

Negative Valve Overlap Reforming Chemistry in Low-Oxygen Environments

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ABSTRACT

Fuel injection into the negative valve overlap (NVO) period is a common method for controlling combustion phasing in homogeneous charge compression ignition (HCCI) and other forms of advanced combustion. When fuel is injected into O₂-deficient NVO conditions, a portion of the fuel can be converted to products containing significant levels of H₂ and CO. Additionally, other short chain hydrocarbons are produced by means of thermal cracking, water-gas shift, and partial oxidation reactions. The present study experimentally investigates the fuel reforming chemistry that occurs during NVO. To this end, two very different experimental facilities are utilized and their results are compared. One facility is located at Oak Ridge National Laboratory, which uses a custom research engine cycle developed to isolate the NVO event from main combustion, allowing a steady stream of NVO reformat to be exhausted from the engine and chemically analyzed. The other experimental facility, located at Sandia National Laboratories, uses a dump valve to capture the exhaust from a single NVO event for analysis. Results from the two experiments are in excellent trend-wise agreement and indicate that the reforming process under low-O₂ conditions produces substantial concentrations of H₂, CO, methane, and other short-chain hydrocarbon species. The concentration of these species is found to be strongly dependent on fuel injection timing and injected fuel type, with weaker dependencies on NVO duration and initial temperature, indicating that NVO reforming is kinetically limited. Further, NVO reforming does not require a large energy input from the engine, meaning that it is not thermodynamically expensive. The implications of these results on HCCI and other forms of combustion are discussed in detail.

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INTRODUCTION

One of the reasons that HCCI combustion has not been realized in a production vehicle is that it is difficult to control, effectively postponing realization of the combustion mode's promise of simultaneous high thermal efficiency with low engine-out emissions. One technique that is capable of exercising some control over HCCI combustion is to use either a single or multi-pulse direct injection (DI) of fuel into the re-compressed residuals of an NVO valve strategy. When NVO fueling is employed, the fuel injection timing and NVO duration are highly effective means of controlling the phasing of the HCCI combustion event [1, 2, 3, 4, 5, 6, 7, 8].

While it's clear that exothermic oxidation reactions are an important part of the chemistry that occurs when NVO fueling is employed, the full range of fuel chemistry that occurs isn't fully understood. Arning et al. [4] concluded that fuel injection was able to control HCCI combustion because this controlled the extent of oxidation reactions in the NVO, thereby changing the start of compression temperature. Fitzgerald and Steeper [7] have also reported significant heat release from fuel injection into the NVO period with a pilot injection. They also showed the main combustion event is affected by the chemical species formed in the NVO, in particular formaldehyde and ethylene. Optical engine results by Berntsson and Denbratt [9] also showed significant interaction between main combustion phasing advance and NVO formaldehyde formation.

The NVO conditions in the aforementioned studies were fuel-lean, thus providing sufficient available O_2 for oxidation reactions to proceed. However, there are other NVO conditions where very low- O_2 , fuel-rich conditions can be present. For example, in order to expand the high load limit of HCCI, a number of researchers have investigated a stoichiometric NVO combustion mode that uses a spark-ignition event to initiate combustion followed by a volumetric HCCI-like heat release [10, 11, 12, 13, 14] (a regime known both as spark-assisted HCCI (SA-HCCI) and spark assisted compression ignition (SACI)). Despite this regime's lack of available O_2 , fuel injection timing into the NVO continues to play a dominant role on the combustion phasing of the main combustion event [12]. Under these fuel-rich conditions the NVO chemistry is not well understood.

Improving the understanding the fuel-rich chemistry that occurs during the NVO period under fuel rich conditions has implications beyond the HCCI and SA-HCCI modes of combustion. Alger and Mangold [15] reported on a dedicated exhaust gas recirculation (D-EGR) concept where they converted one cylinder of a multi-cylinder engine to operate under fuel-rich conditions to produce a reformat stream with significant concentrations of CO and H_2 . The dedicated cylinder reformat is exhausted to the intake of the remaining cylinders and consumed under spark-ignited (SI) combustion conditions. The combination of exhaust gas recirculation (EGR) and reformed fuel offers improved anti-knock characteristics and improved dilution tolerance. These characteristics combine to enable an increase in compression ratio, resulting in up to a 10% reduction in fuel consumption [15].

