

Thermal and Chemical Effects of NVO Fuel Injection on HCCI Combustion

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ABSTRACT

Fuel injection during negative valve overlap (NVO) can extend low-load gasoline HCCI operation through control of main combustion phasing. Reactions and heat release accompanying NVO fuel injection give rise to changes in temperature and composition of the charge prior to main combustion. The extent of reaction of injected NVO fuel and the relative importance of resulting thermal and chemical effects on main combustion are a current research topic.

In this work, bulk temperature computations are used to quantify thermal conditions prior to main ignition for cases with and without NVO fueling. To separate measured thermal effects from chemical effects of NVO fuel reactions on the main combustion, cases without NVO fuel but with similar mixture temperatures and combustion phasing are compared. Effects of varying NVO fuel amount and injection timing on heat release, combustion phasing, bulk temperature evolution, and iso-octane ignition temperatures are analyzed. Chemical kinetic simulations using detailed and reduced mechanisms corroborate some general experimental trends, giving insight into the species and reactions causing observed effects.

INTRODUCTION AND BACKGROUND

After more than two decades of study, benefits and obstacles of engine operation by homogeneous-charge compression ignition are well known. Benefits of HCCI include unthrottled operation, increased compression ratio (relative to typical SI) high efficiency associated with volumetric combustion, and low engine-out emissions from dilute, low-temperature combustion [1,2]. Obstacles include: difficulties controlling combustion phasing; high-load operation, which is generally impeded by excessive pressure rise rates; and

low-load operation, which is kinetically limited by low charge temperatures leading to misfire.

Various strategies have been employed to extend range of operation for both high and low loads. For high load operation, Sjöberg, *et al.* [3] have demonstrated the potential for reducing pressure rise rates through thermal stratification. Others have established operation at low loads by increasing charge temperature through various means. Exhaust gas recirculation, re-breathing, and retention strategies have all been employed to provide additional energy necessary for ignition at low-load. Negative valve overlap (NVO) is one such retention strategy receiving recent attention for its ability to extend the range of low-load operation and to rapidly control main combustion phasing when coupled with diverse fuel injection strategies.

The NVO strategy incorporates early exhaust valve closing (EVC) and late intake valve opening (IVO) in order to retain large quantities of residuals. NVO thereby provides, in an efficient manner, the usual thermal and dilution advantages of residual retention. But in addition, because the residuals are recompressed (reheated), the strategy enables injection and possible reaction or reformation of fuel during the NVO period. In this way, NVO operation potentially provides a means of controlling main combustion by altering both charge temperature and composition (through reforming).

The effects of recycled burned gases are summarized by Zhao [4] and include: charge heating, dilution (reduction in intake oxygen), heat capacity, chemical reactivity, and stratification. The relative magnitude of these effects depends on the fueling strategy employed and the conditions into which fuel is injected.

Effects of NVO fuel-reforming reactions under rich conditions have been investigated by Aroonsrisopon, *et al.*

[5] and Song, *et al.* [6,7]. The latter employed a single injection strategy in which all fuel is injected during NVO. These investigators confirmed earlier conclusions by Koopmans, *et al.* [8] that oxygen-deficient conditions lead to limited heat release during NVO. Song demonstrated that fuel-rich conditions during NVO can lead to net endothermic or modestly exothermic NVO reactions that enhance reforming and its chemical effect on main combustion. All investigators found that leaner conditions during NVO permit more heat release, enhancing thermal effects on main combustion through higher charge temperatures.

