



Full Length Article

Detailed speciation and reactivity characterization of fuel-specific in-cylinder reforming products and the associated impact on engine performance

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HIGHLIGHTS

- The impact of reformat on charge reactivity varied among the fuels tested.
- PIMS can discern between isomers with drastically different effects on reactivity.
- Acetylene has a large impact on increasing reformat reactivity for fuels tested.
- Acetaldehyde may contribute to improved reactivity at low reformat fractions.
- Reformat fraction and compressed temperature dictated combustion phasing trends.

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ABSTRACT

In-cylinder reforming of a gasoline pilot fuel injection during the negative valve overlap (NVO) period of an engine cycle can be used to alter the fuel-air mixture reactivity in low-temperature gasoline combustion (LTGC). In the present study, the impact of the NVO reformat on main-period engine performance was evaluated experimentally for four single-component surrogate gasoline fuels (*iso*-octane, *n*-heptane, ethanol, and 1-hexene) using a custom alternate-fire sequence. For each fuel, the NVO injection mass was held constant as the main-period injection mass was varied. The constant NVO injection mass allowed the NVO reformat product stream to be separately characterized in detail using photoionization mass spectrometry (PIMS). PIMS measurements were performed to characterize the NVO reformates of the four fuels used for main-period engine performance testing, as well as two additional fuels: cyclohexane and a toluene/*n*-heptane blend. All experiments were conducted using a direct-injection, single-cylinder research engine equipped with a custom dump valve apparatus used to perform bulk gas sampling at the end of the NVO period. A constant volume, adiabatic, single-zone reactor model with detailed chemical kinetic mechanisms was used to evaluate the reactivity of each NVO reformat compared to the unreformed parent fuel, the impact of specific species on reformat reactivity, and to examine the factors that influence main-period engine performance. The PIMS measurements and reactor model analysis indicated that all tested fuels (except *n*-heptane) exhibit increased reformat reactivity as compared to the unreacted parent fuel through production of more reactive species, namely acetylene, acetaldehyde, propene, and allene. Main-period engine performance was impacted by changes in reactivity from the reformat fraction of total fueling and compressed temperature (through the ratio of specific heats and differences in charge cooling from the main injection). *iso*-Octane was found to have the largest benefit in reactivity as the reformat fraction of total fueling increased. Alternatively, increases in reactivity for ethanol were primarily due to decreased charge cooling while reactivity increases for 1-hexene were dictated by increased ratio of specific heats. This paper demonstrates that NVO-generated reformat can improve main-period reactivity through both chemical and thermal effects, although significant NVO-period heat losses reduce total-cycle engine thermal efficiency.

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Nomenclature

AHR/AHRR	apparent heat release/rate	PRF	primary reference fuel
CA	crank angle relative to main-period TDC	RGF	residual gas fraction
CA _{NVO}	crank angle relative to NVO-period TDC	RON	research octane number
CoV	coefficient of variation	RPM	revolutions per minute
EVC/EVO	exhaust valve close/open	SNR	signal-to-noise ratio
GC	gas chromatograph	SOI	start of fuel injection
HR/HRR	heat release/rate	TDC	top dead center
IMEP	indicated mean effective pressure	VUV	vacuum ultraviolet
ITE	indicated thermal efficiency	m/z	mass-to-charge ratio
IVC/IVO	intake valve close/open	t_{ign}	constant-volume ignition delay time
LHV	lower heating value	T_{peak}	peak bulk-averaged in-cylinder temperature during the NVO period
LTGC	low-temperature gasoline combustion	$\Delta t_{ign}(T,P)$	difference in t_{ign} between neat PRF60 and the t_{ign} of 95% PRF60 + 5% by mole of a test species at stoichiometric conditions and a given temperature (T) and pressure (P)
MCP	micro-channel plate	γ	ratio of specific heats
NTC	negative temperature coefficient	ϕ	equivalence ratio
NVO	negative valve overlap		
PIE	photoionization efficiency		
PIMS	photoionization mass spectroscopy		
ppm	parts per million		

