

The Reduced Effectiveness of EGR to Mitigate Knock at High Loads in Boosted SI Engines

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ABSTRACT

Numerous studies have demonstrated that exhaust gas recirculation (EGR) can attenuate knock propensity in spark ignition (SI) engines at naturally aspirated or lightly boosted conditions [1]. In this study, we investigate the role of cooled EGR under higher load conditions with multiple fuel compositions, where highly retarded combustion phasing typical of modern SI engines was used. It was found that under these conditions, EGR attenuation of knock is greatly reduced, where EGR doesn't allow significant combustion phasing advance as it does under lighter load conditions. Detailed combustion analysis shows that when EGR is added, the polytropic coefficient increases causing the compressive pressure and temperature to increase. At sufficiently highly boosted conditions, the increase in polytropic coefficient and additional trapped mass from EGR can sufficiently reduce fuel ignition delay to overcome knock attenuation effects. Kinetic modeling demonstrates that the effectiveness of EGR to mitigate knock is highly dependent on the pressure-temperature condition. Experiments at 2000 rpm have confirmed reduced fuel ignition delay under highly boosted conditions relevant to modern downsized boosted SI engines, where in-cylinder pressure is higher and the temperature is cooler. At these conditions, charge reactivity increases compared to naturally aspirated conditions, and attenuation of knock by EGR is reduced.

CITATION: Szybist, J., Wagnon, S., Splitter, D., Pitz, W. et al., "The Reduced Effectiveness of EGR to Mitigate Knock at High Loads in Boosted SI Engines," *SAE Int. J. Engines* 10(5):2017, doi:10.4271/2017-24-0061.

INTRODUCTION

One engine technology to increase spark-ignited engine efficiency is cooled external exhaust gas recirculation (EGR). The attractiveness of cooled external EGR is that it offers thermodynamic advantages to the working fluid while maintaining conventional 3-way catalyst aftertreatment compatibility. The overall efficiency advantages for high EGR conditions are described in detail in a thermodynamic modeling study by Caton [2], and are summarized below. First, additional mass from the EGR causes the manifold pressure to increase without increasing the intake oxygen flow, which at part-load conditions can decrease engine pumping and increase engine efficiency. Second, the peak in-cylinder temperature decreases with EGR, causing the in-cylinder heat transfer to decrease. Third, due to a combined thermal and composition effect, the working fluid ratio of specific heats (γ) increases with EGR.

These three beneficial efficiency effects of EGR have led to modern production spark-ignited engines incorporating increasing levels of EGR. For instance, Hyundai attributed a 3.5% fuel consumption decrease in their new generation of naturally aspirated engine designed for high EGR tolerance in hybrid electric applications [3]. Similarly, Toyota is employing up to 25% external EGR in their new generation of naturally aspirated engine for hybrid electric systems [4], citing EGR as a one of the technologies that enable their engine to achieve 40% brake thermal efficiency.

In addition to these thermodynamic advantages, EGR also reduces the exhaust temperature which can reduce the need for overfueling at high engine speeds [5,6,7] and EGR can reduce the knock propensity [5,6,8,9,10]. This can enable increased engine efficiency as operation approaches full load, through either combustion phasing advance or

increased compression ratio. In this respect, Alger et al. [8] also concluded that every $\sim 1\%$ EGR was equivalent to a 0.5 octane number increase, and that at an engine load of 8 bar brake mean effective pressure (BMEP), it was possible to advance the spark timing and combustion phasing by 15 crank angle degrees (CAD) with the use of 20% EGR.

The knock attenuation effects were discussed by both Hyundai [3] and Toyota [4] as one of the important benefits of EGR. However, these were both naturally aspirated engines for hybrid applications, and a rapidly growing portion of the cars entering the marketplace are boosted. Specifically, in 2006 only 3.2% of new cars sold in the United States (US) were equipped with a turbocharger, but in 2016, 25.2% of cars sold in the US were estimated to be turbocharged [11]. The uptake of turbocharged engines by 2025 is projected to be in excess of 50% [1].