Leaner NVO combustion is enabled by a split-injection strategy in which only part of the fuel is injecting during NVO for reforming [8,9,10,11,12,13]. Koopmans, *et al.* [8] found that greater NVO heat release afforded by these conditions enhances main combustion phasing sensitivity to NVO fuel injection timing and amount. Nearly all investigators report that NVO reactions have thermal and chemical effects on main combustion. Berntsson, *et al.* [11] state that the heat generated by the NVO fuel was a major contributor to the combustion phasing of PRF85 (primary reference fuel comprising 85% iso-octane and 15% n-heptane) based on rough estimates of temperature at intake valve closing (IVC). They also indicate that radicals formed during NVO may influence the phasing. Wermuth *et al.* [13] similarly emphasize that fuel reforming during recompression produces a combination of chemical and thermal effects. The focus of this work is to separate and better understand these two effects of NVO fueling.

APPROACH

EXPERIMENTAL APPROACH

In this work, we have adopted the following experimental approach in order to separate the thermal and chemical effects of NVO fuel injection. Two sets of experiments are compared: those with NVO fuel injection (labeled *NVO-fuel cases*) and those without (labeled *main-fuel cases*). Common to both sets, a fixed mass of fuel is injected at the beginning of the intake stroke (main fuel injection), as indicated in Fig. 1. For the NVO-fuel cases only, an additional, small amount of fuel is injected during recompression (at varying timings), also shown in Fig. 1.

During analysis, each pair of cases (NVO vs. main) is compared at a common main combustion phasing (CA10 from -2 to 6 CAD aTDC-main¹). For the NVO-fuel cases, main combustion phasing is controlled by adjusting the mass and timing of NVO fuel injection while holding intake air temperature constant. For the main-fuel cases, intake air temperature is adjusted (increased by about 100 K) to match

the same phasing range. In the analysis then-given a pair of cases with the same phasing-we are able say that the effect of NVO fuel injection is exclusively thermal if pre-ignition temperatures match during the compression stroke. On the other hand, if the compression-stroke temperatures differ significantly (and yet the main combustion phasing is identical), this implies that the chemistry has changed, i.e., that there is a chemical effect of NVO fuel injection.

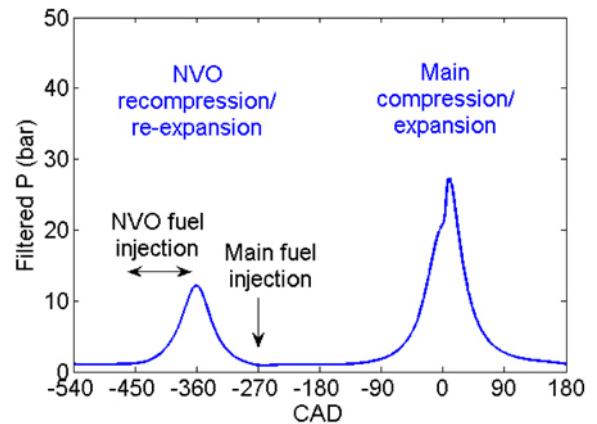


Figure 1. A typical NVO cycle pressure record with main combustion occurring near 0 CAD, preceded by the NVO recompression and re-expansion centered around -360 CAD.

ENGINE SPECIFICATIONS AND OPERATING CONDITIONS

Experiments are carried out in a single-cylinder (0.63 L) automotive HCCI research engine [14] configured for NVO operation. The GM prototype pent-roof head houses two intake valves and a single exhaust valve. 150 CAD of NVO is achieved by early exhaust valve closing and late intake valve opening using short-dwell (145 CAD), low-lift cams. Symmetric valve events are chosen to retain approximately 50% of the main charge during NVO while avoiding additional pumping work. The engine's nominal geometric compression ratio is 11.5 . However, 1-dimensional engine modeling and careful analysis of motored pressure data reveal that the effective compression ratio is 10.6 . This value is used for all analyses in this study. Additional engine specifications are listed in Table 1.

¹For the most part, *relative* crank angles are used in the paper: for example, CAD aTDC-main = crank angle degrees after top dead center of main compression, and CAD bTDC-NVO = crank angle degrees before top dead center of the NVO period. In a few graphs showing the entire cycle, absolute crank angles from -540 to $+180$ are used, with 0 CAD representing TDC of main combustion. CA10 represents the CAD where 10% of total heat release occurs.

