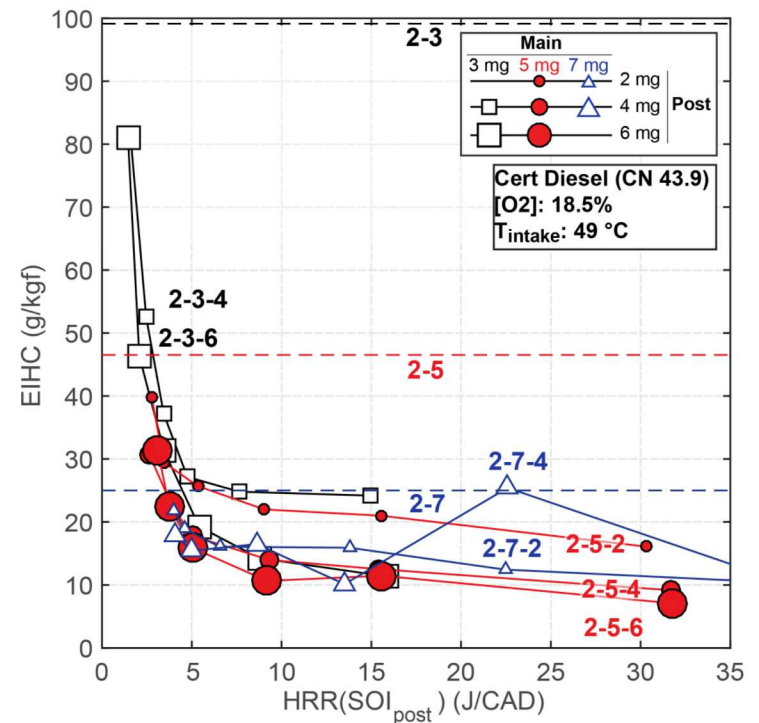
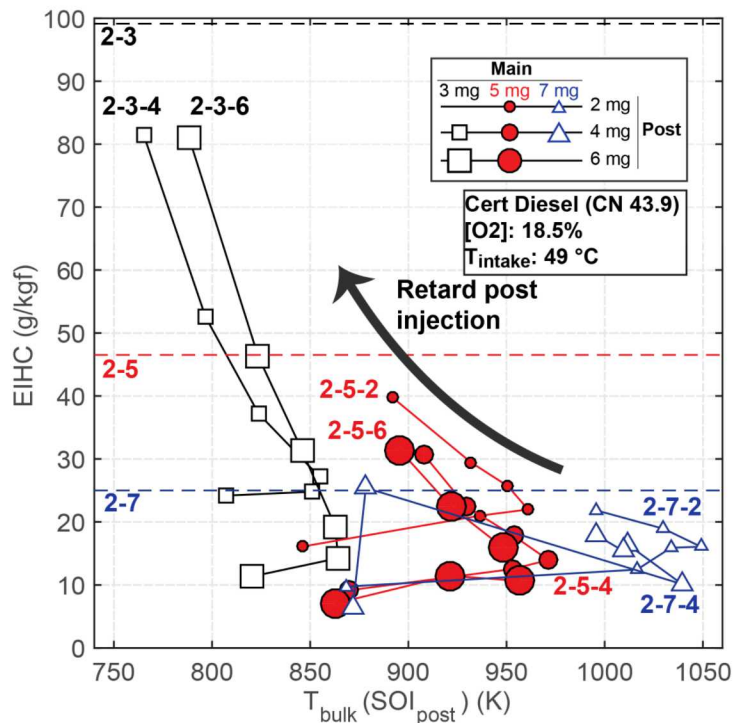
Experimental results: unburned hydrocarbon (UHC) emissions

- Pilot-main only: UHC emissions decrease with increasing main quantity
 - Longer main injection – higher temperatures help oxidation?
 - Possible sources of UHC emissions – overmixing due to long ignition delays? extinction due to expansion?
- Adding a post injection decreases UHC emissions
 - Advantages of post injections become smaller as post injections are retarded
 - UHC increases most with post retard for small main quantities
 - Increasing post quantity may decrease UHC emissions, but not always
- What is important to achieve robust post ignition and combustion?
 - Bulk temperature?
 - Local interactions? Entrainment wave?