Using reformat to improve the anti-knock characteristics and dilution tolerance of the fuel is not new. There are numerous reports where researchers have observed that the higher flame speed of reformat containing H_2 and CO mixture helps to extend the lean burn regime of SI engines [3, 16, 17, 18, 19]. In addition, Topinka and coworkers [16] have observed that the knock limit of the resulting mixture is extended by reducing the autoignition tendency of the mixture. Thus, the fuel properties of the reformat product from fuel-rich chemistry are advantageous and can be exploited with well-understood engine technologies for improved efficiency, such as dilute SI combustion and increased compression ratio.

The present study investigates NVO reforming chemistry through direct sampling and analysis of NVO product species during fired engine operation. The results from two very different engine cycles and facilities are compared. At Oak Ridge National Laboratory (ORNL), a unique 6-stroke engine cycle has been developed that continually exhausts gases following NVO recompression, enabling real-time chemical analysis. Experiments examine a range of operating conditions including multiple parent fuels and varying excess O_2 content, charge temperature, and NVO fuel injection timing.

To confirm the ORNL experimental results, and to extend their applicability to alternative engine configurations, collaborative experiments have been performed at Sandia National Laboratories (SNL). At SNL, NVO gas samples can be captured during conventional 4-stroke operation using a custom dump valve and then analyzed off-line [20]. For the collaboration, results from SNL experiments at similar operating conditions are compared with ORNL data to gain added insight into NVO reforming chemistry.

EXPERIMENTAL APPROACH

This experimental section first describes the ORNL experimental setup and methodology, followed by the SNL experimental setup.

ORNL Experimental Setup

This engine is used to investigate NVO thermo-chemical interactions with 4 single-component fuels at 5 NVO durations and 6 NVO injection timings with 3 different start of NVO thermo-chemical compositions. A highly modified 2.0L GM Ecotec SI engine with stock DI fueling system and an aftermarket port fuel injection (PFI) fueling system is used for the ORNL experiments. The engine geometry is listed in [Table 1](#). Three of the cylinders of the production engine are disabled to allow single-cylinder operation and a custom piston is installed to increase compression ratio to 11.85 (stock 9.2). The engine is equipped with a small research module hydraulic valve actuation (HVA) system from Sturman Industries to enable fully variable valve actuation. To accommodate the HVA system, the cylinder head has been machined, disabling the functionality of the production cam and fuel pump systems.

This engine is operated with a laboratory air handling system. Pressurized and dried facility air containing less than 5% relative humidity is metered to the engine using a mass air flow controller. Separate electro-mechanical valves for backpressure and external EGR enable independent control of intake manifold pressure, exhaust manifold pressure, and EGR. Cooled EGR mixes with fresh air upstream of an air heater, followed by the intake plenum and then the intake manifold. EGR is measured using an EGR 5230 system from ECM, a non-intrusive method that utilizes pressure-compensated wideband O_2 sensors in both the intake and exhaust. When cooled EGR is used, a constant rate of $20 \pm 1\%$ is supplied.

Crank-angle (CA) resolved data is recorded at 1800 samples per revolution (0.2 CA resolution). Cylinder pressure is measured using a spark-plug-integrated piezo-electric pressure transducer from Kistler. Additionally, the DI command signal and intake and exhaust valve lift from each of the four HVA valves is recorded on a crank-angle resolved basis. All indicated results presented in this study represent 300-cycle ensemble averages.

Table 1. Engine geometry.

Bore x Stroke [mm]	86 x 86
Conrod length [mm]	145.5
Compression ratio [-]	11.85:1
Fuel injection systems	1. Side-mounted DI 2. Port fuel injected

Emissions from the spark-ignited (SI) combustion event are measured using a standard emissions bench. NO_x is measured using a heated chemiluminescence analyzer, CO and CO_2 are measured using infrared analyzers, O_2 is measured using a paramagnetic analyzer and unburned hydrocarbon (HC) emissions are measured with a heated flame ionization detector. Smoke measurements are performed using an AVL 415S smoke meter. Exhaust fuel-air equivalence ratio (ϕ) is both calculated from the emissions bench and measured with an automotive wideband O_2 sensor in the exhaust. All emissions but H_2 from the fuel-rich NVO event are measured using a Fourier Transform Infrared (FTIR) instrument from MKS. H_2 is measured using a magnetic sector capillary-inlet mass spectrometer from VTI Instruments.

Two Coriolis-effect mass flow meters are used to separately measure fuel flow rate for the PFI and DI fueling systems. Fuel-rail pressure for the DI fueling system is regulated to a constant 100 bar using a fuel system external to the engine utilizing a closed-loop electro-pneumatically-controlled pressure regulator. Fuel for the PFI fueling system is maintained at 5 bar. The temperature of the engine coolant and the oil are held constant at 90°C , and the intake manifold temperature is maintained to a constant temperature of 52°C regardless of the presence of EGR.