However, the same magnitude of knock suppression at naturally aspirated conditions has not been consistently observed under boosted conditions. At an engine load of 14 bar indicated mean effective pressure (IMEP), Hoepke et al. [12] found that while EGR still provided a substantial knock-mitigation effect, about 8 CAD advance in spark timing and combustion phasing with 20% EGR, it was only about half of what was reported by Alger et al. [8]. Lewis et al. [13] investigated EGR knock mitigation effects at a constant intake manifold density and found they were able to advance spark by as much as 10 CAD at loads over 20 bar BMEP, but this dataset was also accompanied by a decrease in load with EGR, which is a direct result of maintaining a constant intake density. Splitter and Szybist [14] investigated the effect of EGR across the operating load range with three different fuels. While they found a significant attenuation in knock propensity at engine loads below 12 bar IMEP with the use of EGR, the ability to advance combustion phasing when EGR was added at high loads diminished to the point where nearly no benefit was observed at loads above 15 bar IMEP.

The purpose of this study is to investigate how the effectiveness of EGR to mitigate knock changes as engine operating load changes. This is accomplished using a combination of chemical kinetics modeling, adiabatic compression calculations, and the use of experimental data.

METHODOLOGY

Experimental Facility

The experimental apparatus and much of the methodology used in this study has been previously reported [15]. A 2.0 L GM Ecotec LNF engine equipped with the production side-mounted direct injection fueling system was used in this study. Engine geometry details are presented in Table 1. The engine was converted to a single-cylinder engine by disabling cylinders 1, 2, and 3. The combustion chamber geometry and camshaft profiles were unchanged from the stock configuration. Production camshaft phaser timings were applied and maintained constant during each combustion phasing sweep.

Table 1. Engine geometry.

Bore $\times$ Stroke [mm]	86.0 $\times$ 86.0
Conrod length [mm]	145.5
Wrist pin offset toward expansion stroke[mm]	0.8
Compression ratio [-]	9.2 : 1
Fuel injection system	Direct injection, side-mounted, production injector with opposite linear wall directed six-hole spray pattern

The engine was operated using a laboratory fueling system. The fueling system used a pneumatically actuated positive displacement pump in conjunction with an electronic pressure regulator to provide fuel rail pressure. A constant fuel rail pressure of 100 bar was used throughout this study.

A laboratory air handling system was constructed to allow for external EGR while using pressurized facility air and achieving a flipped pumping loop, where the exhaust pressure is lower than the intake pressure. To accomplish this, pressurized and dried facility air having less than 5% relative humidity was metered to a venturi air pump using a mass air flow controller. The venturi created up to an 8 kPa pressure differential, with the vacuum side pulling EGR through an EGR cooler and into the intake. The air pump arrangement, in conjunction with electromechanical backpressure and EGR valves, is shown in Figure 1. A constant intake plenum temperature of 35°C was achieved regardless of the EGR concentration using the combination of an EGR cooler and an electrical heater upstream of the intake surge tank. The EGR used in this study was not treated with an exhaust catalyst before being recirculated to the intake, but was held above its dew point to prevent water condensation ($\geq 70^\circ\text{C}$ upstream of the venturi air pump where it is mixed with fresh air). EGR was measured using a non-intrusive method that utilizes pressure-compensated wideband oxygen sensors in both the intake and exhaust.

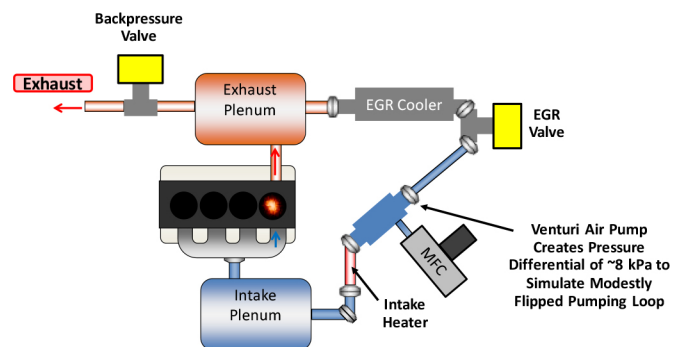


Figure 1. Schematic of the engine air handling system.