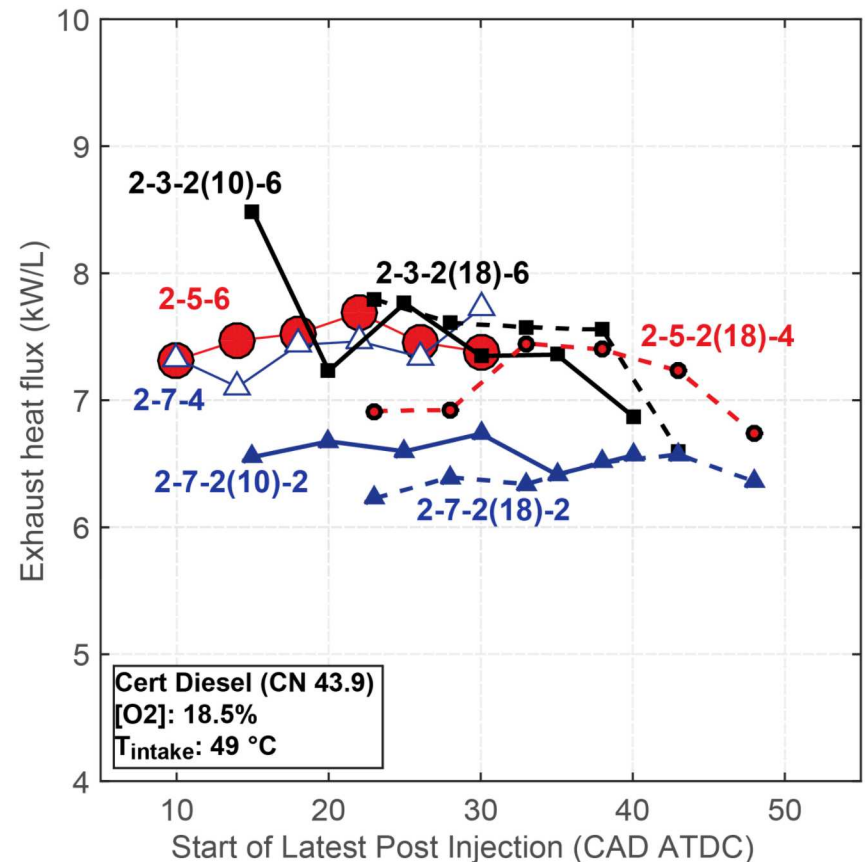
Experimental results: unburned hydrocarbon (UHC) emissions

- UHC emissions tend to increase as T_{bulk} at the start of the post injection decreases, but the behavior is not monotonic, particularly for early post injections
 - Interaction between main and post?
- UHC emissions trend strongly upward as the instantaneous heat release rate at the start of the post injection decreases
 - Curves tend to collapse on one another (but not completely)
 - Do local conditions determine post combustion robustness?



