

Analysis of Thermal and Chemical Effects on Negative Valve Overlap Period Energy Recovery for Low-Temperature Gasoline Combustion

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ABSTRACT

A central challenge for efficient auto-ignition controlled low-temperature gasoline combustion (LTGC) engines has been achieving the combustion phasing needed to reach stable performance over a wide operating regime. The negative valve overlap (NVO) strategy has been explored as a way to improve combustion stability through a combination of charge heating and altered reactivity via a recompression stroke with a pilot fuel injection. The study objective was to analyze the thermal and chemical effects on NVO-period energy recovery. The analysis leveraged experimental gas sampling results obtained from a single-cylinder LTGC engine along with cylinder pressure measurements and custom data reduction methods used to estimate period thermodynamic properties. The engine was fueled by either iso-octane or ethanol, and operated under sweeps of NVO-period oxygen concentration, injection timing, and fueling rate. Gas sampling at the end of the NVO period was performed via a custom dump-valve apparatus, with detailed sample speciation by in-house gas chromatography. The balance of NVO-period input and output energy flows was calculated in terms of fuel energy, work, heat loss, and change in sensible energy. Experiment results were complemented by detailed chemistry single-zone reactor simulations performed at relevant mixing and thermodynamic conditions, with results used to evaluate ignition behavior and expected energy recovery yields.

For the intermediate bulk-gas temperatures present during the NVO period (900-1100 K), weak negative temperature coefficient behavior with iso-octane fueling significantly lengthened ignition delays relative to similar ethanol fueled conditions. Faster ethanol ignition chemistry led to lower recovered fuel intermediate yields relative to similar iso-octane fueled conditions due to more complete fuel oxidation. From the energy analysis it was found that increased NVO-period global equivalence ratio, either from lower NVO-period oxygen concentrations or higher fueling rates, in general led to a greater fraction of net recovered fuel energy and work as heat losses were minimized. These observations were supported by complementary single-zone reactor model results, which further indicated that kinetic time-scales favor chemical energy-consuming exothermic oxidation over slower endothermic reformation. Nonetheless, fuel energy recovery close to the thermodynamic equilibrium solution was achieved for baseline conditions that featured 4% NVO-period oxygen concentration.

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INTRODUCTION

Low-temperature gasoline combustion (LTGC) engines that employ compression induced auto-ignition can achieve good emissions characteristics and excellent fuel economy through the use of staged, flameless combustion. Efficiency gains are achieved through reduced heat transfer, and pumping losses, along with increased thermal efficiency from higher compression and mixture specific heat ratios

[1, 2]. The main challenge has been to achieve stable combustion across a range of relevant engine speeds and loads, while keeping noise and emission characteristics at an acceptable level.

For elevated loads, indicated mean effective pressures (IMEP) of up to 10 bar have been achieved in naturally aspirated engines through the use of positive valve overlap (PVO) strategies that retain exhaust

thermal energy for the subsequent cycle through valve re-breathing [3]. Intake-pressure boost and partial fuel stratification, particularly with the use of ϕ -sensitive fuels, has likewise been used to extend high-load limits above 20 bar IMEP without engine knock [1, 4]. Furthermore, strategies such as spark-assisted compression ignition (SACI), where conventional spark ignition is used to initiate flame-propagation so that combustion phasing is optimized and combustion noise is modulated, have shown promise [3, 5, 6, 7, 8, 9].

Challenges likewise exist at low engine loads where poor combustion stability can lead to partial burns or misfires that adversely impact fuel economy along with carbon monoxide (CO) and hydrocarbon emissions [1]. To extend low-load stability limits, the negative valve overlap (NVO) strategy has been used to retain exhaust thermal energy for the subsequent cycle through modified valve lift and timing events that form a recompression stroke [10, 11]. Often an NVO-period pilot fuel injection is used to further heat the charge [9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24] or alter main-period reactivity and knock resistance through reformation or partial oxidation of the injected pilot fuel [11, 15, 16, 19, 23, 24, 25, 26, 27].

