

The Influence of Residual Gas NO Content on Knock Onset of Iso-Octane, PRF, TRF and ULG Mixtures in SI Engines

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ABSTRACT

Reported in the current paper is a study of the effects of Nitric Oxide (NO) within a simulated Exhaust Gas Residual (sEGR) on Spark Ignition (SI) engine end gas autoignition.

A modified version of the single cylinder Leeds University Ported Optical Engine Version 2 (LUPOE-2) engine was designed to completely eliminate retained residual gas and so allow unambiguous definition of the composition of the in-cylinder charge.

The engine was alternately operated on stoichiometric mixtures of iso-octane, two Primary Reference Fuels (PRF), a Toluene Reference Fuel (TRF), and a commercially available Unleaded Gasoline (ULG) and air. These mixtures were diluted with sEGR (products of the complete stoichiometric combustion of the given fuel/air mixture) in mass fractions ranging from 0-15%; with and without 5000ppm NO (0.52% by mass) within that sEGR.

For those fuels exhibiting little or no Negative Temperature Coefficient (NTC) behaviour, NO addition to the sEGR resulted in increased rate of reaction in the end gas and advanced autoignition and thus knock onset.

Conversely, autoignition (and thus knock onset) was suppressed with the addition of NO for fuels exhibiting strong NTC characteristics if the cycle unburned pressure/temperature history spent a significant period of time to autoignition in the NTC regime.

Ideas relating to the effects of residual gas NO concentration on autoignition, and thus knock onset are subsequently discussed.

CITATION: Roberts, P. and Sheppard, C., "The Influence of Residual Gas NO Content on Knock Onset of Iso-Octane, PRF, TRF and ULG Mixtures in SI Engines," *SAE Int. J. Engines* 6(4):2013, doi:10.4271/2013-01-9046.

INTRODUCTION

To mitigate pollutant and gas emissions from Spark Ignition (SI) engines, a number of advanced combustion systems (direct-injection, multiple injections, Exhaust Gas Residuals (EGR) etc) as well as complex valvetrain arrangements and catalyst aftertreatments have been introduced with some success. However, although these may prove sufficient for the immediate future, one such combustion phenomenon ultimately limits the power output and efficiency of every SI engine currently produced; autoignition.

It is generally accepted that autoignition is the result of spontaneous ignition of the unburned end gas region ahead of the normal propagating flame front. This can be caused by high pressures and temperatures, "hot-spots" on the combustion chamber walls (or valves) or radical "pool" groups that can influence the oxidation process. Although

autoignition is not always detrimental to engine performance, it is nearly always accompanied by knock; the in-cylinder "pinging" noise caused by pressure oscillations interacting with the combustion chamber - a consequence of rapid rates of heat release from autoignition of the unburned end gas [1].

As a result of these autoignition induced pressure oscillations, which are ultimately a function of the pressure/temperature/time history of the unburned mixture, thermal efficiencies are compromised, since compression ratios are restricted to mitigate the high temperatures which promote autoignition of hydrocarbon/air mixtures. Knock also places limitations on the "usefulness" of Homogeneous Charge Compression Ignition (HCCI) engines, seen by some as the solution to the problems caused by engine emissions and the rate of crude oil consumption. However, due to the modest power output generated by such a combustion process (to accommodate the knock phenomenon) hybrid HCCI/SI engines have been suggested; though high thermal

efficiencies of both SI and HCCI engines are still ultimately limited by the effects of autoignition/knock.

While the autoignition phenomenon has not been eradicated completely, a number of techniques are commonly used to mitigate its effects; these include altering ignition timing away from a preferred optimum, addition of anti-knock fuel additives to the fuel itself and addition of EGR, either trapped in-cylinder or re-circulated back into the engine. The latter is perhaps one of the most suitable solutions available to engine manufacturers for suppressing autoignition, since this system offers a secondary benefit; the suppression of Oxides of Nitrogen (NO_x). However, since the addition of EGR to a fuel/air mixture dilutes the combustible mixture, power generation is duly reduced. Another issue associated with the re-introduction of residual gases is the inevitable reactive trace species contained within the otherwise inert mixture. These are primarily produced as a result of insufficient time to achieve thermo-chemical equilibrium and are also associated with non-stoichiometric mixtures accompanied with fast transients experienced with real world driving.

