

Effect of Heat of Vaporization, Chemical Octane, and Sensitivity on Knock Limit for Ethanol - Gasoline Blends

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ABSTRACT

Ethanol and other high heat of vaporization (HoV) fuels result in substantial cooling of the fresh charge, especially in direct injection (DI) engines. The effect of charge cooling combined with the inherent high chemical octane of ethanol make it a very knock resistant fuel. Currently, the knock resistance of a fuel is characterized by the Research Octane Number (RON) and the Motor Octane Number (MON). However, the RON and MON tests use carburetion for fuel metering and thus likely do not replicate the effect of charge cooling for DI engines. The operating conditions of the RON and MON tests also do not replicate the very retarded combustion phasing encountered with modern boosted DI engines operating at low-speed high-load.

In this study, the knock resistance of a matrix of ethanol-gasoline blends was determined in a state-of-the-art single cylinder engine equipped with three separate fuel systems: upstream, pre-vaporized fuel injection (UFI); port fuel injection (PFI); and DI. Constant inlet temperature was held downstream of the injector for UFI and upstream of the injectors for PFI and DI. For each fuel, engine inlet pressure was swept at borderline knocking conditions at constant engine speed using each of the three fuel systems. This test method characterized each fuel's knocking behavior over a wide range of conditions, including those typical of boosted DI engines.

Comparison of UFI and DI results allowed the chemical octane effect on knock to be separated from the evaporative charge cooling effect. These effects were found to be of comparable importance for ethanol blends.

An outcome of the test method was the discovery of an interaction between combustion phasing and the sensitivity of a fuel's autoignition kinetics to temperature. For a given gasoline blendstock, increasing ethanol content significantly increased knock-limited performance with combustion phasing near the thermodynamic optimum, as expected. However, due to ethanol's high sensitivity, knock-limited performance improved to a much greater extent with increasing ethanol content as combustion phasing was retarded. This effect was further enhanced by charge cooling with DI. Increasing ethanol content also significantly increased the knock-limited performance before enrichment was required to control exhaust gas temperature.

The RON ratings of the fuels did not fully reflect the observed knock resistance of mid-to-high level ethanol blends (E20 and higher). K, the weighting factor for MON in the Octane Index, decreased with increasing combustion phasing retard and with increasing evaporative charge cooling, and increased with increasing inlet temperature and increasing compression ratio.

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INTRODUCTION

The 2007 Energy Independence and Security Act mandates the use of 36 billion ethanol-equivalent gallons of renewable fuels in the U.S. by 2022. Fifteen billion gallons of this amount consists of corn ethanol, and it is intended that a significant portion of the remaining 21 billion gallons will be cellulosic ethanol [1]. Use of this quantity of ethanol will require increasing the amount of ethanol blended with gasoline beyond 10%, and/or increased consumption of higher ethanol blends in flexible fuel vehicles. Fuels standards for the future are also currently under consideration with governmental agencies, the oil industry, and automotive manufacturers.

Since the 1930s, RON and MON have been used to characterize the knock resistance of a fuel for automotive engines. RON and MON are measured according to ASTM D2699 [2] and D2700 [3], respectively, in a Cooperative Fuel Research (CFRTM) engine manufactured by GE Energy Waukesha. A comparison of test conditions for the determination of RON and MON are shown in Table 1.

Table 1. Engine conditions for the RON and MON tests.

Parameter	RON	MON
Inlet Air Temperature	52°C	38°C
Inlet Mixture Temperature	*	149°C
Intake Air Pressure	atmospheric	atmospheric
Coolant Temperature	100°C	100°C
Engine Speed	600 rpm	900 rpm
Spark Timing	13° bTDC	14 - 26° bTDC
Compression Ratio	4 - 18	4 - 18

*Not specified, but will be lower than the inlet air temperature.