Resultant reformat products contain a mixture of exhaust gases with high concentrations of CO, hydrogen, and unburned hydrocarbons. The reformat-rich mixture can alter reactivity for LTGC or increase flame speeds for spark-ignited combustion; both features serve to extend dilution tolerances. An example is the dedicated exhaust gas recirculation (D-EGR) concept where a single engine cylinder uses fuel-rich combustion to create power along with a continuous stream of EGR laden with CO and hydrogen reformat to improve the knock-resistance of all cylinders [28]. Szybist et al. [29, 30] further pointed out that NVO-period reformat generated under oxygen deficient conditions can be used to increase the total available chemical fuel energy through the use of exhaust-heat driven endothermic reactions that convert the parent fuel into components with higher overall energy content. The so-called thermochemical recuperation process can offset NVO-period pumping losses [11] by transferring sensible exhaust thermal energy into available chemical energy for subsequent main-period combustion.

A key objective of the NVO-period reactions is to improve the overall cycle efficiency through some combination of extracted work and fuel energy, with minimal period losses. From a full-cycle perspective, work generated during the NVO period is more valuable than fuel energy since inevitable losses during main-period combustion must be considered. However, high losses are expected due to a combination of low compression ratios from non-optimal valve timings and poor thermodynamic efficiency that results from slow reaction rates [2]. Additional thermal energy at IVO will also negatively impact volumetric efficiency during induction. Other considerations include factors that impact main-period reactions such as the formation of reformat species and charge heating from fuel oxidation.

Despite the potential benefits and numerous studies, NVO-period reactions remain poorly understood. The current study objective was to analyze the thermal and chemical processes that impact NVO-

period energy recovery. The thermodynamic analysis presented here focused only on the closed portion of the NVO period; a full-cycle thermodynamic analysis similar to that performed by Dornotte et al. [31] for boosted LTGC will be addressed in a future study. The analysis leveraged experimental gas sampling results obtained from a single-cylinder LTGC engine. Gas sampling at end of the NVO period was performed via a custom dump-valve apparatus described by Steeper and Davisson [23], with detailed sample speciation by an in-house gas chromatograph (GC). Sampling data were complemented by cylinder pressure measurements, with data reduction algorithms used to estimate period thermodynamic properties. The engine was fueled by either iso-octane or ethanol, and operated under sweeps of NVO-period oxygen concentration, injection timing, and fueling rate. Net energy out in terms of fuel energy available for the subsequent period, NVO-period work, and the change in charge sensible energy was calculated at each operating condition. Complementary detailed chemistry single-zone reactor models were performed over relevant mixing and thermodynamic conditions, with results used to evaluate ignition characteristics and expected energy recovery yields across a range of initial equivalence ratios (ϕ) and temperatures under representative engine time scales.

APPROACH

Sandia Single-Cylinder LTGC Engine

An optically accessible single-cylinder research engine configured for LTGC operation was used for all experiments. All-metal components replaced quartz windows, since optical visualization was not required; a metal flat-top piston was retained. Relevant engine geometric characteristics are summarized in Table 1. The pent-roof cylinder head contains one exhaust and two intake valves along with a Bosch, step-hole, valve covered orifice (VCO) injector with 8-holes and a 70° cone angle that was mounted centrally as shown in Figure 1. Exhaust valve closing (EVC) and intake valve opening (IVO) mark the start and finish of NVO recompression, and occurred 75 crank angle degrees before and after NVO top dead center (CAD_{NVO}). Roughly 50% of the residual exhaust gases were retained. Head surface temperature was monitored by an embedded thermocouple placed into one of two available spark plug ports.

The dump valve had an 8 mm head diameter with a 3.2 mm lift, and was housed in a body that fits into the remaining 14-mm threaded spark-plug port. The sampling system consisted of a manifold connected to a vacuum evacuated, 1-liter, Teflon-lined, stainless-steel sample bottle; a schematic of the apparatus is illustrated in Figure 2. Solenoid-operated isolation and vacuum valves were used to minimize gas contamination from subsequent dump cycles and any potential engine blow-by across the dump-valve. All sampling system components were electrically heated to 90° C and insulated to avoid water and hydrocarbon condensation.

Table 1. Engine Specifications and Operating Conditions.