Of the reactive trace gases present within EGR, the effects of Nitric Oxide (NO) on autoignition, thus knock onset have been well documented [2, 3, 4, 5, 6, 7]. In these studies, the effect of NO on autoignition (sometimes added synthetically, or as an “original” species of the residual gas fraction) was found to be contrary for different fuels and conditions; in that autoignition was either promoted or suppressed when NO was present within the mixture. In light of these published results, the current study was designed to reconcile these apparently contradictory effects by conducting experiments with an engine operating with an unambiguous EGR and NO content under knocking conditions for a number of fuels. Determination of the end gas pressure/temperature history of such mixtures was required to understand the mechanisms involved.

EXPERIMENTAL

i. Research Engine

All experiments reported in the current study were performed using the Leeds University Ported Optical Engine Version 2 (LUPOE-2) - the specification of the engine is detailed in [Table 1](#) with the engine shown diagrammatically in [Figure 1](#).

This engine was based upon a commercially available Lister Petter PH1 single cylinder diesel engine which was extensively modified in the workshop in the School of Mechanical Engineering at the University of Leeds. Such modifications included a reduction in the cylinder bore and a change to the “effective” stroke so as to reflect the conventional, approximately “square” geometry of current automotive SI engines.

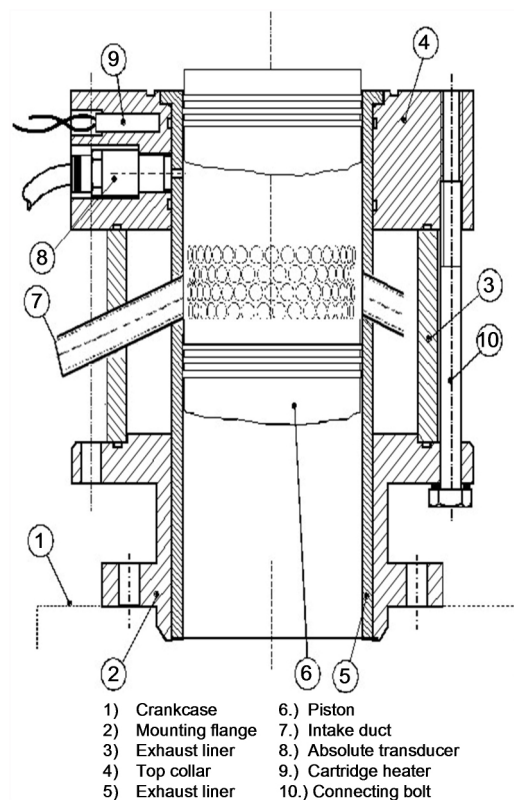


Figure 1. Schematic of the LUPOE-2 engine without the cylinder head

Table 1. LUPOE-2 engine specification

Bore (mm)	80
Stroke (mm)	110
Conrod length (mm)	232
Clearance height (mm)	7.5
Geometric swept volume (cm ³)	552.9
Effective swept volume (cm ³)	361.4
Geometric compression ratio	15.7
Effective compression ratio	10.6
Intake port close (° CA aTDC)	-107.8
Exhaust port open (° CA aTDC)	101.0

Changes to the engine breathing were also implemented where the charge air was essentially “blown” into the engine through two diametrically opposed intake banks angled 20° below the horizontal (the original engine was of over-head poppet valve arrangement). This modification was primarily undertaken to give preferred overhead full-bore optical access for flame structure analysis and visualization of gas motion, as well as allowing an improvement of the definition of the charge mixture's thermodynamic state at the start of compression.

Exhaust gases exited the cylinder via a “colander” arrangement of four rows of 10 mm diameter holes set circumferentially around the cylinder. This was designed to

eliminate strong in-cylinder motion induced by strong exhaust flows.