ORNL Experimental Methodology

To study the chemical species formed during the NVO period, an unconventional 6-stroke engine cycle has been developed. The additional 2-strokes are possible with this engine because there is no mechanical linkage between the crankshaft and the HVA valve train. The modified engine cycle (depicted in Figure 1) uses an SI combustion event to set up an NVO event where a portion of hot exhaust gases are recompressed and fuel is injected in a manner relevant to HCCI and SA-HCCI combustion strategies. However, the additional stroke enables the NVO products to be independently exhausted to a chemical analysis train instead of being consumed by a subsequent combustion event. Thus, the 6-stroke engine cycle is used as a research methodology and is not being proposed as a production-intent engine cycle for automotive applications.

As illustrated in Figure 1, the 6-stroke engine cycle starts at -360°CA after firing top dead center (aTDC_f) with a conventional SI intake stroke of air and fuel. The PFI system is used to deliver fuel for the SI combustion event, and a typical closed-valve fueling strategy is used to deliver this fuel at a timing of approximately -150°CA aTDC_f. Since the NVO and SI combustion events are de-coupled, the combustion phasing of the SI event can be independently controlled by spark timing as EGR level and equivalence ratio vary. Spark timings between -30 and -15°CA aTDC_f are used to maintain CA50 phasing for Conditions 1-3 (Table 2).

Table 2. Experimental SI and corresponding NVO conditions.

	SI Φ (-)	SI EGR (%)	NVO O_2 (%) [*]	NVO T_{EVC}
Condition 1	1	0	~ 0.4	High
Condition 2	1	20	~ 0.4	Low
Condition 3	0.8	0	~ 4.0	Low

^{*} O_2 concentration on a wet basis

The short exhaust event beginning at 170°CA aTDC_f traps a portion of the hot SI combustion products, enabling NVO recompression. During recompression, fuel can be injected into the trapped exhaust with the DI fueling system. Following NVO, reformed products are then exhausted to a chemical analysis train including the FTIR and capillary-inlet mass spectrometer.

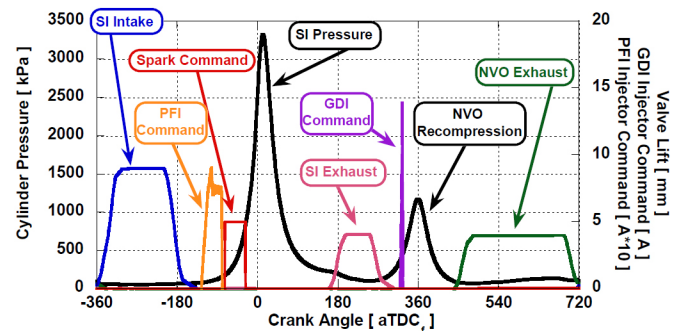


Figure 1. The 6-stroke engine cycle that has been developed to research NVO chemistry.

The two exhaust events depicted in Figure 1 utilize different engine exhaust valves that are controlled independently. NVO duration is investigated parametrically by sweeping SI exhaust valve closing timing and NVO exhaust valve opening timing. To isolate the SI combustion exhaust from the NVO reformat, the engine's exhaust port has been fitted with a divider that directs the flow from each valve to a separate exhaust runner as shown in Figure 2.

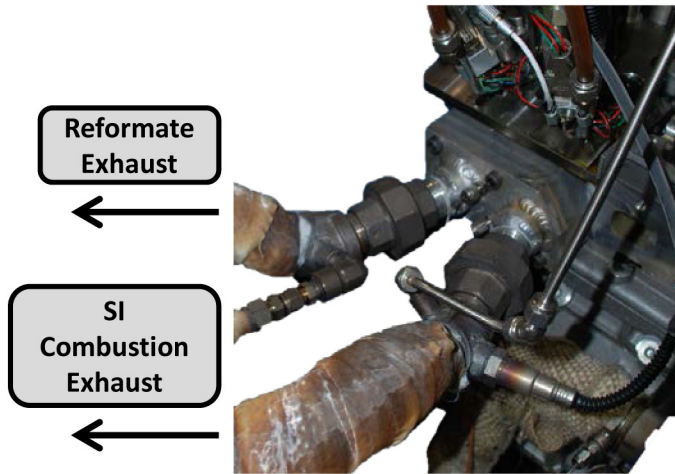


Figure 2. Partitioned product streams from the SI combustion and NVO reforming events.