A Driven engine controller with the Combustion Analysis Toolkit package was used to control the engine and acquire crank-angle (CA) resolved data. For each condition tested, cylinder pressure, spark discharge, and camshaft position data were recorded at 0.2 CAD resolution for 1,000 sequentially fired cycles. Cylinder pressure was measured using a flush-mounted piezoelectric pressure transducer from Kistler (6125C, $\pm 0.4\%$ full scale linearity), and camshaft position was recorded from the production hall-effect sensors. Intake

and exhaust manifold pressure was measured using Omega PX605 pressure transmitters with an accuracy of ± 0.8 kPa. Start of fuel injection timing was commanded during the intake stroke and was held constant at 280 CAD before firing top dead center (TDC). Spark timing was adjusted as needed to achieve the desired combustion phasing, and spark dwell was held constant with the stock ignition coil at 1.8 ms to maintain constant ignition energy. To prevent hot-spot runaway at high load, a spark plug two heat ranges colder than the production engine's plug was used. The colder spark plug is not directly available from the engine or factory original spark plug manufacturer; rather it was identified through cross-referencing current production spark plugs with the same thread and reach as the factory original spark plug. A Denso Iridium HP spark plug was identified as being compatible and was used throughout the study. Engine fuel flow was measured with a coriolis-based fuel flow meter. Engine coolant was circulated with an electric water pump and was maintained at an engine-out temperature of 90°C using a laboratory heat exchanger with facility water, which was controlled using an electronic PID control.

Combustion analysis was performed using a LabVIEW-based routine, which was applied on a per-cycle basis. For each cycle, trapped mass was calculated using the cam position sensor feedback with in-cylinder pressure and by applying the method described by Fox et al. [16] with the measured polytropic expansion coefficient. Apparent heat release was then solved using the zero-phase-filtered in-cylinder pressure and the individual cycle trapped mass with the approach described by Chun and Heywood [17].

Fuels Investigated

In order to test whether the effect of EGR was similar for fuels of varying chemistry, this investigation utilized a set of three fuels that were designed as part of the Co-Optima Initiative. The fuel matrix was designed to hold the research octane number (RON) constant at 98 while investigating two different levels of heat of vaporization (HoV) and two different levels of octane sensitivity (S), where S is the difference between RON and the Motor Octane Number (MON) as shown in Equation 1. At the same time, the fuels were designed to provide substantially different fuel chemistry. The Alkylate fuel, is comprised completely of saturates and has very low S ($S = 1.2$). The Aromatic fuel has $S = 10.7$ and contains over 30% aromatics but doesn't include any oxygenated components. The third fuel, E30, contains 30% ethanol and also has $S = 10.7$. The three fuels were blended by Gage Products, and the fuel properties are presented in Table 2.

$$S = \text{RON} - \text{MON}$$

Equation 1

Engine Operating Conditions

The engine operating conditions investigated utilize a constant mass air flow rate of 900 g/min at 2000 rpm with stoichiometric fueling. Holding airflow and stoichiometry constant provides nearly constant fuel energy flow to the engine, with variations under 0.5%, as seen with the LHV of the stoichiometric mixture per kg of air in Table 2.

Combustion phasing sweeps were collected for each fuel at 0%, 10%, and 20% EGR, with spark ignition timing changing the combustion phasing and all other engine controls held constant. At each EGR level, a constant pressure differential of 8 kPa between the intake and exhaust manifold was maintained (with the intake manifold pressure being higher than the exhaust manifold). Because EGR introduces additional trapped mass in the cylinder, the absolute pressure in the intake and exhaust manifolds increased with EGR. The intake manifold pressure was 147 ± 2 kPa at 0% EGR, 162 ± 3 kPa at 10% EGR, and 180 ± 3 at 20% EGR. Changes in intake manifold pressure at a given EGR level can be attributed to changes in the trapped residual temperature across the combustion phasing sweeps. This equated to engine load of 13.5 - 19.0 bar IMEPg, depending on combustion phasing, as can be seen in the appendix.

Table 2. Fuel properties of the experimental Co-Optima fuel test matrix.