To counter the poor scavenging performance generally associated with engines adopting ported arrangements, the engine was fired at a skip-fire ratio of 9 to ensure “natural” residuals were effectively purged; thus ensuring the in-cylinder charge was the same as that in the intake ducts (Figure 2). In addition, an inverse poppet decompression valve (initially developed to allow skip-fired HCCI operation) mounted within the combustion chamber wall was used to further improve scavenging performance [8].

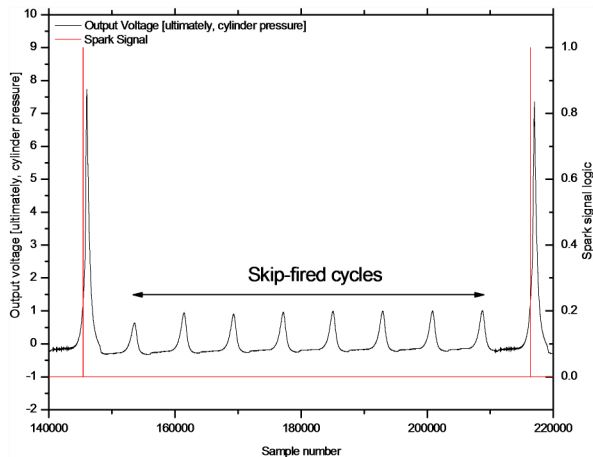


Figure 2. Sample data from skip-fire system

The skip-fire system and installation of the decompression valve within the side of the cylinder head was initially developed to allow full-bore overhead optical access. However, while it would have been advantageous to collect flame and autoignition images to supplement cylinder pressure data, the high intensity knock associated with the fuels used in the current study would have resulted in damage to the quartz window usually adopted. Hence for the duration of the currently reported study a more robust metal blanking plate was installed in the cylinder head.

ii. Fuel, Air & sEGR Supply

The intake fuel and air flowed through two identical intake banks. To promote homogeneous mixing, fuel was added upstream of the intake port via a purpose built fuel injector, located within the “throat” of a venturi; it was located approximately 350 mm from the intake port on each intake. Fuel metering was controlled using a Bronkhorst digital mass flow controller in conjunction with a Bronkhorst E7600 digital readout (one controller and readout per intake). Fuel was pumped to these controllers using an automotive fuel pump which fed the fuel through a filter and past a pressure regulator. As a result of the different fuels used throughout the course of the current study, great care was taken to avoid cross contamination of fuels. To ensure all traces of fuel were removed from the fuel supply system when changing fuels, the mass flow controllers and fuel lines

were purged with nitrogen for approximately 1 hour at a flow rate of 0.5 kg/hr. A full tank of the new fuel was then passed through the system to remove any residuals.

To investigate the effects of residual gas NO concentration on autoignition (thus knock onset), a simulated EGR (sEGR) mass fraction was added to each stoichiometric fuel/air mixture, with and without a representative NO concentration within the residual fraction. Re-introducing the residual content via “synthetic” means (with and without NO), rather than “trapping” or re-circulating EGR as with traditional methods allowed an unambiguous definition of the charge mixture ingested into the engine.

The gaseous element of the sEGR fraction was supplied using pressurised bottles of CO₂ and N₂. Water content was provided using two 50 ml syringes driven by two Braintree Scientific Inc multiphase programmable syringe pumps (one per intake) which delivered water through a multihole injector just before the first heater on each intake. Up to 5000ppm NO (0.52% by mass) was added to the sEGR fraction when required; this is typically the concentration expected for an engine operating at wide-open throttle, an engine speed of 1500 rev/min and with an air fuel ratio (AFR) of 14.7 (similar to those for the experiments reported in the current report). When NO was required it was introduced to the engine from a third bottle containing an NO/N₂ mix supplied by BOC Gases; diluting the NO with N₂ reduced the risk of storing and using the gas in its “pure” form. This mix incorporated 7000ppm NO (accurate to $\pm 3\%$); hence the required in-cylinder sEGR NO concentration was achieved by diluting the NO/N₂ mixture with excess N₂.