Table 1. Engine Specifications

Displacement (single-cylinder)	0.633 L
Bore	92 mm
Stroke	95.25 mm
Effective Compression Ratio	10.6
Intake Valve Opening	75 CAD aTDC-NVO
Intake Valve Closing	220 CAD aTDC-NVO
Exhaust Valve Opening	220 CAD bTDC-NVO
Exhaust Valve Closing	75 CAD bTDC-NVO
Valve Lift	3 mm

The engine hardware includes a low-profile (25-mm tall) fused-silica ring incorporated at the top of the cylinder, and a fused-silica piston top to facilitate optical access. Although optical data are not reported here, measurement of in-cylinder temperatures using tracer PLIF are reported in a companion paper [15] for similar operating conditions as a way of validating the temperature computational algorithm employed in this work.

Fuel is delivered to the cylinder by an 8-hole direct injector, centrally located in the head. As already mentioned, split injections are required for NVO-fuel cases, complicating measurement of injected quantity for each part of the cycle. A positive-displacement flow meter in the upstream fuel line measures the average total fuel delivery per cycle. Correlations between injection duration and delivered fuel mass were determined to quantify average mass delivered by each injection. Iso-octane is exclusively used in this work to study chemical and thermal effects of NVO reactions for a single-stage ignition fuel.

Engine operating conditions are listed in Table 2. Intake air pressure and temperature are controlled by upstream metering valves and auxiliary heaters. Metering orifices are controlled to maintain 100-kPa air pressure at the engine manifold to simulate naturally aspirated conditions. Auxiliary heaters in the supply lines and intake plenum elevate intake temperatures to achieve desired combustion phasing. Of course, higher intake air temperatures (ranging from 420 to 470 K) are required for the main-fuel experiments to obtain similar combustion phasing as the NVO-fuel tests.

Table 2. Engine Operating Conditions

	Main-Fuel Experiments	NVO-Fuel Experiments
Intake Temperature	420 – 470 K	335-360 K
Coolant Temperature	363 K	353-363 K
Main Fuel Mass	7.9 mg	7.9 mg
Main Start of Injection (SOI)	270 CAD bTDC	270 CAD bTDC
NVO Fuel Mass	NA	1.0 – 2.0 mg
NVO Start of Injection (SOI)	NA	100 – 15 CAD bTDC
Fuel Injection Pressure	10 MPa	
Manifold Pressure	100 kPa	
Engine Speed	1200 RPM	

The fuel injection strategy for this work has been chosen to facilitate our comparative study of main-fuel (single-injection) and NVO-fuel (split-injection) operation. To mimic low-load operation (a principal motivation for the NVO strategy), the main fuel injection during the intake stroke is fixed at 7.9 mg (IMEP $\approx$ 190 kPa, global equivalence ratio $\approx$ 0.5). Although this is above the lowest load achievable, 7.9 mg of main fuel is a practical limit for stable operation in our research engine when not injecting additional fuel during the NVO period.

NVO fuel quantity and injection timing serve as the primary independent variables investigated in this study. NVO fuel amounts are varied between 1 and 2 mg in this work, limited by late main phasing and misfire on the low end, and overly advanced phasing on the high end. Resulting in-cylinder equivalence ratios during NVO are consistently lean, varying between 0.1 and 0.4. NVO injection timing is varied from 100 to 15 CAD bTDC-NVO. Early injection timing is limited by apparent fuel loss out the exhaust valve (as shown later). Late injections are limited by unstable engine performance due to piston wetting for NVO SOI later than 15 CAD bTDC-NVO.

Our fueling approach mimics a split-injection strategy adopted by some automotive manufacturers to enable low-load control using small amounts of NVO reforming combined with stratified main fueling. In this study, however, we maintain homogeneous conditions by injecting the main fuel early during intake at 270 CAD bTDC-main to avoid the complication of charge-stratification effects.