The two separate exhaust streams are preconditioned prior to measurement. The SI combustion exhaust passes through heated sample lines and filters held at a constant temperature of 190°C prior to the emissions bench. The NVO exhaust gases are pulled through a heated filter and sample line at 190°C, and the FTIR sample cell is also heated to a constant 190°C. To prevent water or hydrocarbon condensation in the inlet capillary of the mass spectrometer, the NVO sample stream is pre-treated by pulling it through a 2-stage condensation trap. The first stage is an ice water bath (0°C), where the majority of the water and hydrocarbons are removed. The second stage is a mixture of dry ice and acetone (−78°C), where the remaining water and condensable hydrocarbons are removed. A schematic of the experimental setup is shown in Figure 3.

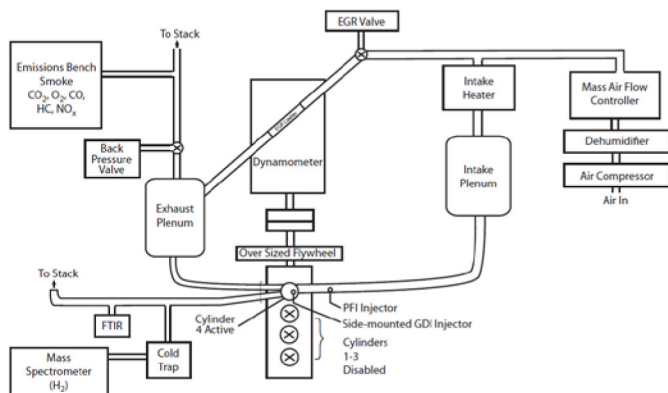


Figure 3. Schematic of experimental setup.

DI fuel injection timing is swept during the NVO event while maintaining a constant SI combustion CA50 of 8-9 CA aTDC_r. The DI fuel injection timing increments consist of a baseline NVO event (no DI fuel injected) and an injection at 310, 320, 330, 340, 350, or 370 CA aTDC_r. The DI fuel energy is held constant at approximately 220 J/cycle resulting in corresponding changes to the injected mass of each fuel.

There is no backpressure applied to the SI combustion exhaust, and as a result, the pressure at the start of the NVO is approximately 1 bar for all conditions.

Start of NVO temperature and O₂ concentration are varied by controlling SI combustion event equivalence ratio and external EGR rate. Table 2 shows the three different SI/start of NVO conditions investigated.

The quantity of PFI fuel supplied is set at 17.3 mg/cycle (740 J/cycle) when no fuel is injected during NVO. Since the operating conditions listed in Table 2 change in the ratio of specific heats, the fixed SI fueling rate varies the gross mean effective pressure (IMEP_g) between 540 and 575 kPa. When fuel is injected into the NVO, it is necessary to reduce the PFI fuel quantity in order to maintain the desired SI equivalence ratio. This is because the internal residuals from the NVO, which contain high concentrations of reformed fuel, are communicated to the subsequent SI combustion event.

ORNL Fuels Investigated

The fuel introduced with the PFI fueling system for the SI combustion event in the present study is an Unleaded Test Gasoline with a research octane number of 96 from Chevron-Phillips Chemical Company with a product name of UTG-96. The properties of UTG-96 are listed in Table 3

Table 3. Fuel properties of gasoline used for PFI fuel injection.

Fuel Property	Test Method	UTG-96
Research Octane Number [-]	ASTM D 2699	96.1
Motored Octane Number [-]	ASTM D 2700	87
Antiknock Index {(R+M)/2} [-]	N/A	91.6
C [wt%]	ASTM D 240	86.5
H [wt%]	ASTM D 240	13.5
Stoichiometric Air-Fuel Ratio [-]	N/A	14.55
Specific Gravity [-]	ASTM D 4052	0.740
Lower Heating Value [MJ/kg]	ASTM D 240	42.8
Reid Vapor Pressure [psia]	ASTM D 5191	9.0

The fuels injected into the NVO event with the DI fueling system in the present study are: iso-octane, iso-butanol, ethanol, and methanol. The iso-octane, iso-butanol, and methanol are reagent grade (obtained from Sigma-Aldrich) with purity >99%. The Decon Labs ethanol is chemically pure (200 proof). The fuel properties for these chemicals, shown in Table 4, are taken from previously reported values in the open literature with references appearing in the table.

Table 4. Properties of fuels injected into the NVO event.