The laboratory air line was used to supply air, regulated to a pressure of 4 bar (gauge) to the engine; note that the in-cylinder mixture (at exhaust port closure) was only fractionally above atmospheric pressure as a result of a number of pressure drops throughout the system and the pressure drop caused by the exhaust extractor. Air flow to each intake was throttled using a needle valve, before being measured using a Brookes 5863S thermal mass flow meter in conjunction with a Brookes 5875 digital display unit. For stoichiometric, residual-free testing at the reference condition (for all fuels), the mass flow rate of air was 6.9 g/sec per intake, accurate to $\pm 1\%$. Schematics of the fuel, air and sEGR delivery systems are shown in Figure 3 and 4. Note the bottle of O₂ shown in Figure 3; although not used during the currently reported study, O₂ was used in later research when adding sEGR to mixtures suitably lean of stoichiometric, required for HCCI operation [8].

Homogeneous mixing of the gaseous sEGR components was achieved using a 5 litre reservoir downstream of rotameters (accurate to within $\pm 2\%$) used for measuring proportions of CO₂, N₂ and NO/N₂ for a given sEGR fraction. Although not directly used to measure specific quantities (but used to keep proportions of gaseous sEGR correct), rotameters were used in conjunction with a needle valve used to throttle the sEGR to the correct mass flow rate

(one per intake); the quantity of which was measured using a Hastings Teledyne HRM-301 mass flow meter (accurate to within $\pm 1\%$) connected to a Chell CMD100 digital display unit (both mass flow meters were connected to the same display unit). A further reservoir was placed within each intake line to allow mixing of air and sEGR as well as to dampen pressure fluctuations caused by engine breathing.

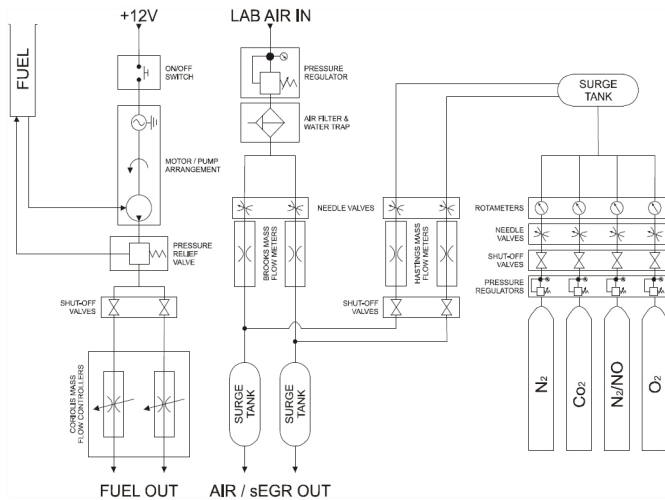


Figure 3. Fuel, air & sEGR experimental setup (i)

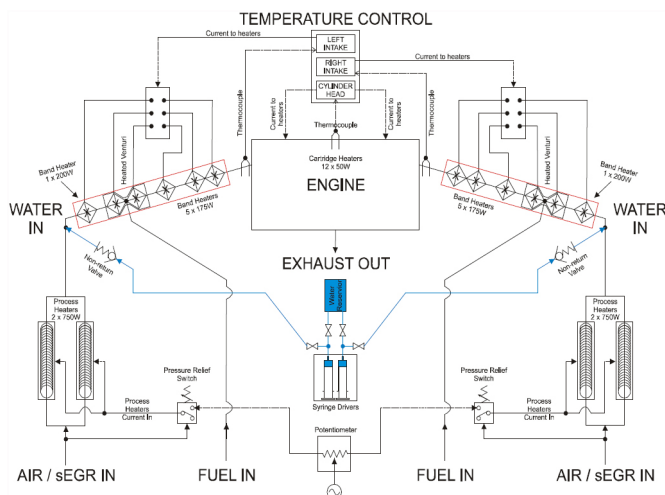


Figure 4. Engine, fuel, air & sEGR experimental setup (ii)