Carburetion is used for fuel introduction in these tests. For the RON test, the inlet air temperature of 52°C is set upstream of the carburetor. For the MON test, the inlet air-fuel mixture temperature of 149°C is set downstream of the carburetor. Although both RON and MON are used to calculate the fuel Anti-Knock Index (RON+MON)/2 which is displayed on retail fuel dispensing pumps in the US, many published papers [4, 5, 6, 7, 8] indicate that the knock resistance of a fuel in modern engines more closely relates to RON.

It is well known that cooling of the fresh charge occurs in direct injection (DI) engines due to vaporization of the fuel. Since inlet temperature in the RON test is set upstream of the carburetor, some cooling of the fresh air occurs due to fuel vaporization. However, the amount of charge cooling which occurs in DI engines may not be accurately replicated. This is of greater importance as the amount of ethanol blended with gasoline increases, due to ethanol's high HoV, which is about 4 times that of gasoline (per unit of heating value). The MON test does not include any effect of charge cooling due to fuel vaporization since the inlet air-fuel mixture temperature is set

downstream of the carburetor, and consequently a fuel's HoV is made irrelevant by supplemental heating.

The above considerations provided the motivation for the current study, whose primary purposes are: 1) understanding the effect of ethanol-gasoline blends on knock-limited performance and thermal efficiency in modern boosted DI engines, both at thermodynamic optimum and retarded combustion phasing, 2) determining if the RON test provides an adequate measure of knock resistance for high ethanol blends in modern boosted DI engines, and 3) separating the inherent or "chemical octane" effect from the charge cooling HoV effect on knock. In this paper, "chemical octane" refers to the effect of the fuel's molecular structure on autoignition kinetics.

FUEL MATRIX

A matrix of test fuels was developed in which both the gasoline blendstock octane rating and the percentage by volume of ethanol were varied (Figure 1 and Table 2).

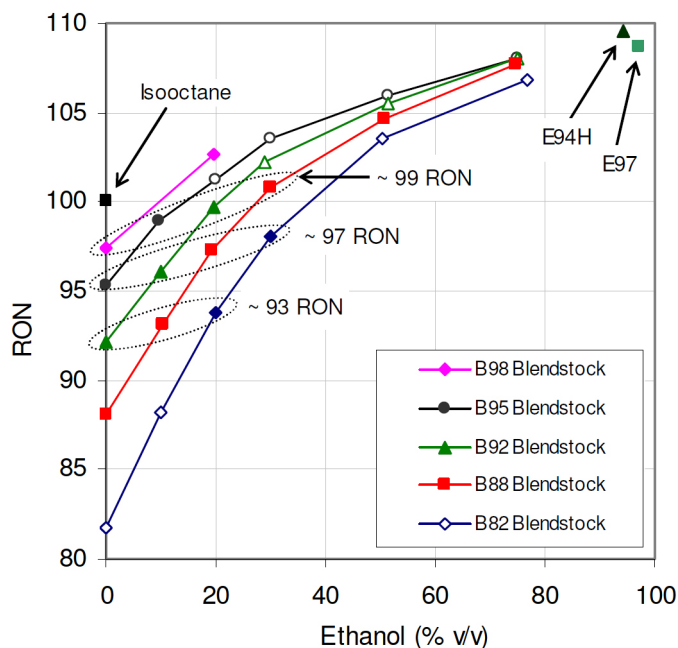


Figure 1. Measured RON vs. ethanol content of test fuels (solid symbols denote engine testing and RON/MON measurement; open symbols denote RON/MON measurement only). Fuels of approximately equal RON indicated by dotted ovals.

The RON and MON were measured both at BP and at GE Energy Waukesha, with very close agreement in measured RON values between the two laboratories. The target RON for the gasoline blendstock is shown in the first column of Table 2, while the average of the RON values measured at BP and GE Energy Waukesha is shown in the remainder of the table and in Figure 1. A detailed report on the composition of the gasoline blendstocks and the composition and characteristics of the test fuels including RON and MON

values is provided in a companion paper [9]. Isooctane was also included in the test matrix to provide a comparison with a Primary Reference Fuel (PRF). By definition, isooctane is 100 RON and 100 MON.

