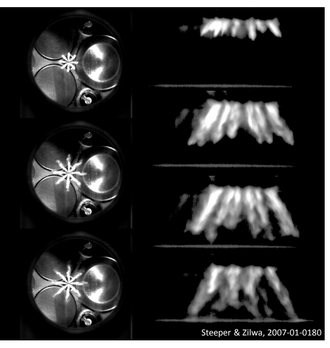
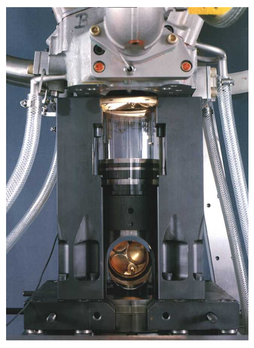
SAND2015-10398C

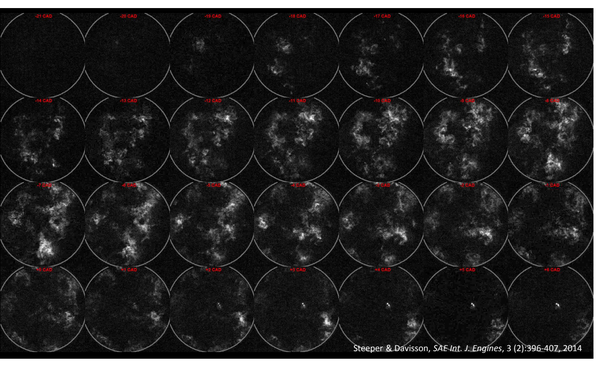
Investigation of Fuel Effects on In-Cylinder Reforming Chemistry using Gas Chromatography

Benjamin Wolk and Isaac Ekoto

Engine Combustion Department, Combustion Research Facility, Sandia National Laboratories







Sandia National Laboratories

Exceptional service in the national interest

Abstract

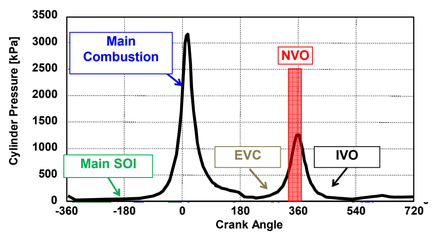
Negative Valve Overlap (NVO) is a potential control strategy for enabling Low-Temperature Gasoline Combustion (LTGC) at low loads. While the thermal effects of NVO fueling on main combustion are well-understood, the chemical effects of NVO fuel reforming have not been extensively studied. The objective of this work is to examine the effects of fuel molecular structure on NVO fuel reforming using gas sampling and detailed speciation by gas chromatography. Engine gas samples were collected from a single-cylinder research engine at the end of the NVO cycle using a custom dump-valve apparatus. Six fuel components were studied at two injection timings: (1) iso-octane, (2) n-heptane, (3) ethanol, (4) 1-hexene, (5) cyclohexane, and (6) toluene. All fuel components were studied neat except for toluene – toluene was blended with 18.9% n-heptane by liquid volume to increase the fuel reactivity. Additionally, a gasoline surrogate matching the broad molecular composition of RD587 research gasoline was formulated using the chosen fuel palette and tested. The energy content of the injected fuel mass was kept constant for the sampled NVO cycle and the excess oxygen was relatively low (2.4%) compared to previous studies. The later injection timing studied resulted in useable energy recovery near 70% and improved reformate yield of hydrogen and C1-C4 hydrocarbons compared to the earlier injection timing for all fuels except toluene/n-heptane. Analysis of the RD587 surrogate reformate compared to the individual component reformates suggests that fuel component interactions depend on injection timing, potentially through the in-cylinder equivalence ratio distribution.

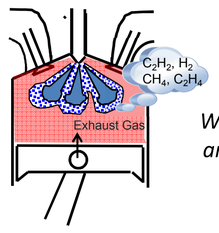
Introduction

The products of fuel-rich combustion can be retained and used to augment main-cycle combustion

Negative Valve Overlap (NVO) improves main-period combustion stability at low loads through…

- Charge heating from retained residuals & heat release
- Enhanced charge reactivity via fuel reforming



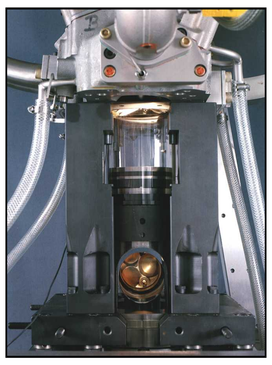


What species are created?

NVO

1. Early Exhaust Valve Closure (EVC) and low valve lifts
   Up to 50% of the exhaust retained
   Low O_2 content (0 – 10% depending on EGR & fueling rates)
2. Pilot fuel injection
3. Concludes with a late Intake Valve Opening (IVO)

Sandia Single-Cylinder LTGC Engine



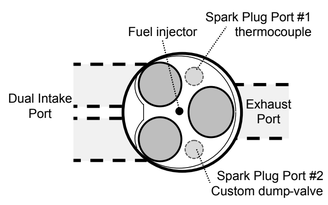
This study evaluates the impact of fuel type (molecular structure) and fuel component interactions on reformate composition and energy recovery.