Displaced volume [liter]	0.633
Bore/Stroke [mm]	92/95.25
Compression ratio	11.3
Inlet Valve Open & Close	+75 CAD _{NVO} & -140 CAD _{MAIN}
Exhaust Valve Open & Close, EVO	+140 CAD _{MAIN} & -75 CAD _{NVO}
Residual Gas Fraction	~0.47
NVO Duration [CAD]	150
Valve Lift [mm]	3
Speed [RPM]	1200
Intake Air Pressure [kPa]	100
Fuel Pressure [bar]	100
Exhaust Excess O ₂ [%]	7, 5.5, 4, & 2.5
NVO (CAD _{NVO})	-65, -40, -10
NVO Injection Quantity [mg/cycle] Iso-octane Ethanol	0, 2, 4, 6, 8, 10 0, 3.3, 6.7, 10.1, 13.4, 16.8
NVO Injection Duration [CAD] Iso-octane Ethanol	0, 1.2, 1.4, 2.3, 2.9, 3.2 0, 1.3, 2.5, 3.2, 3.8, 4.3
NVO Injected Fuel Energy [J] Iso-octane Ethanol	0, 92.2, 184.4, 276.5, 368.7, 460.9 0, 95.4, 191.4, 289.1, 383.0, 478.7
Intake Temperature [°C] 7% Exhaust Excess O ₂ 5.5%, 4% & 2.5% Exhaust Excess O ₂	Iso-octane (Ethanol) 120 (N/A) 88 (93)
EVC Temperature [°C] 7% Exhaust Excess O ₂ 5.5% Exhaust Excess O ₂ 4% Exhaust Excess O ₂ 2.5% Exhaust Excess O ₂	Iso-octane (Ethanol) 432 (N/A) 452 (N/A) 478 (459) 494 (N/A)
Main SOI [CAD _{MAIN}]	-270
Main Fueling Quantity [mg/inj.] 7% Exhaust Excess O ₂ 5.5% Exhaust Excess O ₂ 4% Exhaust Excess O ₂ 2.5% Exhaust Excess O ₂	Iso-octane (Ethanol) 8.3 (N/A) 9.9 (N/A) 11.6 (19.4) 14.3 (N/A)

Iso-octane was used as a gasoline surrogate to simplify the NVO end-period speciation by the GC. Sampling and performance data were also acquired from the engine fueled by anhydrous ethanol. Main and NVO fuel injection rates were set using custom timings from a predefined calibration, with the total fuel injection quantity monitored by a Max Machinery Model 213 volumetric flow meter. The ethanol fueling rate was adjusted such that the total energy injected was equivalent to the corresponding iso-octane condition on a LHV basis. Relevant fuel characteristics are summarized in Table 2.

Table 2. Specifications for the iso-octane and anhydrous ethanol fuels.

Boiling Point [K] Iso-octane Ethanol	372.1 351.5
Heat of Combustion (Exergy) [J/mg] Iso-octane Ethanol	44.5 (46.09) 26.86 (28.56)
Density @ 15.56°C [g/mL] Iso-octane Ethanol	0.692 0.789
Research Octane Number Iso-octane Ethanol	100 108

The operating conditions replicated low-load engine operation where combustion stability can be problematic. The engine speed was set to 1200 RPM, with the intake air pressure fixed at 100 kPa to mimic naturally aspirated operation without throttling. The engine was operated under sweeps of NVO-period oxygen concentration, injection timing, and fueling rate as described in Table 1. To maintain an acceptable 3% gross IMEP coefficient of variation (CoV), the intake air temperature was fixed at 88°C. The exception was for the NVO period with 7% oxygen where to reach 3% gross IMEP CoV, the temperature had to be increased to 120°C. Engine specifications, fueling-rate schedules, and bulk-averaged equivalence ratios for each condition are listed in Table 1.