Table 2. Matrix of test fuels (black font denotes engine testing and RON/MON measurement; red font denotes RON/MON measurement only).

Ethanol (% vol)	Measured RON of test fuels							
	0	10	20	30	50	75	94	97
80	81.7	88.3	93.8	98.1	103.5	106.8		
Base Gasoline	86	88.2	93.1	97.3	100.8	104.7	107.7	
RON (Target)	91	92.2	96.1	99.7	102.2	105.6	108.1	
95	95.4	98.9	101.3	103.5	106.0	108.0		
98	97.4	102.7						
Isooctane	100							
Hydrous Ethanol (E94)							109.6	
Denatured Ethanol (E97)								108.7

The fuel designation convention used in this paper is as follows: the RON of the gasoline blendstock, followed by the ethanol percentage, followed by the measured RON value; for example, B88E10-R93 designates a gasoline blendstock of 88 RON with 10% added ethanol by volume with a measured RON value of 93 for the mixture (Figure 2). For denatured ethanol and hydrous ethanol, designations of E97-R109 and E94-R110, respectively, are used.

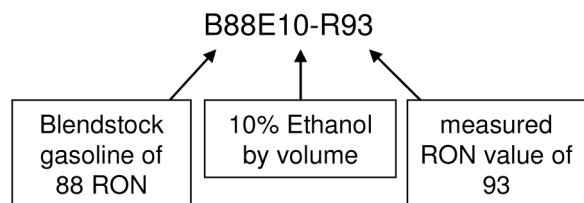


Figure 2. Fuel naming convention.

The intent was to produce diagonal lines in Table 2 of constant RON as ethanol content was progressively increased and gasoline blendstock RON was decreased, according to the linear molar octane blending approach described in [10]. As noted in Table 2 and shown by the dotted ovals in Figure 1, the measured RON values increase somewhat along these diagonals (e.g., from B95E0-R95 to B82E30-R98).

The HoV of the fuels tested in this study are shown in Figure 3. The HoV in Figure 3 is expressed as kJ per kg of air for a stoichiometric mixture, since this relates directly to the amount of charge cooling provided by vaporization of the fuel. Because of ethanol's high HoV, the HoV of the test fuels increase directly with ethanol content. Isooctane has a somewhat lower HoV than the gasoline blendstocks, whereas E94-R110 has a very high HoV due to 6%v water content.

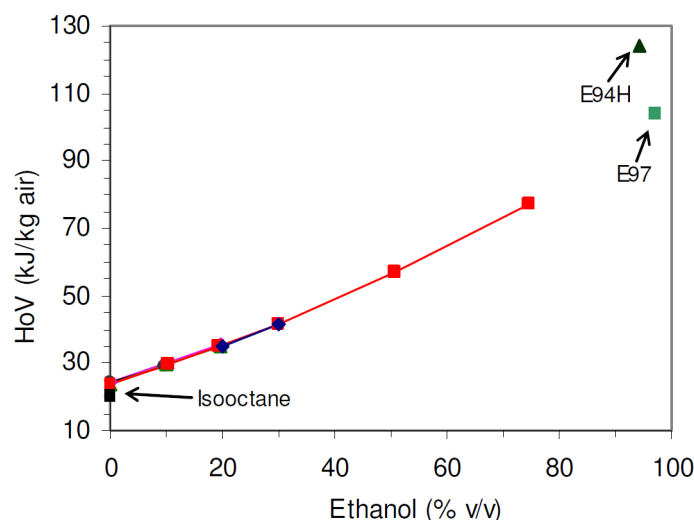


Figure 3. Heat of vaporization of test fuels.