Fuels

iso-octane
n-heptane
ethanol
1-hexene
cyclohexane
toluene / n-heptane
RD587 surrogate

Blends (vol. %)

	T/nH	RD587 Surr.
iso-Oct.	-	54.9
n-Hept.	18.9	11.6
Ethanol	-	9.9
1-Hexene	-	4.7
Toluene	81.1	18.9



Conditions

$[O_{2,exh.}]$ = 2.4%

$m_{inj.}$ = 6 mg iso-octane
(or LHV equivalent)

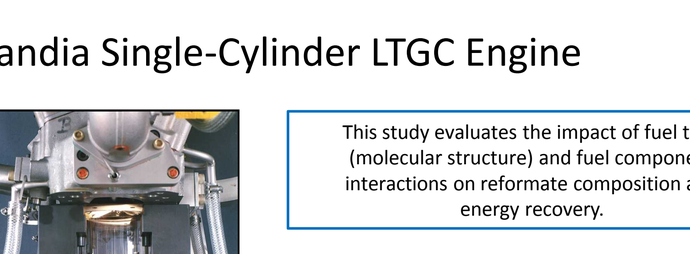
$T_{exh.}$ ≈ 365 °C

SOI_{NVO} = -65, -40 CAD

Engine Specifications

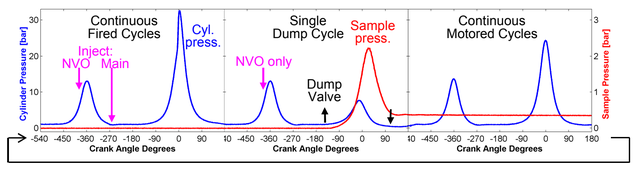
Head design	Pentroof
Displacement	0.63 liter
Bore	92 mm
Stroke	95.25 mm
CR	11.3
Speed	1200 rpm
Intake air pressure	1.0 bar abs.

Sample Collection and Analysis



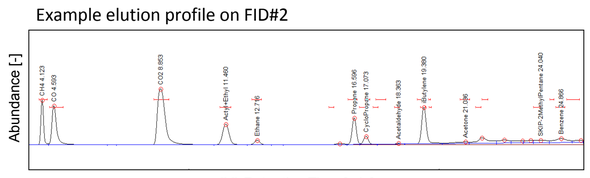
2 x Flame Ionization Detector (FID)
1 x Thermal Conductivity Detector (TCD)

A repeatable NVO environment is established before a single dump sample is taken



Steeper & Davisson, *SAE Int. J. Engines*, 3 (2):396-407, 2014

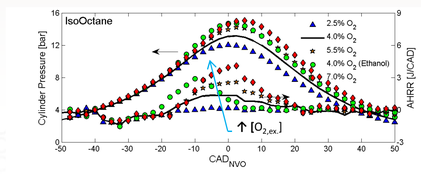
Example elution profile on FID#2

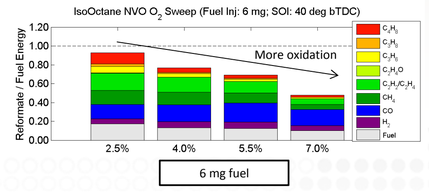


Gas chromatography with 2 FID/1 TCD detectors identifies major and minor reformate species

Results

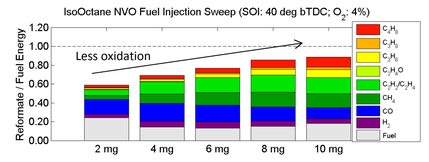
Previous studies





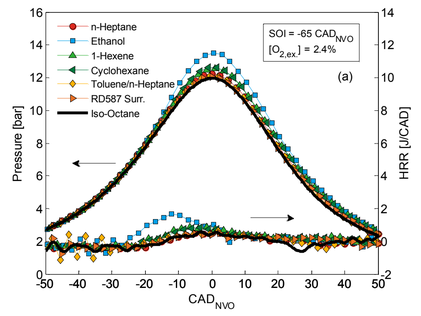
Best fuel energy recovery for ↑ϕ & ↓O_2, with limited oxidation

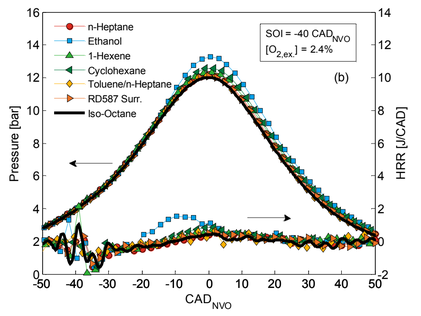
How do different fuels reform in-cylinder during a low-O_2 NVO period?