DATA ACQUISITION AND ANALYSIS

A piezo-electric pressure transducer measures cylinder pressure at $\frac{1}{4}$ CAD increments. To compensate for transducer drift, cylinder pressure for each cycle is “pegged” to manifold pressure measured by a separate transducer. An algorithm was developed to determine an appropriate CAD for equating cylinder and manifold pressures during the intake stroke when flow is at a minimum. More details about the procedure are described in [15]. Cylinder pressures used for the

temperature and heat release analysis discussed below are first filtered and ensemble averaged over 50 consecutive engine cycles.

Strategically placed thermocouples provide mean gas temperature measurements in the intake port and exhaust runner, and near-surface temperatures in the combustion chamber. The intake-port thermocouple is placed in the middle of the inlet manifold airstream. The exhaust thermocouple is placed a few millimeters downstream of the exhaust valve. The combustion-chamber thermocouple is mounted in an aluminum plug (matching the aluminum head) that is inserted in an unused spark-plug hole. The latter provides a time-averaged surface temperature used for computing heat loss from the cylinder.

Intake-air flow rates are measured and controlled by sonic orifices upstream of the intake plenum and auxiliary heaters. As mentioned, average fuel flow is determined using a positive-displacement meter. Based on air and fuel measurements, global equivalence ratio is computed. Equivalence ratio is also extracted from a UEGO sensor measuring O_2 in the exhaust, providing a consistency check on our mass-flow measurements. Exhaust species (CO , CO_2 , NO_x and unburned hydrocarbons-UHCs) are measured on an emission bench, from which combustion efficiency can be quantified.

Measured engine-out emissions indicate exhaust-gas composition after main combustion and prior to NVO reactions. Heat-release computations for NVO and main combustion provide estimates of chemical conversion efficiency, which are in turn used to look up product compositions predicted by chemical simulation. Once in-cylinder gas compositions are estimated, thermodynamic properties including gas constants, specific heats, and specific heat ratios are computed for use in subsequent analyses. Further details are given in [15].

Mass-averaged cycle temperatures are computed from measured pressure records using the algorithm described in [15]. Computations are based on mass conservation and a simple equation of state for steady-state operation. Required trapped mass temperatures are estimated by relating measured exhaust-runner temperatures to in-cylinder gas temperatures at the beginning and end of exhaust. A variety of validation techniques have been applied to test algorithm assumptions and predictions. As an example, comparisons of computed temperatures with a GT-Power 1-D engine simulation showed agreement within 5 K for the broad range of fired conditions tested in this work.

Apparent heat release is computed from pressure, volume, temperature, and specific heats using energy conservation by accounting for differential work and internal energy changes

throughout the cycle. Crank-angle-resolved specific heats, determined by composition and temperature are employed in the computation. Combustion phasing during main and NVO heat release is quantified using the standard definitions of CA10 and CA50, i.e., the angle at which 10% or 50% of the total heat release for that period has been released. Estimates of chemical heat release rates are computed by correcting apparent heat release for convective heat-transfer losses to the wall. The well-known Woschni correlations [16] are used to compute estimates of convective heat transfer assuming a cycle-average wall temperature determined by our combustion-chamber thermocouple.

COMPUTATIONAL APPROACH

To assist in determining the chemical effects of NVO fueling, chemical kinetic simulations are performed for NVO-fuel and main-fuel test conditions. NVO-fuel cases require simulation of reactions during NVO followed by intake air mixing and finally reactions during main compression and expansion. Of course, main-fuel cases only require simulation of main reactions using appropriate initial conditions. In all cases, the primary experimental data to be matched by the simulations are the extent of reaction (fuel-conversion efficiency) during the NVO period and CA10 during main combustion. The primary prediction of interest is chemical composition following NVO reaction/reformation.