Experimental results: effect of multiple post injections on exhaust enthalpy

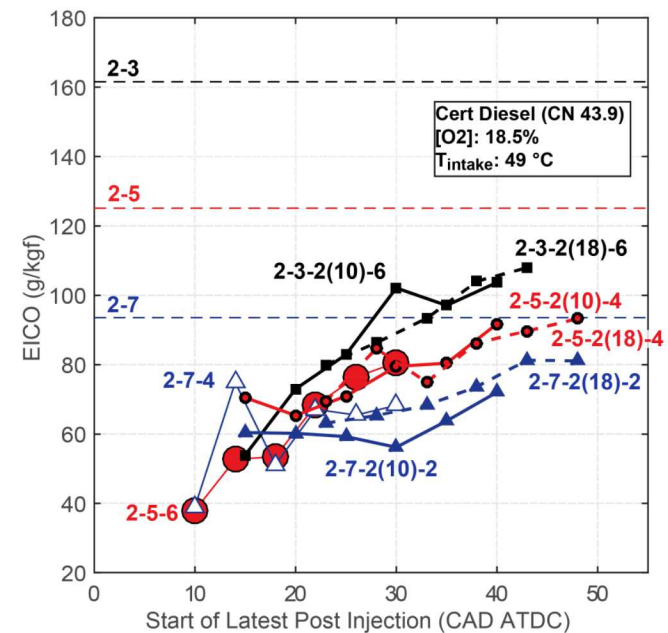
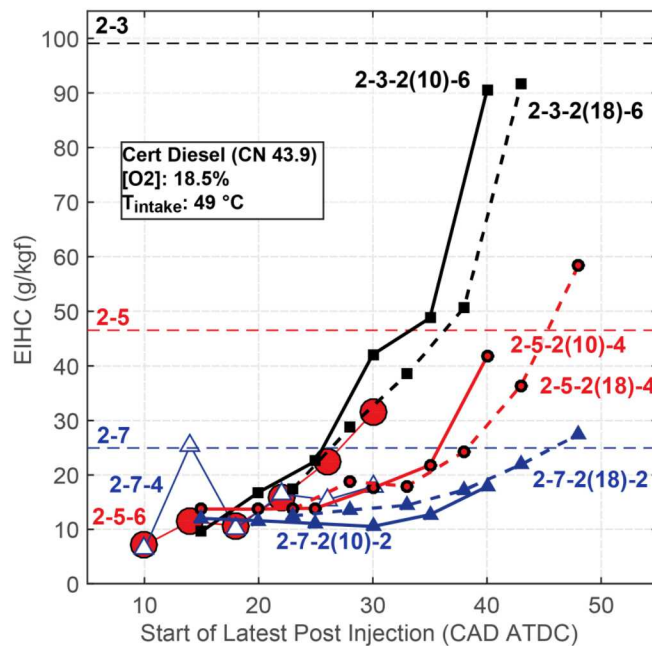
- Total injected mass (nominal): 13 mg
- No one strategy emerges as a clear winner
- Adding multiple small posts to a large main seems to be less effective than adding one large post
 - 2-7-2-2 vs. 2-7-4
- These preliminary results are not conclusive
- Experiments with Sandia's new medium-duty diesel should improve the quality of these data
 - Online fuel flow measurement
 - Continuously fired operation
 - Direct measurement of exhaust temps



Caveat: different injector needed for double-post strategy

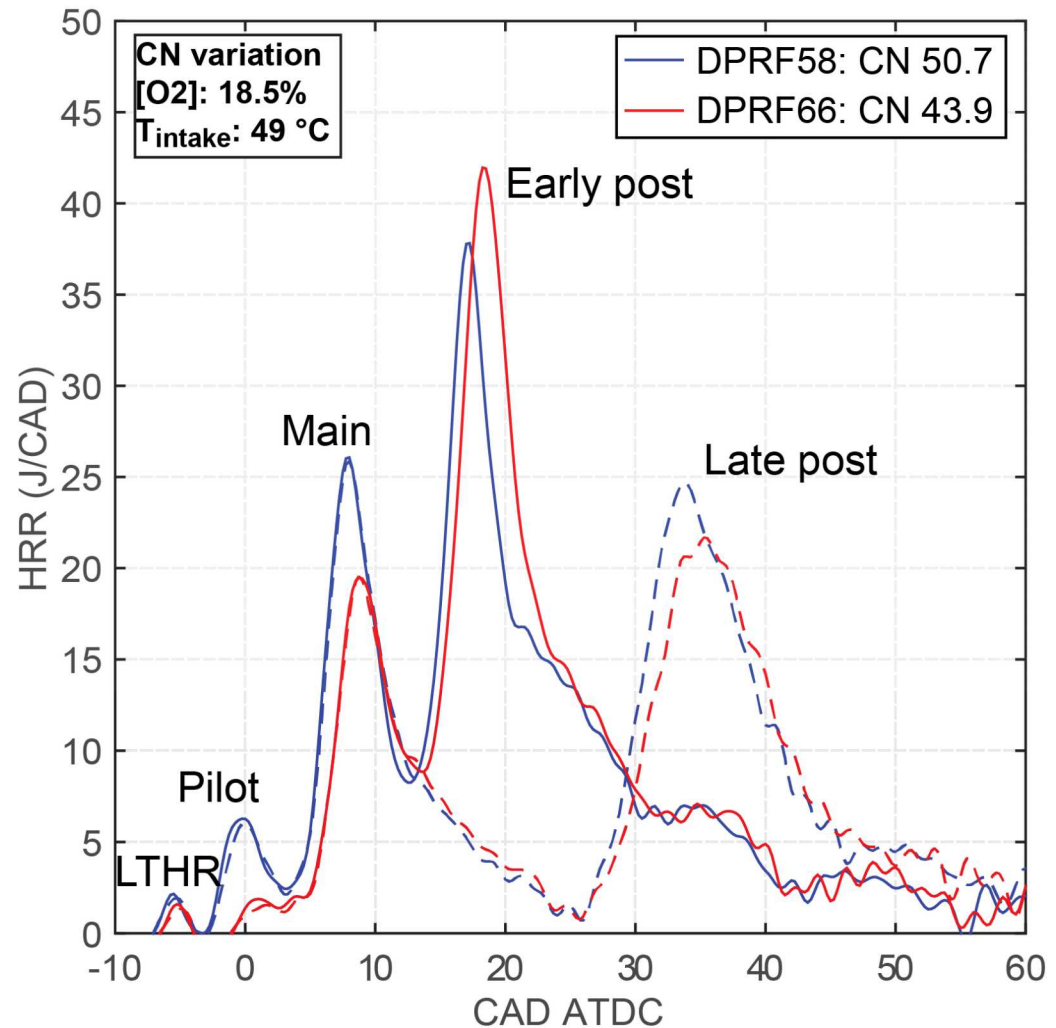
Experimental results: effect of multiple post injections on UHC/CO emissions

