Full Length Article

The impact of nitric oxide on knock in the octane rating engine

Zhongyuan Chen, Hao Yuan, Tien Mun Foong, Yi Yang*, Michael Brear

Department of Mechanical Engineering, University of Melbourne, Parkville, Victoria 3010, Australia

ABSTRACT

Nitric oxide (NO) is a trace species that is always present in reciprocating engines, and can significantly affect fuel autoignition. This work presents a systematic investigation of the impact of NO on fuel autoignition in a standard, octane rating engine. Knock onset timing is investigated over a wide range of equivalence ratios, intake temperatures, and fuel compositions with increasing levels of NO added via the engine intake. NO is observed to both promote and retard autoignition in different cases. In particular, NO added via the engine intake can often promote autoignition when the engine is operated at sufficiently rich conditions such that there is negligible, combustion-induced residual NO in the fresh charge. Increasing the intake air temperature with iso-octane fuelling further enhances NO's promoting effect. The promoting effect of NO is also found to be stronger for fuels containing higher toluene and ethanol content rather than paraffins, suggesting that the autoignition of fuels with higher octane sensitivity is also more sensitive to NO addition. These observed impacts of NO are discussed using a current understanding of the interaction chemistry between NO and the studied fuels. This suggests that new, fuel-specific NO mechanisms are required as an integral part of the kinetic modelling of engine combustion.

1. Introduction

Knock in spark ignition (SI) engines fundamentally limits engine efficiency, and is a process that results from the interaction of the fuel autoignition chemistry and the thermo-chemical conditions inside the engine cylinder. For reciprocating engines, these in-cylinder conditions commonly involve the products of combustion as part of the auto-igniting mixture due to the presence of residual gases. The increasing use of exhaust gas recirculation (EGR) to control engine emissions and to enable advanced, low temperature combustion [1] also makes the residual combustion products even more significant in the engine autoignition process.

Amongst the various combustion products, nitric oxide (NO) has been reported to have a pronounced and complex impact. NO was reported to promote autoignition (and therefore knock) of iso-octane in SI engines [2–5] and in homogeneous charge compression ignition (HCCI) engines [6–9]. For example, Sheppard et al. [3] reported that knock onset of iso-octane in an optical SI engine was monotonically advanced with increasing NO addition up to 387 ppm. Contino et al. [9] studied the impact of NO (from 0 to approximately 500 ppm) in an HCCI engine and found that the CA50 (50% mass fraction burnt point) of iso-octane was consistently advanced as more NO was added.

This promoting effect of NO was, however, generally observed at low levels of NO addition or high autoignition temperatures, with high levels of NO addition at low temperatures found to retard autoignition [2,3,6,7,10]. For example, Prabhu et al. [11] conducted a motored engine study using PRF81 (iso-octane/n-heptane mixture at 81:19 ratio by volume), and reported that for intake temperatures below 70 °C, NO addition up to 100 ppm promoted the fuel autoignition as indicated by the CO formation, but higher levels of NO addition inhibited the reactivity. A similar, non-monotonic impact was reported by Dubreuil et al. in an HCCI engine [6] fueled with n-heptane and the mixtures of n-heptane/iso-octane and n-heptane/toluene with research octane numbers (RON) of 25 and 24, respectively. They found that the first-stage ignition (low temperature heat release) was advanced with NO addition up to 100 ppm but was delayed by further NO addition. The second-stage ignition (hot ignition) was also advanced with NO addition up to 100 ppm but remained almost unaffected at higher NO levels.

The impact of NO has also been reported to be fuel dependent. Sheppard et al. [3] reported that NO tended to suppress the autoignition of fuels with strong negative temperature coefficient (NTC) behaviors (e.g. paraffins), but promote the autoignition of fuels with weak NTC behaviors (e.g. aromatics). More fundamental experiments have also been conducted in flow reactors, jet stirred reactors, and a rapid compression machine to understand the chemistry between NO and C1-C5 hydrocarbons [12–19], n-heptane, iso-octane and toluene [6,20,21]. Similar to the engine studies, the impact of NO in these experiments exhibited a complex dependence on temperature, NO concentration and

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fuel composition [21].

Such investigations show that the impact of NO in SI engines is complex and challenging to study experimentally. This is in part because NO in the residual gases varies with engine operating conditions. Techniques such as skip-firing [2,3] and Ar-O$_2$ combustion [4] have been used to remove the impact of residual NO at the cost of altering the engine combustion environment. Also, production engines are often unable to withstand continuous knocking combustion, and the borderline knocking condition commonly used in these engines makes it difficult to examine the impact of NO on engine autoignition.

To address such issues, this study therefore uses a Cooperative Fuel Research (CFR) engine, which is the standard octane rating engine [22,23] and is designed for continuous knocking operation. Fuel rich conditions are a focus in order to suppress combustion generated NO, thereby enabling study of the impact of NO addition via the engine intake. Although these conditions differ from normal, stoichiometric SI engine operation, they permit continuous firing and thus maintain more realistic temperatures for the cylinder walls and residual gases, both of which are important to autoignition. The adjustable compression ratio of the CFR engine further allows knocking to be studied over a wide range of operating conditions, particularly the varied intake temperatures, equivalence ratios and fuel compositions that are considered in this work.