A measure of the sensitivity of a fuel's autoignition kinetics to unburned gas temperature which has been commonly used is the difference between the RON and MON values for the fuel: $S = \text{RON} - \text{MON}$. The sensitivity for the matrix of fuels of Figure 1 is shown in Figure 4.

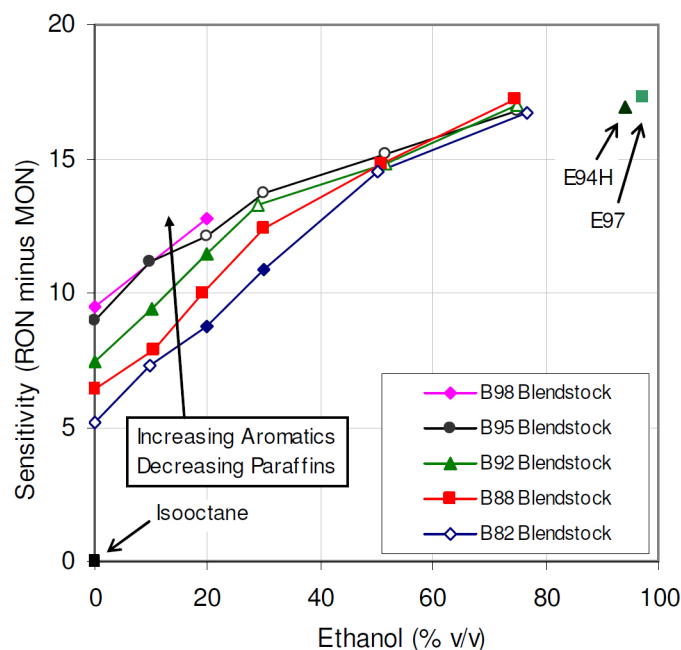


Figure 4. Sensitivity of test fuels (solid symbols denote engine testing and RON/MON measurement; open symbols denote RON/MON measurement only).

Sensitivity increases as n-paraffins are replaced with aromatics to increase blendstock RON [9]. Sensitivity also increases with increasing ethanol content. At an ethanol content of 50% by volume and greater, the sensitivity is nearly independent of the gasoline blendstock because the knock related properties are dominated by ethanol. By

definition, the sensitivity of isooctane as measured by RON minus MON is zero.

As discussed in [4,5,6], sensitivity has a profound impact on the knock behavior of a fuel as a function of the engine operating conditions. Sensitivity is a measure of how dependent the autoignition kinetics of a fuel are to the temperature of the unburned end gas. Plots of autoignition delay time vs. temperature for hypothetical fuels with high sensitivity and low sensitivity are shown in Figure 5, which is a conceptual illustration adapted from Figure 6 of [4].

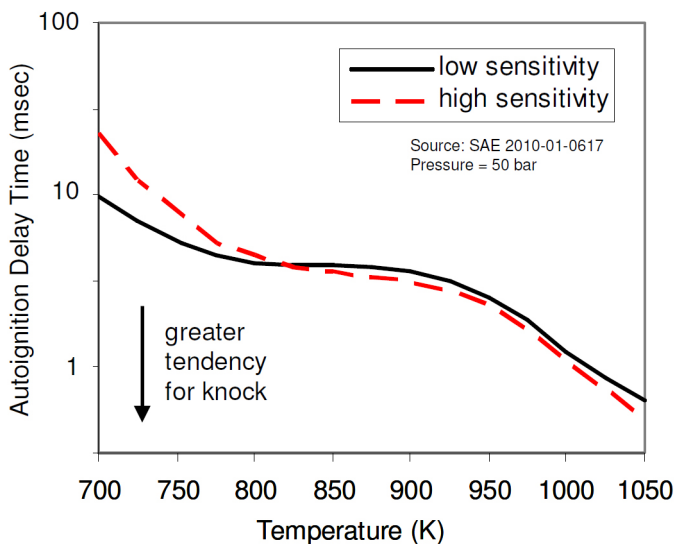


Figure 5. Autoignition delay time vs. temperature.