- UHC and CO emissions are typically highest for small main quantities
- Excessive post retard increases pollutant emissions without increasing exhaust enthalpy
- Large main and small posts produces fewer pollutants, but the exhaust enthalpy is lower than for other cases – why?
 - Next step: energy balance analysis



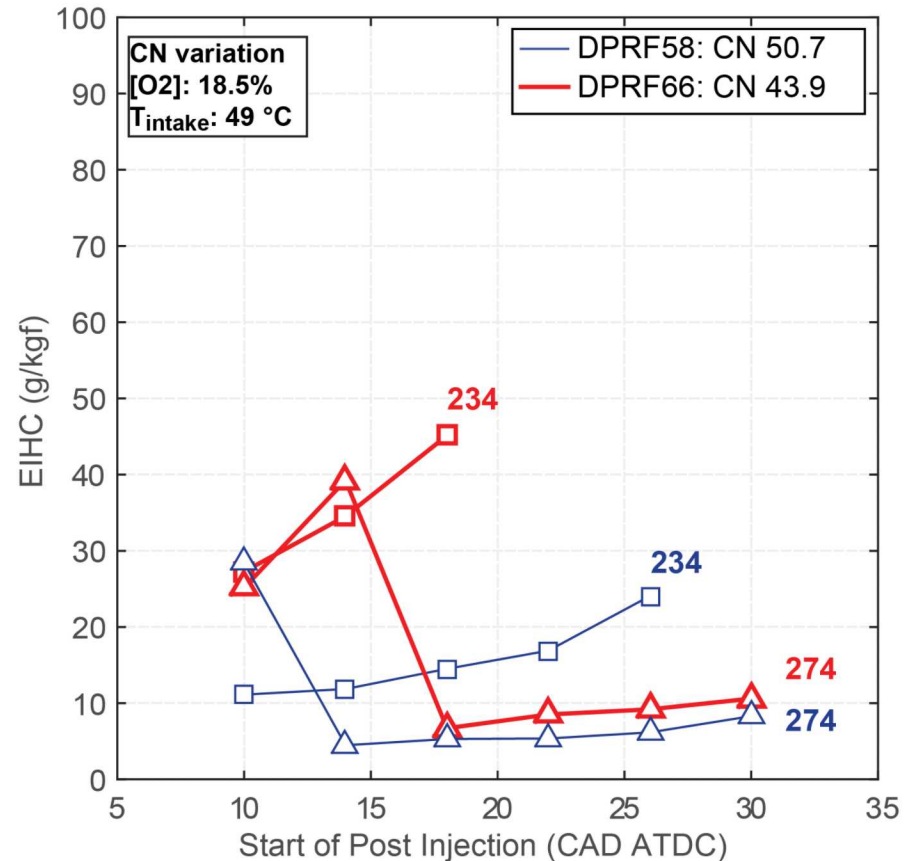
Cetane number effects on heat release rate

- Representative results shown for 2-3-6 case
- LTHR of the pilot is only slightly affected by cetane number
- Pilot combustion overlaps with the main injection
- Cetane number influences the combustion of every injection
 - Not just ignition delay/phasing, but also peak heat release rate