1. Introduction

The Low-Temperature Gasoline Combustion (LTGC) strategy, where combustion is initiated via compression-induced auto-ignition of dilute charge mixtures, can reduce nitrogen oxide (NO_x) and soot emissions while improving cycle thermal efficiency. The central challenge has been to achieve effective ignition control at low engine loads, where slow burn rates due to elevated dilution fractions and low in-cylinder temperatures can lead to partial burn or even misfire [1]. Proposed strategies to improve low-load auto-ignition control include intake air heating [2], exhaust valve re-breathing [3], spark-assist [4] and partial fuel stratification [5,6]. However, intake heating leads to large parasitic losses and is not practical for engine transients, spark ignition is ineffective at low loads under heavy dilution, and fuel stratification can increase soot and NO_x emissions due to the formation of locally rich regions.

A viable alternative is to use in-cylinder combustion or reformation of fuel injected during an auxiliary negative valve overlap (NVO) recompression period to heat the charge and alter reactivity characteristics [7–9]. Reformate speciation at the conclusion of the NVO period has been performed for a range of mixture stoichiometry, with energy analyses used to determine the tradeoffs among recovered chemical energy, NVO-period work, and NVO-period heat losses [9–11]. Moreover, it was demonstrated that partially oxidized species, when fed into the intake, can increase cycle thermodynamic efficiency through increased charge specific heat ratios [12].

For NVO periods with low amounts of excess oxygen (O_2), kinetically limited pyrolysis and partial oxidation reactions result in a reformate-rich product stream laden with small hydrocarbons, carbon monoxide (CO), and hydrogen (H_2). Reformate speciation was previously performed through dump sampling at the conclusion of the NVO period with sample characterization by gas chromatography (GC) [13,14]. Although GC can effectively measure the general classifications of hydrocarbon species present in the reformate, it is less accurate at quantifying isomers with similar column elution times that have been observed to have significantly different oxidation pathways [15]. That is, GC provides sufficient information to perform a chemical energy balance of the NVO-period injected fuel, but it does not provide the detail needed to accurately model the impact of the reformate on auto-ignition reactivity during the main period. Additionally, the previous work by the authors

[13,14] did not include experimental measurements of the influence of the reformate on main-period engine performance.

In this work, the impact of NVO reformate on main-period engine performance for four single-component surrogate gasoline fuels (*iso*-octane, *n*-heptane, ethanol, and 1-hexene) was evaluated using a custom alternate-fire sequence at a range of main-period injection mass. The NVO-period reformates for the four tested fuels, as well as cyclohexane and a blend of toluene/*n*-heptane, were separately characterized through detailed speciation using photoionization mass spectrometry (PIMS) with synchrotron-generated vacuum ultraviolet (VUV) light. A single-cylinder research engine equipped with a custom dump-valve sampling system was used for all experiments. An adiabatic, single-zone reactor model was used to evaluate the charge reactivity of the PIMS-measured reformates compared to the unreformed parent fuels (e.g. *iso*-octane) and to examine the factors influencing main-period engine performance.

2. Experimental

2.1. Single-cylinder research engine

Engine experiments were conducted in two parts: (1) main-period engine performance measurements and (2) dump-sampling of the NVO reformate with speciation by PIMS. An optically accessible single-cylinder research engine outfitted with a pent-roof cylinder head, central direct injection, and a flat-top piston was used for all experiments. The cylinder head has one exhaust and two intake valves. All-metal components replaced quartz windows and liners for the current experiments; crevice volumes are ~ 3 –4 times larger than a comparable production engine. The Bosch, step-hole, valve covered orifice injector has 8 nozzles and a 60° included angle. The 150 crank angle (CA) duration NVO recompression was centered around NVO top dead center (TDC_{NVO}), achieved by modifying the exhaust valve closure (EVC) and intake valve opening (IVO) events (geometric recompression ratio of 5.51:1). The modified valve timing along with the use of low-lift cams (3 mm lift) resulted in $\sim 46\%$ retained burned gases into the subsequent main portion of the cycle. Bulk temperatures and residual gas fractions (RGF) at EVC were calculated using a custom 1-D engine model previously described by Fitzgerald et al. [16]. The head surface temperature was monitored by an

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