	Alkylate	Aromatic	E30
RON (ASTM D2699)	97.9	98.0	98.3
MON (ASTM D2700)	96.7	87.3	87.6
S (RON-MON)	1.2	10.7	10.7
IBP ^a (ASTM D86)	50.3	34.4	38.2
T10 (ASTM D86)	93.1	59.4	60.7
T50 (ASTM D86)	100.3	108.1	74.3
T90 (ASTM D86)	105.9	157.9	155.2
FBP ^a (ASTM D86)	161.3	204.4	204.1
C wt % ASTM D5291	83.75	87.22	74.78
H wt % ASTM D5291	15.80	13.12	13.79
O wt % ASTM D5599	<0.1	<0.1	11.19
Stoichiometric AFR	15.07	14.43	12.84
HoV [kJ/kg] ^b	307.8	361.2	532.4
LHV ^a [MJ/kg] ASTM D4809	44.52	42.95	38.17
LHV of stoichiometric mixture per kilogram of air [MJ]	2.97	2.97	2.98
Aromatics ASTM D1319	0	30.8	8.1
Saturates ASTM D1319	100	65	57.1
Olefins ASTM D1319	0	4.2	5.0
Ethanol ASTM D4815	0	0	29.95

^aFBP = final boiling point; IBP = initial boiling point; LHV = lower heating value.

^bHoV values measured at NREL using methodology described in Reference [18].

Computational Methods

To understand the chemical interactions for each of the three fuels with increasing EGR at high loads, a recently developed comprehensive detailed kinetic mechanism for transportation fuels by LLNL was used in simulations for ignition delay times [19]. The kinetic mechanism under consideration has been validated across the broad range of thermodynamic conditions and mixtures explored in this work (~1-50 bar, ~600-1000 K). Briefly, the kinetic mechanism merged published mechanisms for smaller (H_2 to C_4 [20]) and larger (hexenes [21], n-heptane [22]) compounds with updated or new submechanisms for iso-octane and methyl substituted aromatics (toluene, xylenes, trimethylbenzenes). In the mechanism [19], NO_x related pathways were modeled with a submechanism from Politecnico di Milano [23].

For each of the three Co-Optima fuels, simpler surrogates for kinetic modeling were developed by matching RON, S, molar H/C ratio, hydrocarbon classes (PIONA), and distillation properties. Constant volume homogeneous reactor ignition delay time simulations from ZeroRK, which is an advanced kinetic solver [24], were used to predict RON and S of the surrogates based on new correlations from Mehl et al. [19]. Distillation properties were calculated using a simple equilibrium model for ideal mixtures based on Antoine's coefficients from Yaws' Handbook [25]. Table 3 provides the predicted values of the fuel surrogates' targeted properties.

Table 3. Co-Optima fuel surrogate properties for kinetic modeling.

	Co-Optima Alkylate	Co-Optima Aromatic	Co-Optima E30
RON	98.5	98.9	96.2
S	2.2	10.6	11.0
molar H/C	2.233	1.865	2.341
IBP ^a	84.7	59.2	64.9
T10	91.9	71.2	69.9
T50	100.2	115.1	84.9
T90	105.2	163.3	120.4
FBP	151.1	169.4	169.3
Aromatics	2	33	7.7
Saturates	98	62	57.4
Olefins	0	5	4.9
Ethanol	-	-	30
Stoichiometric AFR	15.04	14.60	12.90
HoV [kJ/kg]	313.1	353.6	539.7
# of components ^a	4	7	8

^aSee the Appendix for the components and liquid volume compositions

The chemical kinetic model was used to generate ignition delay maps for each of the three Co-Optima fuels covering the range of in-cylinder pressures and temperatures considered. Adiabatic constant volume homogeneous reactor simulated ignition delay times were determined from a temperature threshold of 500 K from the initial temperature of the simulation. This threshold was used as a marker for the second stage (or overall) ignition event. Temperatures from

600 to 1000 K in 5 K increments, and pressures of 1 to 50 bar in 3 bar increments were considered for stoichiometric mixtures. Nominal composition of the air was $O_2 + 3.76 N_2$ and EGR was considered on a mass basis. Simulations covered 0%, 10%, and 20% EGR where the EGR composition was assumed to be equivalent to complete products of stoichiometric combustion (i.e. CO_2 , H_2O , and N_2). All simulations considered in this study included 150 ppm of NO to account for in cylinder residual NO_x, unless stated otherwise. In total, there were over 25,000 simulations completed in 20 minutes of wall-time on 128 processors using the ZeroRK solvers.