Port-fueled dimethyl ether injections were used to rapidly warm engine cylinder surfaces before being replaced by direct injections of iso-octane or ethanol. Total fueling rates were set to reach the desired exhaust oxygen concentration. Once cylinder wall temperatures (measured in the head) reached 127°C, the dump-cycle sequence illustrated in Figure 3 was activated. The sequence featured a custom NVO injection rate, no main injection, and activation of the dump-valve system shortly after IVO (-200 CAD_{MAIN} to 50 CAD_{MAIN}), before concluding with continuous motored cycles. Accordingly, the dump cycle collected a mix of end-period NVO mixtures and heated intake air. Dump-sampling was repeated until the sample bottle pressure exceeded atmospheric pressure (~6-8 dump samples). The engine was then stopped with the sample bottle isolated. Due to the unique nature of the NVO dump-cycle, exhaust-gas emissions measurements, lambda values, and main-period engine performance data for this cycle are unavailable. Bulk temperatures and residual gas fractions (RGF) at EVC were calculated using a custom 1-D engine model previously described by Fitzgerald et al. [32], that was validated over a wide range of NVO operation. The calculated RGF was used to account for charge composition due to intake air dilution. Peterson et al. [26] confirmed that exhaust gas speciation results were not significantly impacted by intake air scavenging.

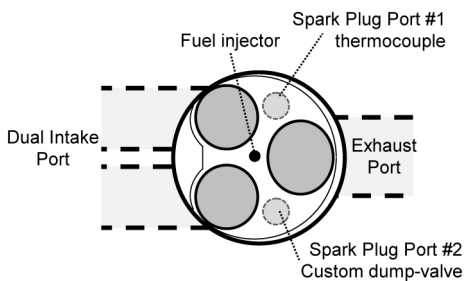


Figure 1. Pent-roof cylinder head valve, spark plug, and injector schematic.

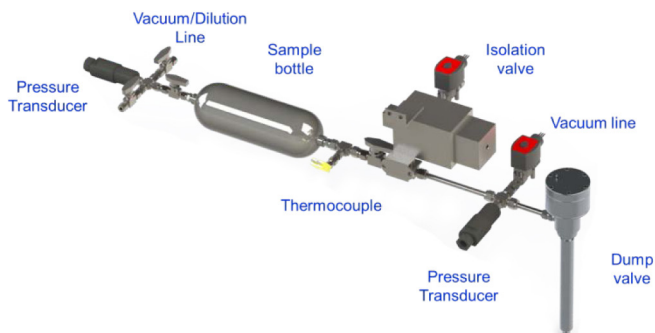


Figure 2. Illustration of the custom dump valve system and sample bottle.

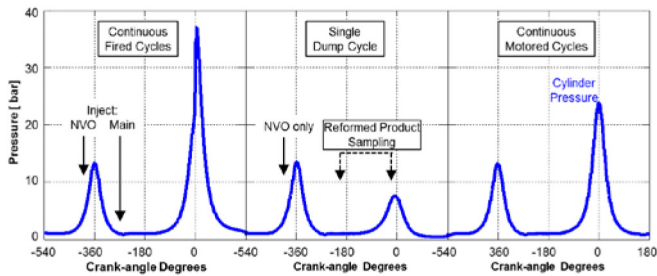


Figure 3. Description of dump-cycle-sequence.

The sample bottle was connected to a compact SRI Instruments Multi-Gas Analyzer #3 gas chromatograph (GC) that housed three gas column detectors capable of speciating a wide range of sample stream constituents. The first of two flame ionization detectors (FID#1) was connected to a Restek MXT-1 60 m capillary tube and was primarily used to identify large intermediate hydrocarbons. A second FID (FID#2) with a slower eluting 2 m Restek Haysep-D column was used to resolve smaller hydrocarbons (C_1 - C_2), with a methanizer used to detect CO and CO_2 . Note that FID#2 could not distinguish between acetylene (C_2H_2) and ethylene (C_2H_4) due to similar column elution times. Nonetheless, each species has a similar GC response, with the cumulative values reported here. A 2 m Restek Molecular Sieve-13x column that fed a thermal conductivity detector (TCD) was used to detect hydrogen and oxygen, and was connected in series to the FID#2 column. The gas sample characterization methodology was similar to the procedures described in [23], with an updated calibration gas mix based on detailed NVO-period speciation measurements obtained via photo-ionization mass spectrometry [33].

