

Investigation of Negative Valve Overlap Reforming Products Using Gas Sampling and Single-Zone Modeling

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ABSTRACT

Negative valve overlap (NVO) is a viable control strategy that enables low-temperature gasoline combustion (LTGC) at low loads. Thermal effects of NVO fueling on main combustion are well understood, but fuel reforming chemistry during NVO has not been extensively studied.

The objective of this work is to analyze the impact of global equivalence ratio and available oxidizer on NVO product concentrations. Experiments were performed in a LTGC single-cylinder engine under a sweep of NVO oxygen concentration and NVO fueling rates. Gas sampling at the start and end of the NVO period was performed via a custom dump-valve apparatus with detailed sample speciation by gas chromatography. Single-zone reactor models using detailed chemistry at relevant mixing and thermodynamic conditions were used in parallel to the experiments to evaluate expected yields of partially oxidized species under representative engine time scales. Modeling efforts help identify physical mechanisms that further describe experimental findings with regards to anticipated fuel-fraction and temperature fields.

For the NVO fueling sweep, end-cycle CO_2 concentrations remained essentially flat, while intermediate species concentrations rose as fueling rates increased. The rate-of-increase was most pronounced for the C_3 - C_4 hydrocarbons whose rate-of-increase was greater than the relative increase in fueling rate. Modeling results suggest that oxygen depleted environments coupled with lower heat release temperatures result in slower reforming rates, which yielded higher C_3 - C_4 production. For the oxygen concentration sweep with fixed NVO fueling, CO and CO_2 products increased as the amount of oxidizer likewise increased. These increases came at the expense of intermediate hydrocarbon yields.

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INTRODUCTION

Ambitious automotive fleet-wide CO_2 targets of less than 100 g/km (~ 54.5 mpg) in Europe by 2020 and in the US by 2025 have created increased demand for high-efficiency engines that can meet ever tightening air-quality standards while maintaining acceptable consumer price points. To meet these targets, the U.S. DRIVE (Driving Research and Innovation for Vehicle efficiency and Energy sustainability) partnership has established an overarching mission "to accelerate the development of pre-competitive and innovative technologies to enable a full range of efficient and clean advanced light-duty vehicles" [1]. Within U.S. DRIVE, the Advanced Combustion and Emission Control (ACEC) Tech Team has

established a stretch goal to improve engine efficiency 20% relative to a 2010 gasoline engine benchmark by 2020 through the removal of technical barriers.

Novel low-temperature gasoline combustion (LTGC) strategies have achieved excellent fuel economy while maintaining low engine-out emissions in research settings through the use of staged, flameless combustion modes. Reactivity Controlled Compression Ignition (RCCI) is a promising variant that uses a combination of gasoline and diesel-like fuels to customize charge reactivity across the engine speed/load map for optimal performance characteristics [2, 3, 4]. A main drawback is the requirement for separate fuel systems and injectors, which adds significant cost and complexity to the vehicle.

Accordingly, the most recent ACEC roadmap [1] calls for low-cost yet efficient onboard means of tailoring fuel properties. Traditionally this has been through onboard reformers that extract hydrogen from the parent fuel and seed it into the intake charge to extend achievable dilution rates [5]. However, large endothermic barriers for gasoline and diesel steam reformers require the use of oxidation catalysts [6] that can impose fuel economy penalties or require costly precious metal catalysts [7, 8] that may be subject to poisoning. While ethanol reformers have lower thermodynamic barriers that enable them to be driven by exhaust heat alone, ethanol fuel volume fractions of 25% or more are still required [9]. Alternatively, dedicated exhaust gas recirculation (D-EGR) strategies where a single engine cylinder is reserved to reform parent fuel components into lower heat capacity intermediates (i.e., carbon monoxide and hydrogen), which are then fed into the main intake charge to increase overall engine thermal efficiencies [10]. Challenges such as cylinder load balance and transient response have been addressed in a demonstrator vehicle [11]. While D-EGR eliminates the need for a second fuel system, it nonetheless increases engine complexity in ways that can limit the application of other high-efficiency strategies such as cylinder deactivation.