A fuel with high sensitivity has greater temperature dependence of the autoignition kinetics compared to a PRF or a fuel with low sensitivity. Therefore engine conditions which reduce the temperature of the unburned gas result in a greater improvement of performance for a high sensitivity fuel compared to a low sensitivity fuel. These conditions include retarded combustion phasing (reduced adiabatic compression of the end gas during combustion), increased charge cooling due to fuel vaporization (lower charge temperature), lower compression ratio (reduced compression of the end gas), and lower inlet temperature (lower initial temperature at the start of compression). Data will be shown in this paper which illustrates these effects.

Because a fuel's sensitivity to unburned gas temperature plays a key role in understanding the knock behavior of the fuel, the focus in this paper is on the effect of engine operating conditions on unburned gas temperature. However, it should be noted that autoignition kinetics are also affected by the pressure of the unburned end gas [4].

TEST HARDWARE

This study used the single cylinder engine hardware described in [11] and shown below in Figure 6, with the exception of the piston bowl. For this study, the piston dome did not include a bowl for cold start catalyst heating mode. Three compression ratios were used during the course of testing, 10.0:1, 12.0:1, and 14.0:1. Piston domes are shown in Figure 7.

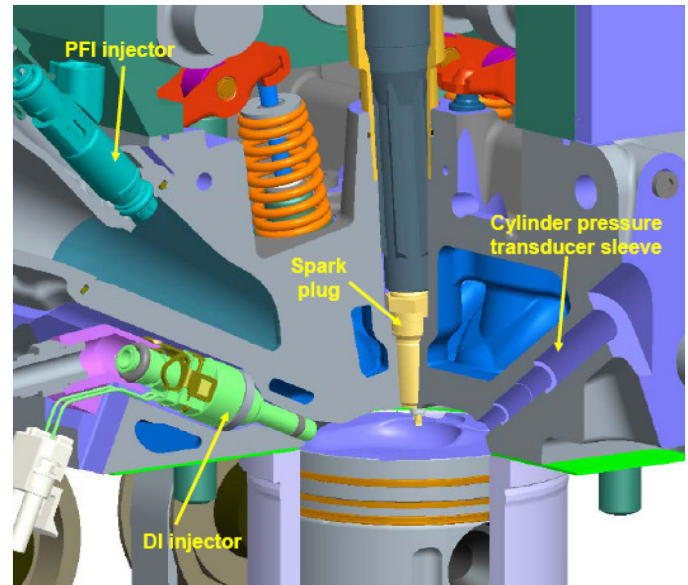


Figure 6. Single cylinder engine hardware.

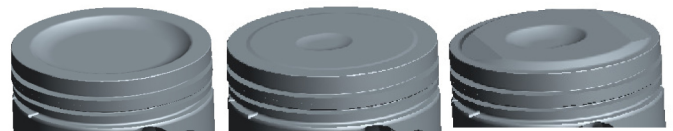


Figure 7. Piston domes for 10:1, 12:1, and 14:1 CR.

The engine is a state-of-the-art automotive design with high tumble intake ports. The engine structure supports a peak cylinder pressure (mean + 3 sigma) of 160 bar, which is required to determine the knock limit of the high ethanol blends. The engine is equipped with both direct injection (DI) in the side location and port fuel injection (PFI). As described in detail in [11], the fuel targeting and spray pattern were validated for both the DI and PFI fuel systems. In addition, the capability to supply fuel upstream in the heated intake piping was added in the test cell, and this is termed "upstream fuel injection" (UFI) in this paper. A schematic of the single cylinder engine showing the fuel injector locations is shown in Figure 8.