Single-Zone Modeling

To better understand the NVO-period energy balance - defined here as the relative change in period chemical energy, sensible energy, and work - single-zone reactor models were performed using Cantera; an open-source chemical modeling software run in the Matlab programming environment. Although in-cylinder conditions were neither well mixed nor isothermal, concentration maps over a range of equivalence ratio and temperature have been used by the authors in a previous paper [26] to explore in-cylinder regions conducive to forming intermediate gas species. Here, similar maps were generated from single-zone constant volume adiabatic models to help understand domains where NVO reforming can realistically yield the higher degrees of thermochemical recuperation. Modeling results were further used to better understand auto-ignition characteristics.

Constant volume reactor simulations were run over a range of relevant equivalence ratios ($\phi = 0.5$ –8) and initial temperatures (800–1100 K) using detailed Lawrence Livermore National Laboratory (LLNL) iso-octane [34] and ethanol [35] kinetics mechanisms. A thermodynamic equilibrium model and a kinetic model with an 8.3 ms residence time comparable to the NVO period were separately considered. All simulations had a constant initial 8 bar pressure, with initial mole fractions taken from experimental sampling data for both iso-octane and ethanol with 4% exhaust excess oxygen. Resultant species mole fractions, gas temperatures, and pressures were post-processed to calculate product chemical energy.

RESULTS AND DISCUSSION

Engine Performance Data

The NVO SOI considered included a -40 CAD_{NVO} baseline along with an advanced -65 CAD_{NVO} condition that occurred shortly after EVC and a -10 CAD_{NVO} retarded condition. The sweep was used to evaluate the influence of period residence time and mixing rates on heat release characteristics. Initial oxygen concentration and fueling rates were fixed at 4% and 6 mg/cycle respectively when the engine was fueled by iso-octane. For ethanol fueling, the injection quantity was increased to 10.1 mg/cycle so that fuel energy injected was equivalent as described earlier. Ensemble-averaged cylinder-pressure and AHRR traces are displayed in Figure 4, with reference traces for the condition without NVO fueling also included.

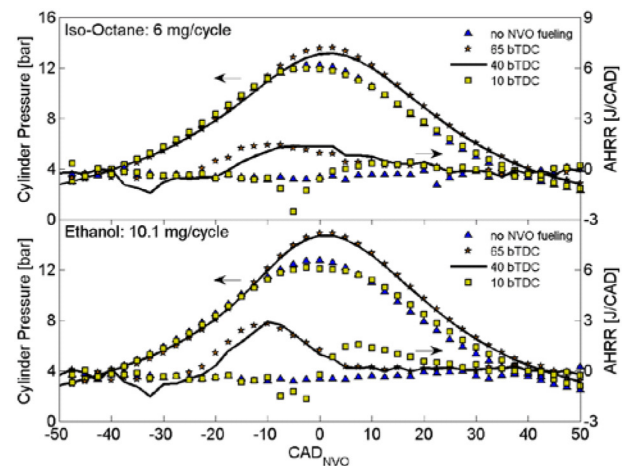


Figure 4. In-cylinder pressure and AHRR traces for a sweep of NVO SOI with 4% oxygen and the engine fueled by iso-octane (top) or ethanol (bottom).

As would be expected given the lack of available oxygen, slow NVO-period heat-release rates extended heat release over much of the period. For the advanced and baseline NVO SOI, the AHRR traces were relatively uniform regardless of fuel-type. For the retarded NVO SOI, slow reaction rates coupled with previously observed piston surface fuel spray impingement [23] limited oxidation opportunities. For all NVO SOI, ethanol fueling exhibited earlier NVO-period ignition relative to equivalent iso-octane conditions, with more substantial AHRR and a shorter duration of heat release.

Differences in NVO AHRR for the two fuels may result from iso-octane ignition being influenced by negative temperature coefficient (NTC) behavior, where ignition delay times increase with higher intermediate temperatures due to altered chain-branching chemistry [36]. To clarify the impact of NTC chemistry for the highly-dilute mixtures with globally-rich equivalence ratios, ignition delay times - defined here as the 10% burn time - were calculated at relevant conditions. Results for a range of ϕ are plotted in Figure 5 for isobaric (8 bar) simulations with an oxidizer stream composition matched to the 4% oxygen NVO-period speciation measurements.