In-cylinder charge heating and fuel reformation via negative valve overlap (NVO) is another viable pathway. For the NVO strategy, residual combustion products from the previous cycle along with a fraction of the subsequent cycle's fuel are trapped through modified valve and injection timings and recompressed in a truncated exhaust stroke [12, 13]. NVO period reactions can impact main combustion in two important ways: (1) through a fairly well-understood combination of retained exhaust energy and fuel oxidation to elevate intake charge temperatures [12, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31], and (2) through a less understood chemical mechanism where fuel-rich reformation can produce intermediate hydrocarbon species with improved reactivity [18, 19, 20, 24, 26, 31, 32]. Steeper et al. [31] observed that for fuel-lean NVO with large amounts of excess oxygen in the exhaust, reactive intermediate production requires the presence of locally rich piston- or wall-spray interaction regions that may be difficult to control. Alternatively, enhanced charge reactivity has also been achieved in low-oxygen NVO environments through more controllable bulk-gas reformation [19, 33, 34], though the reaction details remain unknown.

There have only been a few documented attempts to model NVO period reactions [18, 20, 26, 35]. The earliest example is by Koopmans et al. [18] who used a single-zone Senkin model to identify the role of reaction intermediates on main combustion, but provided only sparse information on NVO period species concentrations. A few years later, engine performance data from Waldman et al. [19] were compared to sector mesh numerical results by Aroonsrisopon et al. [20] in complementary studies that examined sweeps of NVO-to-main injection splits and global equivalence ratios. For low-oxygen NVO environments ($\sim 3.8\%$), the authors attributed most of the main combustion phasing advance to reactivity enhancement effects from NVO period bulk-gas chemistry. In particular, Aroonsrisopon noted a substantial increase in formaldehyde, ethylene, and propene yields in their simulation results, although they did not indicate the relative importance of

each species on reactivity enhancement. More recently, detailed multi-zone simulations by Hessel et al. [35] verified the experimental findings by Fitzgerald et al. [26, 27] that for high-oxygen NVO environments ($\sim 7\%$) the thermal effects dominate. It should be noted that none of the cited numerical studies used detailed experimental speciation data to serve as input boundary conditions for the start of the NVO period at exhaust valve closure (EVC) or benchmark data at the end of the NVO period to compare against. This is an important detail, since Steeper and Davisson [31] have noted that even small intermediate hydrocarbon concentrations of certain species such as acetylene (hundreds of parts-per-million) can significantly alter charge reactivity.

Validation datasets of mixture composition are difficult to acquire during the NVO period since intermediate residuals are retained and consumed during the subsequent main combustion cycle. Laser-based absorption and fluorescence diagnostics have been successfully used to resolve charge temperatures and composition information for select species [22, 25, 27, 36, 37, 38], but are generally insufficient for comprehensive mixture speciation. More recently, direct sampling experiments with follow-on sample analysis by either Fourier transform infrared spectroscopy (FTIR) or gas chromatography (GC) diagnostics has been an effective tool to comprehensively clarify the NVO chemistry details [31, 33, 34, 39, 40]. These methods hinge on the application of suitable gas-sampling systems that are free of biases from quenching or mixture stratification. A recent series of engine experiments have performed detailed measurements of NVO end-product constituents through the use of custom macro-gas sample valve systems [31, 33, 34] in conjunction with either FTIR or GC diagnostics.

The goal of the present study is to enhance the understanding of the NVO reaction chemistry through a combination of controlled engine experiments over sweeps of NVO period oxygen concentration and fueling rates. Macro gas sampling was performed both before and after the NVO period, with samples analyzed by a 3-column GC. Results from detailed chemistry homogeneous reactor models of representative mixtures and initial temperatures during the NVO period were used to augment the analysis. The modeling analysis helps identify mixing and thermodynamic environments that yield the formation of key intermediate species identified in the gas sampling experiments. In-cylinder pressure and NVO apparent heat release rate curves are evaluated to understand the mixture reactivity during NVO to support trends presented in the gas sampling findings. Performance characteristics of the engine during main combustion are not presented due to the dump-valve sampling procedure (i.e. gas is sampled during intake and compression so that main combustion does not take place during sampling), but rather the results focus on analyzing the production yields for different intermediates for the sweeps of NVO oxygen concentrations and NVO fueling rates.