Air temperature was increased and maintained using a series of five 175 W and one 200 W band heaters located along each intake; these provided sufficient heat to vaporise the fuel (and sEGR water content when required) when it was added (the addition of two 750 W air process heaters arranged in parallel per intake were used during later HCCI work). Cylinder barrel and head heating was similarly maintained using twelve 50 W cartridge heaters spaced equidistant around the cylinder barrel; the corresponding temperatures were then monitored and controlled using a

purpose built control unit comprised of three Digitron 4801 slim-line panel thermometers and Type K thermocouples placed inside the cylinder barrel and just before the intake port on each intake.

iii. Data Acquisition

The data acquisition system used throughout the study is presented diagrammatically in Figure 5. Dynamic in-cylinder (gauge) pressure was measured using a Kistler piezoelectric pressure transducer Type 601A mounted flush to the cylinder wall with only the diaphragm exposed to the chamber surface. The charge output from this transducer was amplified using a Kistler charge amplifier Type 5007 set to 10 mechanical units per volt (0-10 v range). The dynamic (gauge) pressure was referenced using a Kistler absolute pressure transducer (Type 4045A5) mounted lower in the piston barrel (60° before Top Dead Centre (bTDC)). This transducer was located in such a position that it was cut off by the piston and was therefore protected from the high temperatures and pressures experienced later in the cycle. A Kistler piezoresistive amplifier Type 4601A set to 0.5 mechanical units per volt (0-10 v range) was used in conjunction with this absolute sensor.

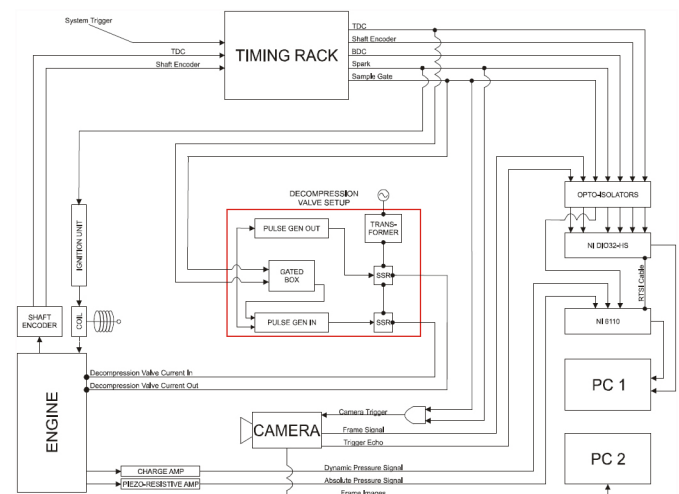


Figure 5. Data acquisition system & wiring schematic

A Hohner 3202 shaft encoder, located at the torque free end of the crank shaft, was used to record Crank Angle (CA) data. The encoder produced 1800 pulses per revolution as well as a separate single pulse for Top Dead Centre (TDC) so piston position could be referenced. In addition, a dedicated timing rack (built in the School of Mechanical Engineering workshop at the University of Leeds) was used for generating timing signals for the ignition, decompression valve, camera (when required) and data acquisition system given TDC and external clock signals from the shaft encoder.

All engine data were recorded using a data acquisition system which incorporated two National Instruments data acquisition Peripheral Component Interconnect (PCI) cards, a LabVIEW programme and a personal computer (a description

of this system in found in Hattrell [9]). Dynamic and absolute pressure signals were recorded using two separate channels of a National Instruments 6110 analogue PCI card (accurate to 12 bits) whereas digital signals (TDC, BDC etc) were recorded using a National Instruments DIO-32HS digital PCI card. Simultaneous recording of analogue and digital timing signals was achieved by linking the cards via a Real-Time System Integration (RTSI) cable which synchronised their internal sample clocks in a master/slave type orientation. Data sampling from the analogue and digital signals began at a Bottom Dead Centre (BDC) pulse before a firing cycle, therefore ensuring the data recorded always began with a complete firing cycle. Sampling of all signals was at 200 kHz, equivalent to 22.2 samples per CA at 1500 rev/min.

iv. Fuels and Testing Procedure

A total of five fuels were tested through the course of the current study. These fuels took the form of one single component reference fuel (iso-octane), two PRFs, one Toluene Reference Fuel (TRF) and one Unleaded Gasoline (ULG) - the components of which constituted approximately 60% isoparaffins, 8% normal-paraffins, 21% aromatics and 11% naphthenes (the exact chemical components were not known). The specification of each fuel is set out in [Table 2](#) where RON is the Research Octane Number, MON is the Motor Octane Number and AFR_s is the stoichiometric air/fuel ratio.