The 0-D Closed Internal Combustion Engine Simulator by Reaction Design [17] is used with chemical kinetic mechanisms distributed by Lawrence Livermore National Laboratory (LLNL) [18] and Nissan [19]. The LLNL mechanism models combustion using a *detailed* set of reactions (4,236 reactions involving 1,034 species) for PRF fuels. The Nissan mechanism employs a *reduced* set of reactions (38 reactions involving 33 species) for PRF fuels. Our rationale for using PRF mechanisms (rather than a pure iso-octane mechanism) is to facilitate simulation of low-temperature reactions that may be important when reformed fuel is present. However, simulations also have been performed using pure iso-octane mechanisms and results show almost no discernable differences.

The closed system during NVO recompression and expansion is simulated beginning after NVO injection. Initial charge pressure, temperature, and composition are estimated using experimental data and an assumption of well-mixed constituents. Heat loss, and if necessary, initial temperature, are then adjusted to match measured levels of NVO heat release (and efficiency). Simulations are carried out well into NVO expansion to insure frozen composition. In a recent study, Song *et al* [6] showed that assuming frozen NVO products during intake had a negligible impact on simulated composition at IVC.

The closed system during main compression and expansion is simulated beginning at IVC using experimental pressure, temperature, and composition (again, assuming a well-mixed charge). IVC composition is estimated from the results of NVO simulation combined with measurements of intake air and injected fuel. The simulation is then tuned (via heat loss and, if necessary, IVC temperature) to duplicate main combustion phasing.

The results of the simulations include pressure profiles, heat releases rates, and species time histories, all of which are useful for investigating the chemical effects of NVO products on main combustion.

EXPERIMENTAL RESULTS AND DISCUSSION

OVERALL EFFECTS OF NVO FUEL

As a starting point in our study, we examined the overall effect of NVO fuel injection on main combustion phasing (main CA50) in our optical engine. As have many other groups, we found that both quantity and timing of NVO fuel injection give sensitive control of main CA50. The effect of varying NVO fuel mass while holding injection timing constant is shown in Fig. 2. Each data point represents the average of 50 cycles, and several such averages are plotted for each NVO fuel amount. The scatter in the data (seen in many of the plots presented) is attributed to difficulties duplicating experimental wall temperatures during repeated runs. For the early start of injection case shown in Fig. 2, increasing the NVO fuel quantity from 1 to 2 mg advances main CA50 from 9 to 0 CAD aTDC. Similarly, Fig. 3 demonstrates that retarding injection of NVO fuel from 100 to 15 CAD bTDC advances main CA50 by 4 CAD.

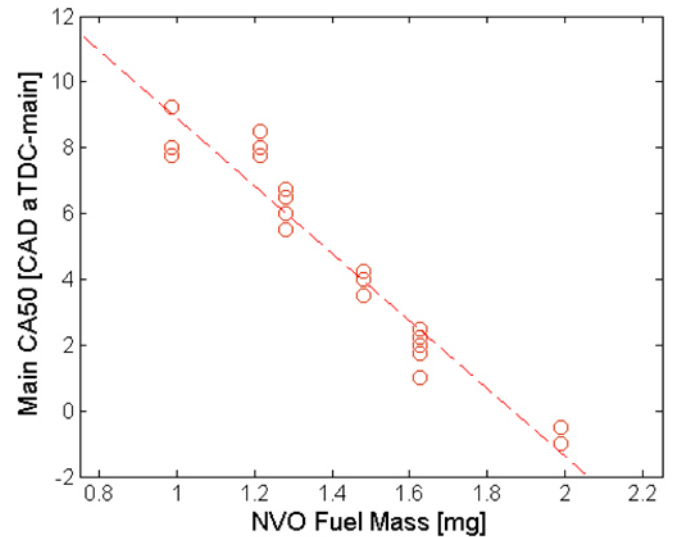


Figure 2. Change in main combustion phasing (CA50) with NVO fuel mass for constant NVO SOI = 80 CAD bTDC. Multiple measurements (each based on 50 cycle averages) are shown for each fuel amount to indicate data variation (a few points are coincident).