APPROACH

Engine

A single-cylinder optical engine configured for LTGC operation was used for the sampling experiments. For the duration of the experiments, metal parts replaced all quartz components. The cylinder head has a

pent-roof design that contains three valves (two intake, one exhaust), along with a centrally mounted 8-hole injector orientated vertically toward a flat-top piston (see Figure 1). An embedded thermocouple in one of two spark plug ports was used to monitor head surface temperature, while the other spark plug port housed a custom dump-valve assembly described in the following section. Engine specifications are shown in Table 1.

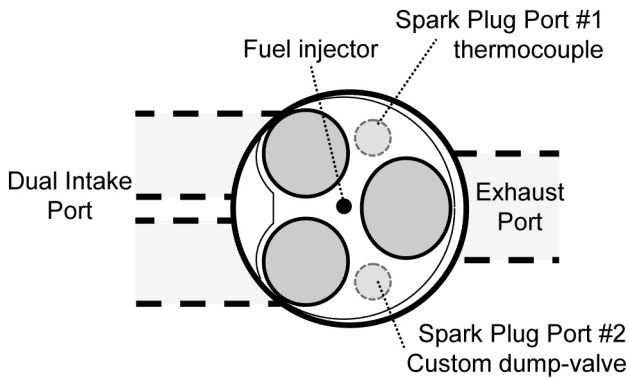


Figure 1. Schematic of the pent-roof cylinder head valve, spark plug, and injector arrangement.

A low pressure (4 bar) injector was used upstream of the intake port to introduce dimethyl ether (DME) into the engine so that reliable compression-ignition could be established when initially firing the engine. The exhaust valve closing (EVC) and intake valve opening (IVO) events occurred 75 crank angle degrees (CAD) on either side of TDC_{NVO} to retain roughly 50% of the residual exhaust gases. To simplify sample gas speciation and facilitate modeling, iso-octane was selected as a surrogate fuel for gasoline. The amount of iso-octane injected was controlled by selecting the injection duration which was measured by a Max Machinery Model 213 flow meter.

Experiments were performed to analyze the NVO gas composition with respect to a sweep of oxygenated environments and NVO fueling rates. For the oxygenated NVO environment sweep, the main injection fueling rates were varied by adjusting the injection duration (14.3, 11.6, 9.9, 8.3 mg/cycle) to produce the desired EVC oxygen concentration (2.5%, 4.0%, 5.5%, 7.0% O₂, respectively). For each condition, a fixed injection pressure (100 bar), NVO fueling rate (6 mg/cycle) and start-of-injection (SOI) for both the main (−270 CAD_{MAIN}) and NVO period (−40 CAD_{NVO}) was maintained. The exhaust stream oxygen concentration was measured by a lambda sensor (ECM OXY 6200-2) located in the exhaust manifold. Intake temperature was held constant at 88°C, except for the 7.0% O₂ case where it was increased to 120°C to maintain combustion stability and reach the target cylinder wall temperature of 127°C. For NVO fueling rate sweeps, the main-cycle fueling rate was fixed at 11.6 mg/cycle (4.0% O₂ environment), with NVO fueling rates varied from 0 to 10 mg/cycle in 2 mg/cycle increments to analyze the impact of NVO period stoichiometry on intermediate species production. Engine specifications and operating conditions used in the sampling experiments along with NVO period fueling rates, oxygen concentrations, and bulk-averaged equivalence ratios for each condition are listed in Table 1.

Table 1. Engine Specifications and Operating Conditions.

Displaced volume [liter]	0.633
Stroke [mm]	95.25
Bore [mm]	92
Compression ratio	11.3:1
Number of Valves	3 (2 intake, 1 exhaust)
Inlet Valve Open, IVO	+75 CAD _{NVO}
Inlet Valve Close, IVC	−140 CAD _{MAIN}
Exhaust Valve Open, EVO	+140 CAD _{MAIN}
Exhaust Valve Close, EVC	−75 CAD _{NVO}
NVO Duration	150 CAD
Valve Lift [mm]	3
Speed [RPM]	1200
Intake Air Temperature	88°C (120°C for 7.0% O ₂ at EVC)
Intake Air Pressure	100 kPa
Fuel, Fuel Pressure	Iso-octane, 100 bar
Main SOI	−270 CAD _{MAIN}
NVO SOI	−40 CAD _{NVO}
NVO Fueling Sweep (4% O ₂ at EVC) Global NVO Equiv. Ratio	0, 2, 4, 6, 8, 10 mg/cycle $\phi = 0.01, 0.73, 1.37, 2.00, 2.63, 3.23$
NVO O ₂ Sweep (NVO fueling: 6.0 mg) O ₂ % at IVC Global NVO Equiv. Ratio	8.3, 9.9, 11.6, 14.3 mg/cycle O ₂ = 7.0%, 5.5%, 4.0%, 2.5% $\phi = 1.10, 1.53, 2.13, 3.46$