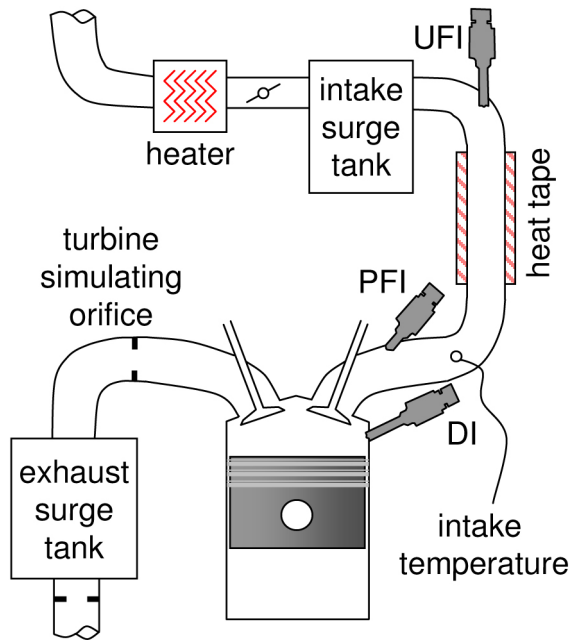


Figure 8. Schematic illustrating fuel injector locations.
UFI injector is ~1 meter from the cylinder head.

TEST CONDITIONS

For most of the testing of this study, a constant inlet temperature of 52°C was set in the intake runner upstream of PFI. The choice of inlet temperature is an important factor in knock testing, as it influences a fuel's knocking behavior relative to that of PRF blends. (PRF blends are binary blends of isooctane and n-heptane, where the octane number of the fuel is defined as the percentage of isooctane.) Fuels with high sensitivity are less knock resistant at high temperature conditions compared to a PRF blend having an equivalent octane rating at a lower temperature condition [4]. The 52°C inlet temperature was chosen for three reasons: 1) for consistency with the RON test, since it has been shown that the knock behavior of a fuel in a modern engine more closely relates to RON than to MON, 2) to increase the tendency to knock relative to cooler inlet temperature, and thereby improve the likelihood of achieving knocking conditions with the high ethanol blends within the structural peak pressure constraint of the engine, and 3) to replicate the high observed inlet temperature of modern intercooled boosted engines under adverse, but realistic, operating conditions.

Valve overlap was set at a fixed value of 20°, with 10° bTDC intake valve opening and 10° aTDC exhaust valve closing. Although modern gasoline turbocharged direct injection (GTDI) engines with variable cam timing employ high valve overlap at low engine speeds to scavenge the exhaust gas out of the cylinder, a fixed valve overlap was chosen for this study to limit the scope of the testing to a reasonable level when testing a large number of fuels. Another reason to avoid scavenging is that the in-cylinder

lambda (the air-fuel ratio divided by the stoichiometric air-fuel ratio) is affected by scavenging if fresh air blows through the cylinder. Evaluation of a fuel's knock resistance would be confounded by this difference in lambda. Additionally, correlation of knock models with the test data is simpler if the in-cylinder lambda is equal to the measured exhaust lambda.

Coolant temperature was set at 100°C to be consistent with both the RON and MON tests. A 25 mm orifice was used in the exhaust piping to simulate the restriction imposed by a turbocharger turbine. This orifice was sized such that the cylinder pressure during the exhaust stroke of the single-cylinder engine matched that of the multi-cylinder turbocharged engine at 2500 rpm and high load with the same valve timing.

PFI injection timing was set such that the end of injection was 15° before BDC of the intake stroke. Open valve injection (OVI) was chosen for two reasons: 1) to maximize the amount of charge cooling due to fuel vaporization in the cylinder, and 2) to avoid smoke under boosted conditions. With closed valve injection under throttled conditions, backflow of hot exhaust into the intake port helps vaporize and mix the fuel, however, under boosted conditions this backflow does not occur. Fuel which has been sprayed into the intake port which has not vaporized can then enter the cylinder as very large droplets and consequently produce particulates.