RESULTS

Knock Limited Combustion Phasing

The addition of EGR slows the combustion process, making it necessary to advance spark timing to achieve comparable combustion phasing. Figure 2 shows that there is a linear relationship between spark timing and the CA50 combustion phasing at each EGR level. Additionally, no major fuel-specific differences are observed. For 20% EGR, it is necessary to advance spark timing by approximately 20 CAD to achieve the same CA50 combustion phasing.

Figure 3 shows the knock response for each fuel as a function of combustion phasing for the three EGR levels investigated: 0%, 10%, and 20%. As stated in the methodology section, air and fueling rates were held constant, so engine load changes with combustion phasing, but is approximately the same for all fuels, as can be seen in the appendix. Knock is represented as the fraction of individual engine cycles with a peak-to-peak knock intensity (KI) of more than 1 bar. Sufficiently retarded combustion phasing mitigates knock propensity for all of the fuels, and for all fuels, the transition to knock is abrupt over a change in combustion phasing of 2-3 CAD.

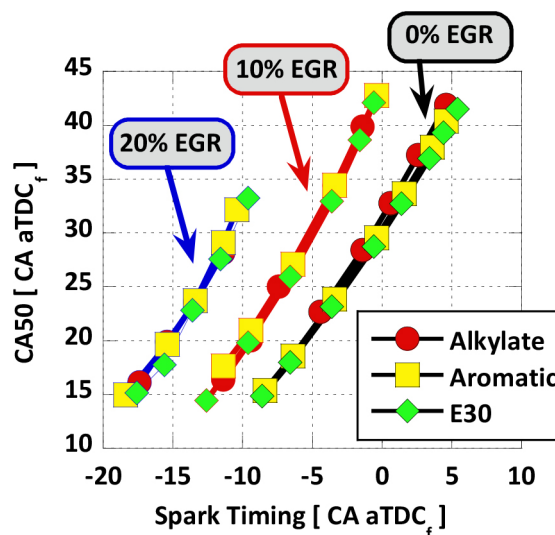


Figure 2. CA50 combustion phasing as a function of spark timing.

It can also be observed in Figure 3 that the response to adding EGR is fuel-specific. For the aromatic and E30 fuels, the phasing of knock onset remains nearly constant. In contrast, an advance of combustion phasing of about 5 CAD is observed for the alkylate. This is quantified further in Figure 4, where the knock limited combustion

phasing is plotted as a function of EGR. The knock-limited combustion phasing is quantified as the CA50 combustion phasing where more than 10% of the engine cycles had a peak-to-peak KI of > 1.0 bar. This phasing was found by performing linear interpolation between the two bounding data points in Figure 3.