Gas-Sampling System

Micro-gas sampling devices have been used previously to characterize NVO cylinder contents [40]. However, these devices are subject to external quenching processes that can introduce measurement uncertainty. Furthermore, the devices capture only a localized portion of the cylinder contents, which can supply incomplete information for a stratified charge. Instead we have used a custom solenoid actuated dump valve assembly, described by Steeper and Davisson [31], to scavenge a significant fraction of the cylinder contents into an evacuated stainless sample cylinder.

The custom dump valve (illustrated in Figure 2) was designed to operate in a conventional 14-mm threaded spark-plug port. The dump valve has an 8 mm head diameter and 3.2 mm maximum valve lift. An automotive valve spring and retainer sit atop the valve stem next to a 3/16" Swagelok fitting that provides a passage for the sampled gas. Solenoid-operated isolation and vacuum valves were activated before each sampling event to minimize gas contamination that may have leaked into the system. A gas manifold connected the dump valve to a 1-liter, Teflon-lined, stainless steel sample bottle. Prior to gas sampling, the gas manifold and sample bottle were evacuated to a pressure of 0.505 kPa, which was measured with a pressure transducer placed on the opposite end of the sample bottle. The manifold, sample bottle, and gas line components were insulated and equipped with electric tape heaters to maintain the sample temperature at 90°C so that condensation of water and heavier hydrocarbons was avoided. Further details about the sampling apparatus can be found in Steeper and Davisson [31].

The sample bottle was connected to a compact SRI Instruments Multi-Gas Analyzer #3 gas chromatograph (GC) machine that housed three gas columns and detectors capable of speciating a wide range of sample stream constituents. The first of two flame ionization detectors (FID#1) was connected to a 60 m capillary tube (Restek MXT-1) to identify large intermediate hydrocarbons (HC) from iso-octane combustion. The second FID (FID#2) and a thermal conductivity detector (TCD) were mounted in series on a pair of packed columns (2-m Restek Haysep-D and 2-m Restek Molecular Sieve-13x). FID#2 was equipped with a methanizer to detect CO and CO₂, and was further able to detect smaller hydrocarbons (C₁-C₂) that were insufficiently resolved by the faster eluting column used by FID#1. Ultra-pure nitrogen was used as the GC carrier gas, which enabled the detection of hydrogen within the TCD detector. Identification and calibration of each gaseous species of interest was similar to the procedure described in [31]. The only difference was that each calibration gas was heated to the 90°C temperature sample bottle to eliminate the need for a calibration species temperature correction during post-processing.

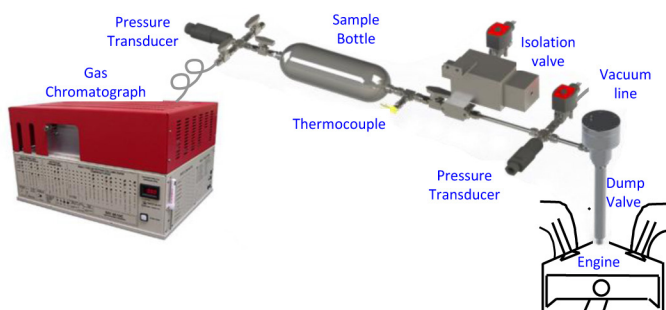


Figure 2. Experimental setup of custom dump valve system, sample bottle, and gas chromatograph for sampling experiments.