The test fuels were evaluated at the engine speeds and compression ratios shown in Table 3. The fuels shown as solid symbols in Figure 1 were tested at 10:1 CR, with the exception of E94-R110 and E97-R109. A subset of these fuels was also tested at 12:1 CR. In addition, the high ethanol content fuels and isooctane were tested at 14:1 CR.

Table 3. Matrix of engine test conditions.

CR	10:1			12:1			14:1		
RPM	1500	2500		1500	2500	3500	1500	1500	2500
Inlet Temp (°C)	52	52		52	52	52	Varied	52	52
Isooctane	x	x		x	x	x	x	x	x
B82E20-R94	x	x							
B82E30-R98	x	x							
B88E0-R88	x	x		x					
B88E10-R93	x	x		x	x	x	x		
B88E20-R97	x	x		x					
B88E30-R101	x	x		x					
B88E50-R105	x	x		x	x	x	x	x	x
B88E75-R108	x	x		x			x	x	x
B92E0-R92	x								
B92E10-R96	x			x					
B92E20-R100	x			x					
B95E0-R95	x								
B95E10-R99	x			x					
B97E0-R97	x	x		x					
B97E20-R103	x								
E97-R109								x	x
E94-R110								x	x

TEST PROCEDURE

Inlet pressure was swept at constant engine speed, and spark timing was set to borderline knocking at each inlet pressure. The resulting combustion phasing, as measured by the location of 50% mass fraction burned in degrees aTDC (CA50), was plotted as a function of the 720°-based Net Mean Effective Pressure (NMEP), as shown in the top plot of Figure 9. (Note that in this paper the x-axis scale of these plots was adjusted according to the range of the data.)