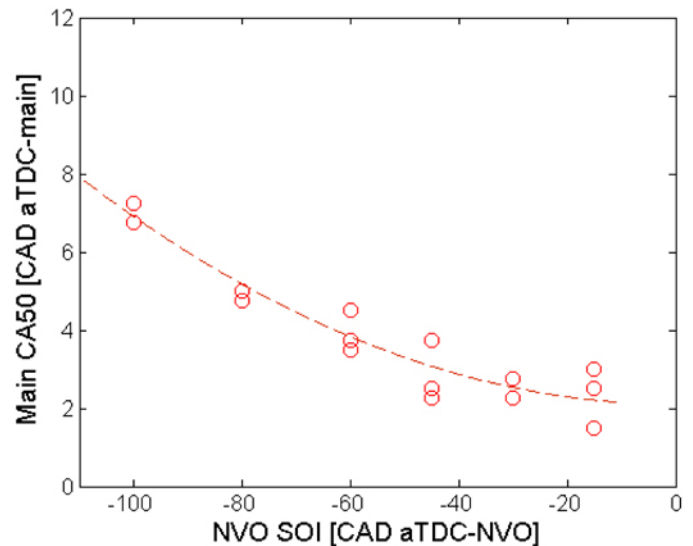


Figure 3. Change in main combustion phasing (CA50) with injection timing of 1.2 mg NVO fuel. Multiple measurements (each based on 50-cycle averages) are shown for each injection timing to indicate data variation (a few points are coincident).

These results show clear trends in engine performance as NVO fueling parameters are changed. However, to understand the observed trends, we need to examine the cycle in finer detail. In the following subsections, we trace the impact of NVO fueling on temperature, composition, and heat release starting with the NVO period and progressing through intake, compression, and main combustion.

NVO INJECTION TIMING EFFECTS

Reaction of NVO fuel is characterized in Fig. 4 by apparent heat-release rate (AHRR) curves near NVO TDC. The collection of curves represents a sweep of NVO injection timing from 100 to 15 CAD bTDC while NVO fuel mass is held constant at 1.2 mg. (As for all experiments, main injection fuel mass is held constant at 7.9 mg.) Earlier injection advances heat release, and all but the most retarded NVO SOI produce a peak heat release prior to TDC of NVO. For the three latest timings (45, 30, and 15 CAD bTDC), a drop in AHRR below zero is visible near the time of injection that is due to cooling by the evaporating fuel spray. (Earlier timings exhibit similar negative AHRR excursions that are out of the visible range of Fig. 4).

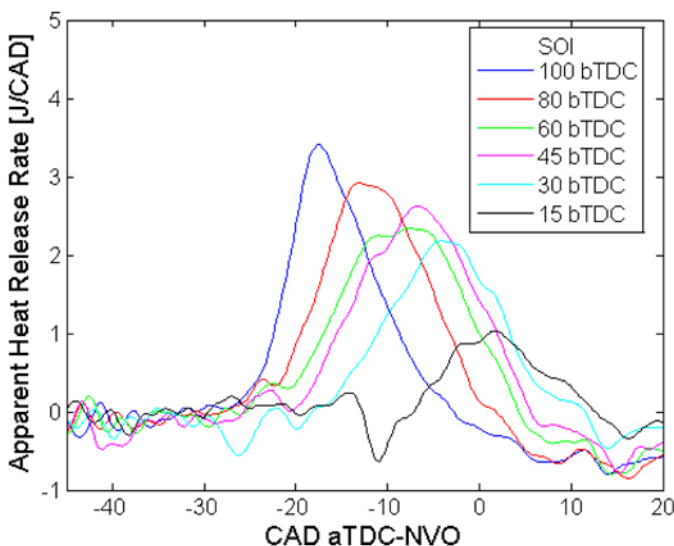


Figure 4. Heat release profiles for a sweep of injection timings with a constant 1.2 mg of NVO fuel.