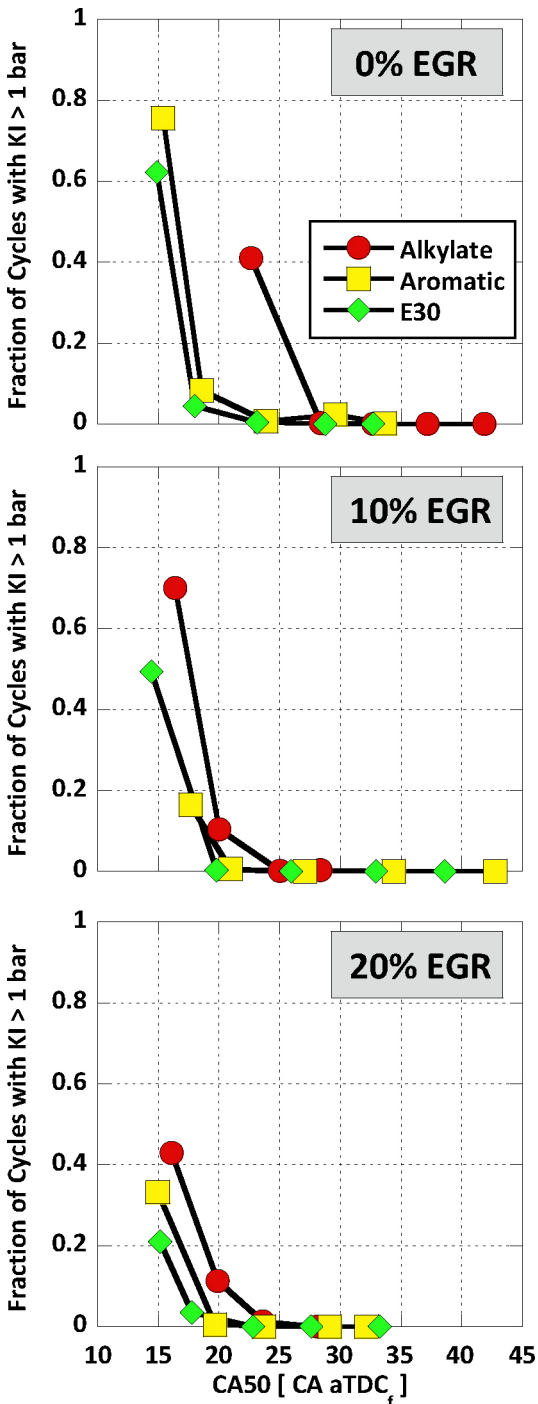


Figure 3. Fraction of engine cycles with KI > 1.0 bar as a function of combustion phasing.

Figure 4 shows that for the alkylate fuel, the addition of 10% EGR advances the knock-limited combustion phasing by approximately 7 CAD. However, the change from 10% to 20% EGR does not yield further benefit. Further, the addition of EGR for the aromatic and E30 fuels at either the 10 or 20% level does not change the knock-limited

combustion phasing. That is much less significant than the 15 CAD advance with 20% EGR reported by Alger et al. at 8 bar BMEP [8], and less than the 8 CAD advance with 20% EGR reported by Hoepke et al. at 14 bar IMEP [12]. The subsequent sections will focus on understanding why the effectiveness of EGR to reduce knock is not observed at this boosted operating condition.

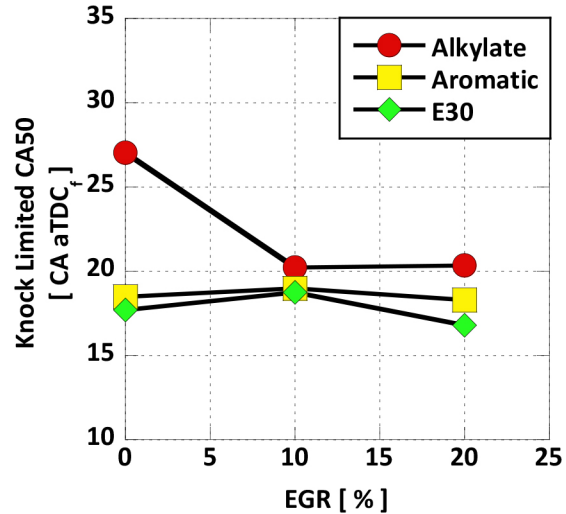


Figure 4. Knock-limited CA50 combustion phasing as a function of EGR for each fuel.

Pressure-Temperature Trajectory with Engine Load

We hypothesize that the effectiveness of EGR is dependent on the trajectory of the unburned gas through the pressure-temperature domain. To support the hypothesis, this section consists of three parts. First, the dependence of knock propensity on the pressure-temperature conditions is reviewed. Second, pressure-temperature trajectories of the unburned gas are calculated without EGR to develop a notional model of how pressure-temperature trajectory is affected by engine load. The third part investigates the effect of EGR on pressure-temperature trajectory in the unburned gas.

Knock Dependence on Pressure-Temperature Trajectory

In the US, gasoline is sold with an antiknock index rating that is the average of the Research Octane Number (RON) [26] and the Motor Octane Number (MON) [27]. The RON test was originally introduced in 1928, but the MON test was not developed until 1932, motivated by a finding that real-world fuels were underperforming the certification results by 2.5-3.0 octane rating points [28]. The MON test introduced a higher engine speed (900 rpm vs. 600 rpm) and a higher intake temperature (149°C downstream of the carburetor vs. 52°C upstream of the carburetor). The MON test conditions were an effort to address the reality that the relative ranking of knock resistance among a set of fuels changes as the engine conditions change. As a measure of this, the concept of octane sensitivity (S), defined as the difference between RON and MON, was introduced.

Independent kinetic modeling studies performed by Yates et al. [29] and Mehl et al. [30] both show the relative dependence of the pressure-temperature trajectory on the knock propensity. The RON and MON tests represent two different pressure-temperature