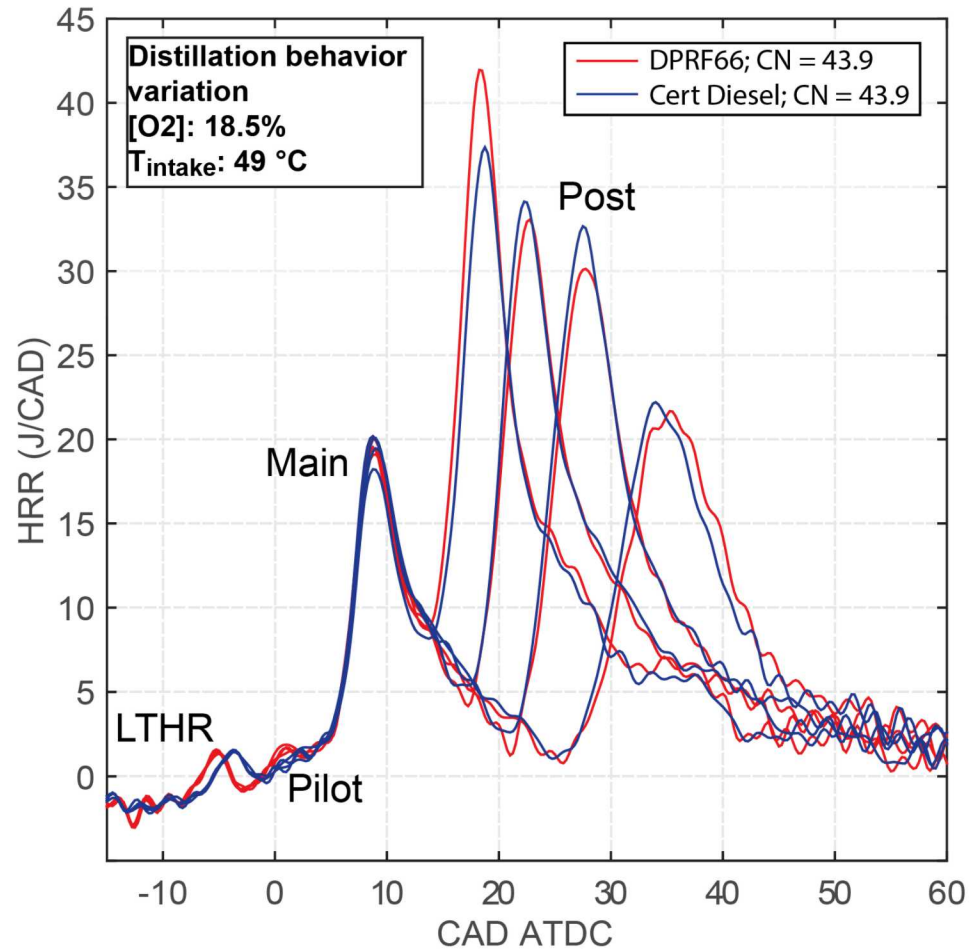
Cetane number effects on UHC emissions

- Results shown for 2-3-4 and 2-7-4 cases
- UHC emissions typically decrease as CN increases
 - Some exceptions for early posts
 - CN effects are larger for smaller main injection quantities
- Further analysis: CN's impact on tradeoffs between pollutant emissions and exhaust enthalpy