Table 2. Fuels tested in currently reported study

Fuel	Blend (by volume)	RON	MON	AFR _s
Iso-octane	100% iso-octane	100	100	15.03
95PRF	95% iso-octane, 5% <i>n</i> -heptane	95	95	15.04
90PRF	90% iso-octane, 10% <i>n</i> -heptane	90	90	15.04
90TRF	71.5% toluene, 28.5% <i>n</i> -heptane	90	79.4	15.04
90ULG	100% Shell gasoline (FB040887)	90	84.7	13.82

Each fuel was initially characterised with the engine operating at the reference condition detailed in [Table 3](#) to generate baseline combustion data under residual free running conditions. Following this, sEGR was supplied to the engine as a proportion of the total charge fed to the engine in the range 0-15% (by mass). With sEGR addition, the combustible components of the charge mixture were inevitably diluted, which therefore affected the unburned end gas composition and temperature and so the tendency for autoignition to occur, (vis à vis the residual-free reference condition). As such, to induce knock of such mixtures it was necessary to alter the engine operating conditions. Unfortunately as a result of this it was not possible to study the sole effects of sEGR on knock onset, since experiments with residuals were conducted at different ignition timings (required to induce knock with dilute mixtures), to those of

the residual-free reference condition. Accordingly, there was insufficient cyclic variation “overlap” in the data from condition to condition (for each fuel tested) to allow comparison of cycles of similar pressure/temperature history and so infer the “sole” effects of sEGR on knock onset. This was the case for all subsequent tests involving sEGR.

Table 3. Reference condition

Engine speed (rev/min)	1500
Equivalence ratio (ϕ)	1.0
Mass flow rate of air (g/sec)	13.8
Intake (gas) and cylinder head (metal) temperature (K)	343
EGR content (% by mass)	0
NO concentration within EGR (ppm)	0
NO concentration within charge (ppm)	0

As alluded to elsewhere in this report, one of the inevitable consequences of the re-introduction of a proportion of the burned gases back into the engine (used for emissions control purposes) is that some trace species are present within the residual gas fraction. A number of researchers [2, 3, 4, 5, 6, 7] have reported that the addition of small quantities of NO can influence the autoignition behaviour of many fuels. It has been suggested in [10] that up to 5000ppm NO can exist within the exhaust gases, which are either trapped in-cylinder as “residuals” or deliberately re-circulated back as “EGR” into the engine. Therefore to explore the influence of NO within the residual on knock onset, 5000ppm NO was added to each sEGR fraction when required. Smallbone [3] had previously explored the effect of a number of different in-cylinder NO concentrations on knock onset for a single condition (achieved by varying the NO concentration within a fixed sEGR fraction). However, it was not considered practical to vary the NO concentration for the wider range of conditions explored here and so a constant NO concentration (within a sEGR fraction), close to the maximum expected within the residual, was adopted in the current study.

To quantify the difference in reactivity promoted by the addition of NO within the sEGR to fuel/air mixtures, “selected” engine cycles of similar unburned pressure vs. CA history for experiments with and without NO for each sEGR condition were compared. It follows that if the pre-knock pressure history for cycles with and without NO were similar then the corresponding pre-knock temperature history should also have been similar. As such, any difference in knock onset must be due to the addition of NO, since all other variables remained the same. This was considered more meaningful than comparing ensemble average cycles from conditions with and without NO because of the inevitable variation in knock onset times and knock intensities caused by variations in the pre-knock burn rate.

To match “selected” cycles with and without NO, it was nevertheless necessary to calculate a pre-knock ensemble average pressure vs. CA record for each condition. Following this, “selected” engine cycles (with and without NO) exhibiting the closest match to the pre-knock ensemble average cycle calculated for a specific sEGR fraction were