Figure 4 shows a clear retard in NVO heat release phasing with injection timing that is explicitly plotted in Fig. 5. The NVO CA50² curve is smooth for SOI between 100 and 30 CAD bTDC, with a shape dictated by increasing charge temperatures, associated evaporation, mixture formation, and kinetic rates. However, for injection timing later than 30 CAD bTDC, the CA50 curve bends distinctly upward. This change in trend is likely the result of piston wetting. At these late NVO injection timings, the piston is close to the injector so that wetting is likely and fuel films may form. The fact that we observe bright yellow combustion luminosity and find characteristic piston-top soot deposits under these conditions suggests the occurrence of pool fires. Such rich combustion could be expected to have a notable impact on chemical composition following NVO.

Figure 4 also shows that peak heat-release rates generally decline with SOI retard. Since most of the heat release occurs prior to TDC of NVO, expansion cooling cannot explain the trend. Higher rates of heat loss are expected for the later heat release cases (due to higher temperatures), but this explains only about 30% of the observed reduction in peak AHRR.

Another factor is an increase in thermal stratification (associated with delayed fuel injection) that has been shown to increase burn duration and reduce peak heat release rates [3]. A final effect of delayed injection is a reduction in time available for fuel evaporation, mixing, decomposition, and radical formation prior to ignition-factors that may change reaction pathways and reduce peak reaction rates.

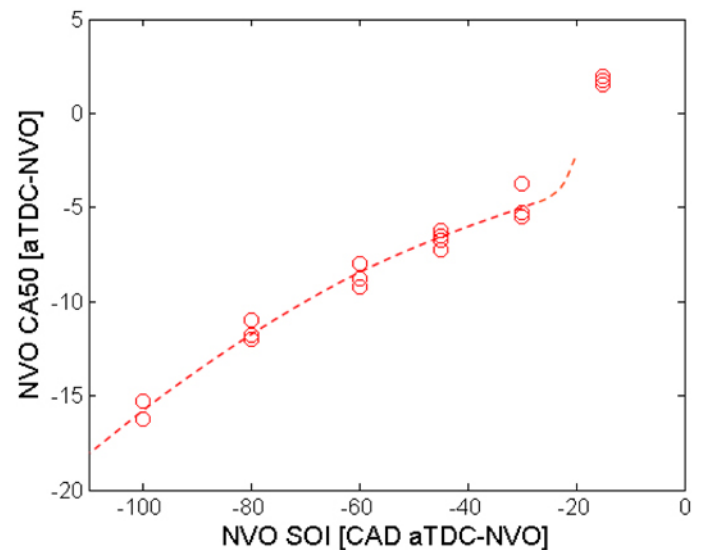


Figure 5. NVO combustion phasing (NVO CA50) for variable injection timing of 1.2 mg NVO fuel.

The percentage of injected chemical energy released as heat during NVO is plotted in Fig. 6 for our injection-timing sweep. After correcting for convective heat loss, the heat release is normalized by injected chemical energy on the y axis, providing a measure of NVO fuel-conversion efficiency.³ Average absolute heat release values are indicated by numbers next to the data points. For SOI earlier than 40 CAD bTDC, the heat release is relatively constant, indicating that fuel oxidation is not limited by residence time. Generally, for these cases of early injection, NVO fuel-conversion efficiency ranges from 80-90%, likely limited by initial temperature and local oxygen concentration. Note the modestly lower heat release for the earliest injection timing (100 CAD bTDC)-we attribute this decline to small amounts of fuel lost out the exhaust due to the fact that SOI occurs

² Again, NVO CA50 is defined as the CAD where 50% of the NVO apparent heat release occurs (not 50% of the chemical energy injected).

³ In calculations of NVO fuel-conversion efficiency, we have ignored the energy contribution associated with unburned fuel carried over from main combustion. For the experiments in this paper, main combustion efficiency is steady at about 93%.