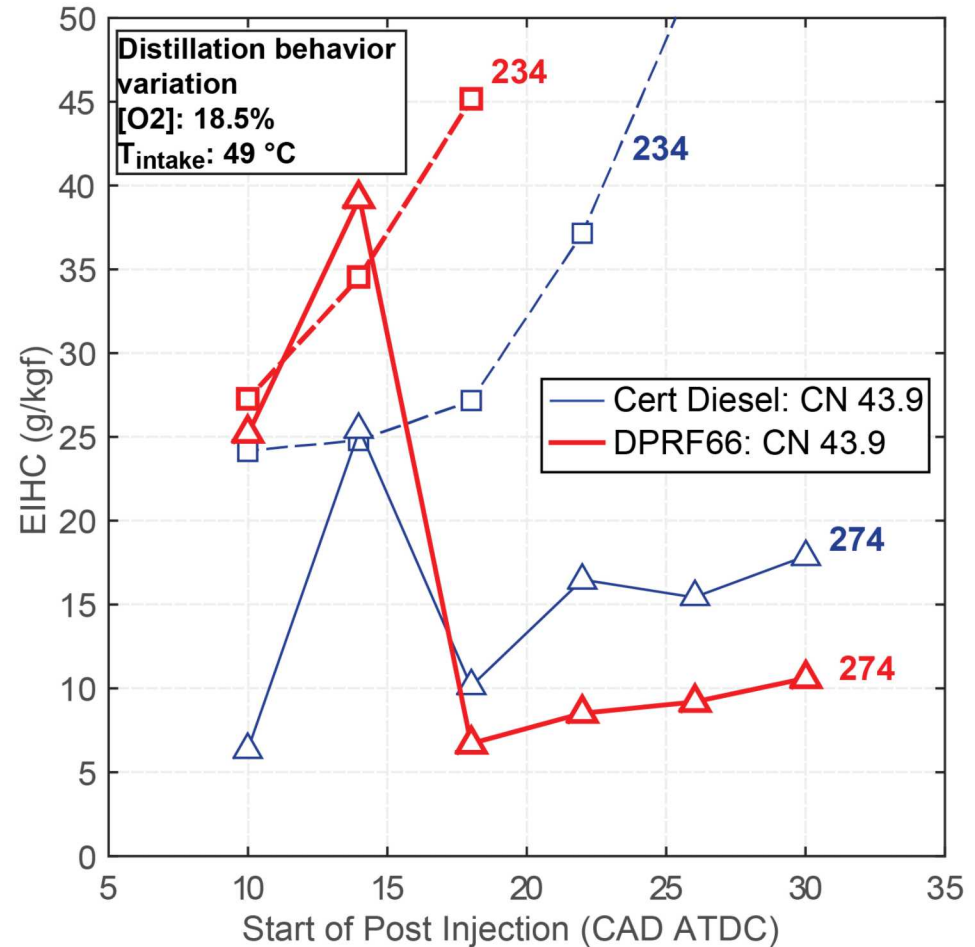
Experimental results: fuel distillation effect on heat release

- Representative results shown for 2-3-6 case: DPRF66 vs. cert diesel
 - Both fuels: CN 43.9
 - CN seems to capture much of the combustion behavior
- Pilot heat release is affected by distillation behavior
 - Cert diesel: retarded onset of LTHR, less pronounced HTHR
- No changes observed in main heat release
- Post heat release profiles differ slightly, but not consistently
 - Significance/cause unclear



Experimental results: fuel distillation effect on UHC emissions

- For a given post timing and small main injection quantities, cert diesel produces fewer UHCs
- The trend is more complex for higher main injection quantities
 - Late posts: cert diesel produces more UHC emissions
- Further analysis and investigation are needed



Conclusions

Thermodynamic analysis (neglecting combustion efficiency)

- Post injections increase work output, but also internal energy available for catalyst heating
- Retarding post heat release reduces work and possibly wall heat loss, increases exhaust heat
- Larger post quantities provide more benefit

Experimental results (preliminary)

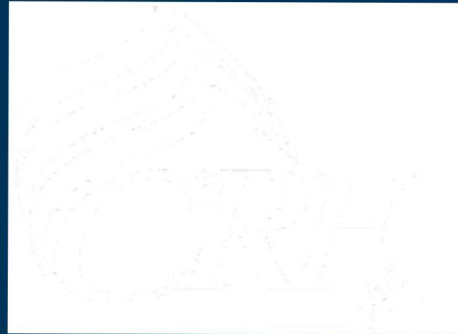
- Exhaust temperature and enthalpy depend most strongly on total fuel mass; improvements are only sometimes realized as post injections are retarded
- Post injections reduce the hydrocarbon emissions resulting from the pilot and main alone
- Combustion efficiency is degraded as post injection timing is retarded; increasing the main quantity improves combustion efficiency
- Some evidence exists to suggest that post injections into an environment with ongoing heat release may be important for reducing hydrocarbon emissions
- Multiple posts may not improve exhaust enthalpy and do not provide clear advantages in UHC emissions – later post injections most often lead to increased CO and UHC emissions
- Cetane number impacts the combustion of each injection, but the impacts on unburned hydrocarbon emissions depend on main quantity
- Fuel distillation effects are not observed to have a strong impact on heat release rates, but the impact on unburned hydrocarbon emissions also depends on main quantity



Next steps in catalyst light-off project

- Co-Optima experiments
 - Thermal testing of fuel blends
- Continued analysis of experimental data
 - Establish experimental objectives for optical studies
- Optical studies
 - High-speed liquid scattering imaging
 - High-speed natural luminosity imaging
 - Infrared imaging: C-H stretch and (potentially) aldehyde
- Transition to medium-duty platform





Thank you for your attention

Questions?