	MeOH	EtOH	i-C ₄ H ₁₀ O	i-C ₈ H ₁₈
LHV [MJ/kg]	20.0 [21]	26.9 [21] 26.8 [22]	33.1 [22]	44.3 [21]
C [wt%]	37.5	52.2	64.9	84.2
H [wt%]	12.5	13.0	13.5	15.8
O [wt%]	50.0	34.8	21.6	0
Research Octane Number [-]	106 [21]	107 [21] 109 [22]	105 [22]	100 [21]
Motor Octane Number [-]	92 [21]	89 [21] 90 [22]	90 [22]	100 [21]
Anti-knock Index $\{(R+M)/2\}$ [-]	99.0	98.0 [21] 99.5 [22]	97.5	100.0
Latent Heat of Vaporization [kJ/kg]	1103 [21]	919.6 [22]	646.4 [22]	308 [21]

SNL Experimental Setup

Sandia's gasoline low-temperature combustion facility houses a single-cylinder optical research engine configured with metal components for the NVO sampling experiments. The three-valve, pent-roof head is equipped with a central, vertical direct injector and two peripheral spark-plug ports. One of the plug ports houses a custom dump valve for capturing NVO samples. The second houses a spark plug, although in these experiments, combustion is primarily initiated by compression ignition. Fuel injection is split between NVO and main portions of the 4-stroke cycle. Further specifications of the setup are listed in Table 5.

Table 5. SNL engine specifications and operating conditions. (Crank angles labeled as in Figure 1.)

Displacement	0.633 liter
Bore	92 mm
Stroke	95.25 mm
Effective Compression Ratio	11.3
Intake Valve Opening	+435 CA aTDC _i
Intake Valve Closing	-140 CA aTDC _i
Exhaust Valve Opening	+140 CA aTDC _i
Exhaust Valve Closing	+285 CA aTDC _i
NVO duration	150 CA
Speed	1200 rpm
Intake air temperature	361 K
Intake air pressure	100 kPa
Intake air flow	~240 mg/cycle
Coolant temperature	363 K
Fuel	Iso-octane
Fuel pressure	10 MPa
Fuel inject: NVO / Main	6.0 / 13.6 mg/cycle

The design of Sandia's dump valve mimics a conventional engine valve but with a scaled-down head diameter of 8 mm and lift of 3.2 mm. During steady firing, a solenoid actuates the dump valve at intake valve closing to vent a large fraction of cylinder contents for a single cycle. The sample is captured in a heated and initially evacuated, 1-liter sample bottle. This process is repeated several times until bottle pressure is about 1 bar. The final sample comprises a cycle-averaged specimen of NVO reformat gases diluted with intake air.

Speciation of the samples is performed using a gas chromatograph equipped with 3 columns, 2 flame-ionization detectors, and a single thermal-conductivity detector. Quantified species of interest include C1 through C8 hydrocarbons, H₂, H₂O, CO₂, CO, and O₂. A more complete description of NVO sampling and analysis conducted at SNL is provided in reference [20].

To facilitate data comparison, the SNL experiments duplicate a subset of ORNL operating conditions. The fuel used is iso-octane, and, as for Condition 3 of Table 2, the exhaust equivalence ratio is adjusted to 0.8 and the associated NVO O₂ concentration is approximately 4% on a wet basis. NVO timing matches the range established in the ORNL experiments, and the fuel energy injected during NVO is scaled up from 220 J/cycle to 264 J/cycle because of the larger displacement and additional NVO trapped mass of the SNL engine. Intake and exhaust temperatures differ substantially, but peak estimated NVO temperatures are similar (1120-1200K for the operating conditions that are compared).

RESULTS

The results section is divided into three subsections. The first characterizes the thermodynamic behavior of the NVO period with and without fuel injection. The second provides insight into the reforming chemistry by comparing ORNL and SNL results. The third presents an energy balance of the in-cylinder NVO fuel reforming.

Thermodynamic Characterization of the ORNL 6-Stroke Engine Cycle

Defining Terminology

Because the ORNL 6-stroke engine cycle is unconventional, it is useful to define appropriate mean effective pressures, as shown graphically in Figure 4. The IMEP_g represents the compression and expansion of the SI combustion event (-180 to +180 CA aTDC_i). The indicated mean effective pressure of the NVO event (IMEP_{NVO}) is during the compression and expansion of the NVO (+180 to +540 CA aTDC_i), while the pumping mean effective pressure (PMEP) accounts for the remaining portion of the 1080 CA 6-stroke cycle (+540 to -180 CA aTDC_i). Additionally, while a net mean effective pressure could be defined and reported, it is not included because this engine cycle is a research tool and is not being proposed as a