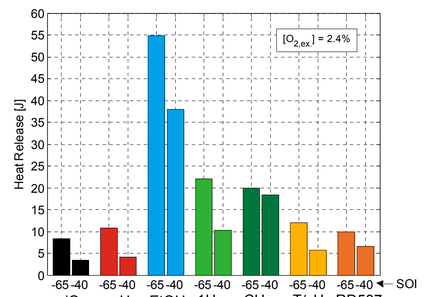


Current study

Cylinder Pressure and Heat Release

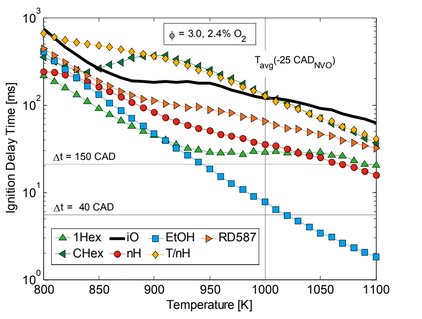




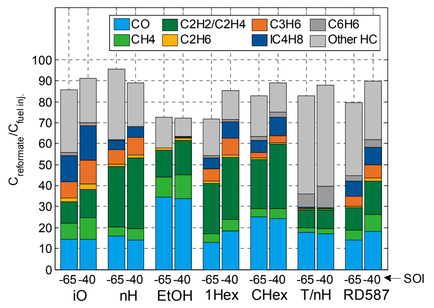


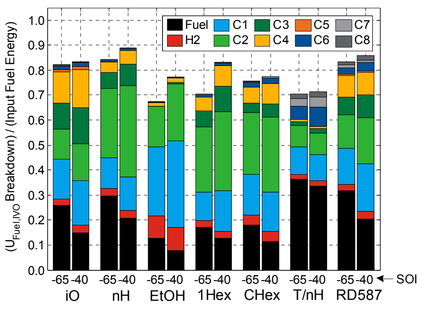
Lower heat release for later injection timing indicates less oxidation

Ethanol is the only fuel with fast enough ignition chemistry relative to the NVO residence time



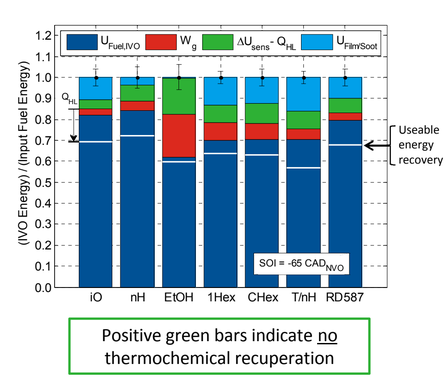
Speciation and Energy Recovery

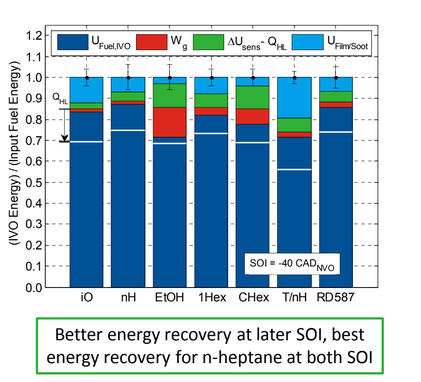




Best reforming to lower hydrocarbons for n-heptane (C7H16) and ethanol (C2H5OH)

Less parent fuel for later SOI, suggests less fuel in crevice regions





Positive green bars indicate no thermochemical recuperation

Better energy recovery at later SOI, best energy recovery for n-heptane at both SOI

Conclusions

In the current study, the effects of fuel molecular structure on NVO fuel reforming were examined for 6 fuel components and a 5-component surrogate for RD587 gasoline using gas sampling and detailed speciation. The major findings of the study are:

- Ethanol released the most NVO-period heat among the fuels tested due to sufficiently short ignition delay time relative to the residence time in the NVO period.
- On an energy basis, the amount of unreformed parent fuel decreased as the NVO injection timing was delayed from -65 CAD_{NVO} to -40 CAD_{NVO} for all fuels, with a corresponding increase in the total reformate chemical energy.
- The closed-period energy analysis revealed that iso-octane, n-heptane, and the RD587 surrogate had ~70% useable energy recovery for both injection timings studied. Ethanol, 1-hexene, and cyclohexene also had near 70% useable energy recovery for the later injection timing, with useable energy recovery being about 10 percentage points lower for the earlier injection timing.

Acknowledgements

This work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. Financial support was provided by the U.S. Department of Energy, Office of Vehicle Technologies. The authors gratefully acknowledge the engineering support provided by Alberto Garcia. The contributions of Brian Peterson, William Northrop, and Richard Steeper are also acknowledged.