Gas Sampling Collection

The engine was operated at 1200 RPM at low-load compression-ignition conditions. During engine warm-up, port-fuel injections of DME were used to quickly heat cylinder surfaces. Once cylinder wall temperatures exceeded 120°C the port fueled DME injections were cut, with the engine instead fueled by direct-injections of iso-octane. The direct-injection system operated with a constant main and NVO fueling rate. The main fueling rate was selected to provide a desired exhaust O₂ concentration, while NVO fuel injection was 2 mg/cycle to provide an initial firing sequence with iso-octane.

The engine operated with this initial firing sequence until cylinder wall temperatures reached 127°C, at which point the dump-valve cycle sequence was activated. The dump-valve cycle sequence consisted of two engine cycles (illustrated in Figure 3); the first cycle preserved the main fueling rate, with NVO fueling set to the desired rate (i.e. 0 - 10 mg/cycle). For the second cycle, the dump valve was activated and the in-cylinder gas contents were scavenged into the sample bottle during the intake and compression stroke of the proceeding cycle. At this point, main and NVO fueling were automatically cut and the engine was transitioned to motored operation. The process was repeated multiple times until the sample bottle pressure reached ~110 kPa. Because the dump-valve was activated to sample the in-cylinder contents during the compression

stroke of the proceeding cycle, main combustion did not take place following the NVO cycle of interest. For this reason, the focus of this work is not to investigate the performance characteristics of the engine, but rather to investigate the production yields for different intermediates for different NVO oxygenated environments and NVO fueling rates.

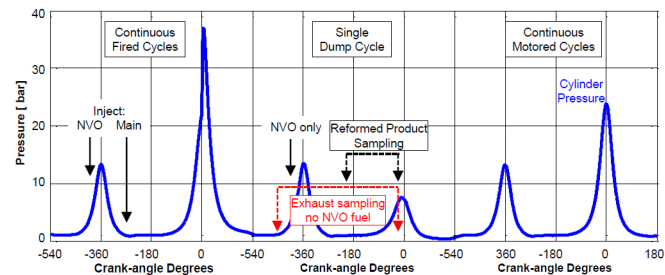


Figure 3. Description of dump-valve cycle-sequence.

The aforementioned dump-valve cycle sequence was performed for two separate sampling operations: (1) exhaust gas sampling from main combustion and (2) reformed product sampling from NVO. Exhaust sampling from main combustion allowed the gas composition prior to NVO compression to be characterized, which aided in identifying initial conditions for chemistry modeling efforts. Dump-valve actuation started at $-135 \text{ CAD}_{\text{NVO}}$ and continued until $-50 \text{ CAD}_{\text{MAIN}}$ (i.e., 445 CAD or 62 ms at 1200 RPM), while the NVO and main injection were suspended during the sample cycle. Approximately five dump-valve sampling events of exhaust gas were performed at each operating condition in order to fill the 1-liter sample bottle to 110 kPa. For the NVO products sampling sequence, dump-valve activation started during the second cycle from -200 to $-50 \text{ CAD}_{\text{MAIN}}$ (i.e., 150 CAD or 21 ms at 1200 RPM), while main fuel injection was suspended during the sample cycle. Roughly ten dump-valve sampling events of the NVO products were needed to fill the sample bottle. The charge composition was diluted by fresh intake charge for both operations. Concentrations determined from the GC were divided by the residual gas fraction to represent species concentrations indicative of those found before IVO. Both sampling operations were separately performed at each operating point.

Once the sample bottle was filled to ~110 kPa, the engine was stopped and the GC analysis commenced. To ensure the 2 ml GC sample loop was completely free of residual air, roughly 25 ml of sampled gas was pulled through the sample loop before the last 2 ml of sample was automatically isolated and injected into the GC columns. Each run required 33 minutes to analyze and the slightly positive sample bottle pressure allowed for three runs.

Additional tests for exhaust gas sampling were performed to assess the differences of sampling with and without intake air dilution. For this operation, both NVO and main fuel injection were suspended during the sample cycle. For sampling without intake air dilution, the dump valve was activated from $-135 \text{ CAD}_{\text{NVO}}$ until $-10 \text{ CAD}_{\text{NVO}}$ (i.e. 125 CAD or 17.35 ms) during what would be identified as part of the NVO duration. A comparison of these sampling operations helps identify any systematic errors caused by the dump-valve sampling system or sample timing. For example, the dump-valve timing can change the effective in-cylinder conditions during intake to not only