2. Experimental methods

2.1. Engine setup

A Waukesha CFR engine is used in this work. The engine is in the standard setup for octane number testing with minor modification for this study. Engine specifications are shown in Table 1. A schematic of the setup is shown in Fig. 1. Ambient air is dehumidified by a chiller operating at 3.5 $\pm$ 1.5 °C. NO (10 vol% in N$_2$) is injected into the air flow upstream of a surge tank. Pure O$_2$ (99.999%) is added at the same location to maintain the intake O$_2$ at the same level as air (20.95%). The gases are mixed in the 10-L surge tank, where turbulence blades are used to facilitate mixing. An electrical heater is installed downstream of the surge tank to control the gas temperature ($\pm$ 1 °C) for the mixed air and NO. A fraction of this gas mixture is sent to a Horiba exhaust emission bench for NO and O$_2$ measurement.

The fuel is supplied via a carburetor downstream of the heater, as per the standard setup of the CFR engine. The gas temperature past the carburetor is reduced due to fuel vaporization. The equivalence ratio (φ) is measured with a Bosch LSU 4.9 wideband universal exhaust gas oxygen sensor and a MoTeC Professional Lambda Meter. The detonation pickup and knock-meter are used to determine the baseline operating condition. The detonation pickup is then replaced by a Kistler (6125C) pressure transducer for the in-cylinder pressure measurement at 0.1 crank angle degree (CAD) resolution. Data acquisition is achieved with an in-house LabVIEW program.

Table 1
Specifications of the CFR engine.

Engine type	Single-cylinder, unthrottled, spark ignition
Combustion chamber shape	Pancake
Spark plug location	Side-mounted
Compression Ratio	Adjustable from 4:1 to 18:1
Cylinder Bore	82.55 mm
Connecting Rod	254.0 mm
Stroke	114.3 mm
Displacement	611.7 cm3
Fuelling	Carburettor
Number of Valves	2
Inlet Valve Closing	146°BTDC
Exhaust Valve Opening	140°ATDC

2.2. Definition of knock onset timing

The impact of NO on fuel autoignition is quantified by the resulting changes in knock onset timing. At each operating condition, the knock onset timing is determined from a single, representative cycle selected from the 600 cycles sampled. To ensure that the selected cycle is representative of the operating condition, the following cost function is used for which the minimum value is reached by the representative cycle

$$\text{COST} = \left(\frac{MFB50_i - MFB50_{avg}}{MFB50_{avg}} \right)^2 + \left(\frac{KP_i - KP_{avg}}{KP_{avg}} \right)^2 \qquad (1)$$

where MFB50 is the crank angle for 50% mass fraction burned and KP is the 'knock onset point'. Subscripts *i* and *avg* denote the value for the ith cycle and the average of all 600 cycles respectively. The MFB50 is evaluated with the approach developed by Rassweiler and Withrow [24]. The 'knock onset point' is defined as the crank angle where the second derivative of the pressure vs. CAD first equals 2000 kPa/deg^2 [25]. Figure 2 shows an example of a representative trace at the standard knock intensity (SKI) condition for iso-octane's RON test.

2.3. O$_2$ compensation

Since the NO used in this study is 10 vol% in N$_2$, the intake O$_2$% will be reduced as NO is added. To examine the impact of reduced O$_2$%, an O$_2$ displacement test is conducted, where pure N$_2$ is added at the engine intake to simulate the O$_2$ dilution from using the NO/N$_2$ mixtures. Experiments are conducted using PRF91 at a compression ratio of 6.73 and an intake temperature of 52 °C. Figure 3(a) shows representative pressure traces at different O$_2$ displacement levels. Retarding of the knock onset timing is observed as in Fig. 3(b). For example, a delay of knock onset by approximately 0.4 CAD results as O$_2$% drops from 20.95% to 20.75%, equivalent to 900 ppm NO addition. This is comparable to the effect of NO reported in previous engine studies [2,3]. Therefore, O$_2$ compensation is considered necessary and thus used throughout this study to maintain 20.95% O$_2$ at the engine intake.

2.4. NO-NO$_2$ conversion

The residence time of the NO/air mixture in the CFR engine intake system is approximately 5 s, during which NO could be potentially converted to NO$_2$. To evaluate the extent of conversion, tests are conducted with different NO addition levels at the intake air temperature (IAT) of 52 °C and 200 °C. Measurements are conducted between the point of NO addition and a point approximately 40 cm before the intake port (Fig. 1). The results are shown in Fig. 4, where the NO$_2$ formation is indicated by the difference between the NO$_x$ and NO.

It is evident that NO$_2$ is only produced significantly at high temperature and high NO addition levels. NO$_2$ production is low for NO addition below 600 ppm where most of the experiments in this work are conducted. NO to NO$_2$ conversion in the engine intake is therefore considered insignificant in this study.

2.5. Test conditions

The CFR engine experiments adopt the RON-like conditions for all cases studied in this work. The conditions shared by these experiments are shown in Table 2.

2.5.1. Impact of NO at different engine operating conditions

Two engine operating parameters, the equivalence ratio and the intake temperature, are swept to study the impact of NO on the autoignition of iso-octane (Table 3). The equivalence ratio is first varied from 0.91 to 1.43 with a fixed intake air temperature of 52 °C (Set 1). Second, the IAT is varied from 52 °C to 200 °C with a fixed φ of 1.43 (Set