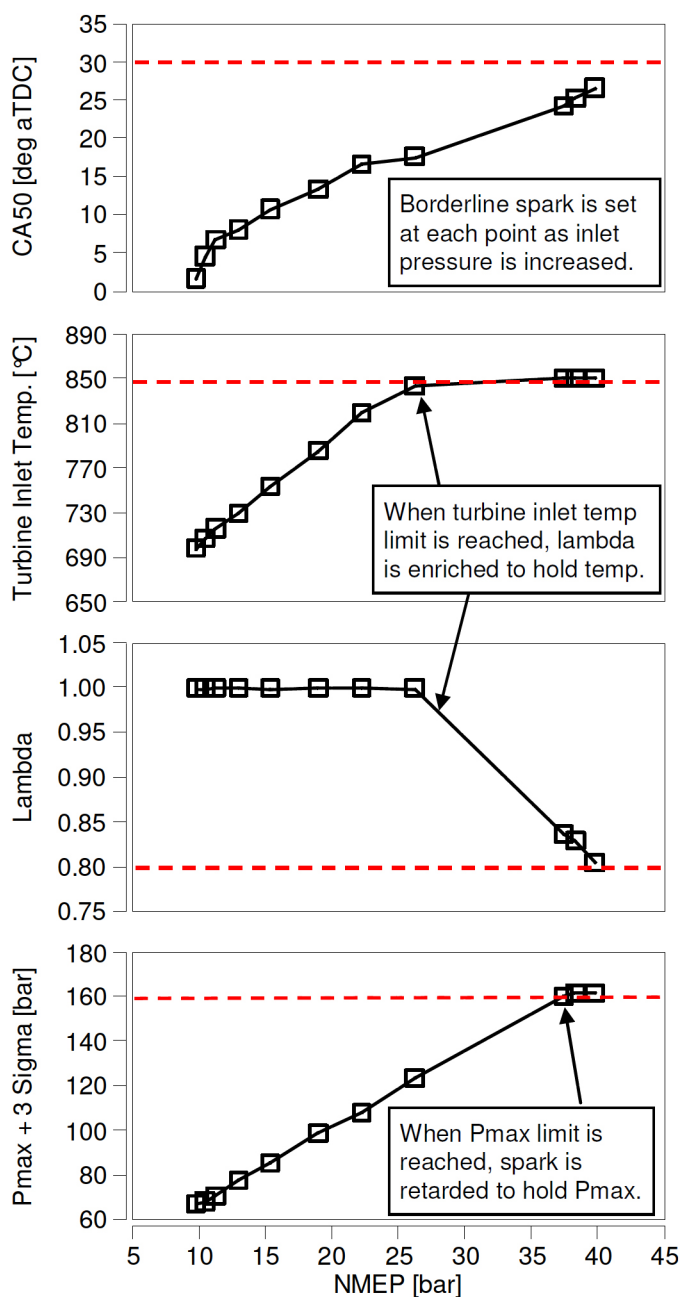


Figure 9. Illustration of test method and operating limits.

At light loads, spark was advanced beyond MBT to achieve borderline knocking. (MBT, or “Minimum spark advance for Best Torque”, is the spark timing for

thermodynamic optimum combustion phasing at a given engine air flow.) As inlet pressure and NMEP are increased, the engine becomes more knock-limited and spark timing must be retarded, resulting in later CA50. Based on experience with boosted GTDI engines, a testing limit of 30° aTDC CA50 was set. Beyond a CA50 of 30° aTDC, engine combustion stability tends to become unacceptable.

As NMEP increases and combustion phasing is retarded, the exhaust temperature increases both due to the higher load, which reduces heat transfer per unit mass, and due to degraded efficiency, which results in increased energy in the exhaust gas. Typical modern gasoline engine wastegated turbochargers have a turbine inlet temperature limit of 950°C. For a single cylinder engine, a limit of 850°C has been found to correspond to a multi-cylinder engine exhaust temperature of 950°C, due to the reduced exhaust mass flow of the single cylinder engine compared to a multi-cylinder with 3 or more cylinders exhausting into the same exhaust manifold. When the exhaust temperature reaches the limit of 850°C, lambda must be enriched to control exhaust temperature to the limit (second and third plots of Figure 9). An enrichment limit of 0.8 lambda was set for this study. Since enrichment suppresses knock, data at rich conditions cannot be directly compared to data at stoichiometry, and hence all data shown in this paper is at stoichiometry unless noted otherwise.

As inlet pressure and NMEP are increased, the peak cylinder pressure can also increase, depending on the amount of combustion phasing retard. If the peak cylinder pressure reaches the engine structural limit of 160 bar (mean + 3 sigma), then the spark timing must be retarded to limit the peak pressure as inlet pressure is further increased (bottom plot of Figure 9). Note that in this event the data no longer represents a knock-limited condition, and therefore does not quantify the knock resistance of the fuel, but does illustrate the increased NMEP potential of the fuel.

The test series is completed when the CA50 limit or the lambda limit is reached, since further increase of inlet pressure would require further spark retard, and one of these two limits would be exceeded.

EFFECT OF ETHANOL CONTENT ON KNOCK LIMIT WITH DIRECT INJECTION

The effect of ethanol percentage on knock limit with direct injection at 10:1 CR at 1500 rpm (with 88 RON gasoline blendstock) is shown in Figure 10. With the low ethanol content fuels, the engine appears to be more knock-limited than a typical GTDI engine, achieving only about 9 bar NMEP at 1500 rpm at a CA50 of 30° aTDC with B88E10-R93 fuel. However, this same single cylinder engine demonstrated values of NMEP in [11] typical of a modern GTDI engine, and the multi-cylinder engine with the same combustion system also achieves typical values [12]. There are two reasons why the engine is more knock-limited in this study: 1) GTDI engines use variable camshaft timing to

increase valve overlap at low engine speed for scavenging of residual exhaust gas from the cylinder, whereas this study was run with a constant valve overlap of 20°, and 2) 52 °C is higher than the inlet temperature that is usually set when assessing full load performance on engine dynamometer (even though higher temperatures can be observed under adverse conditions in the vehicle).

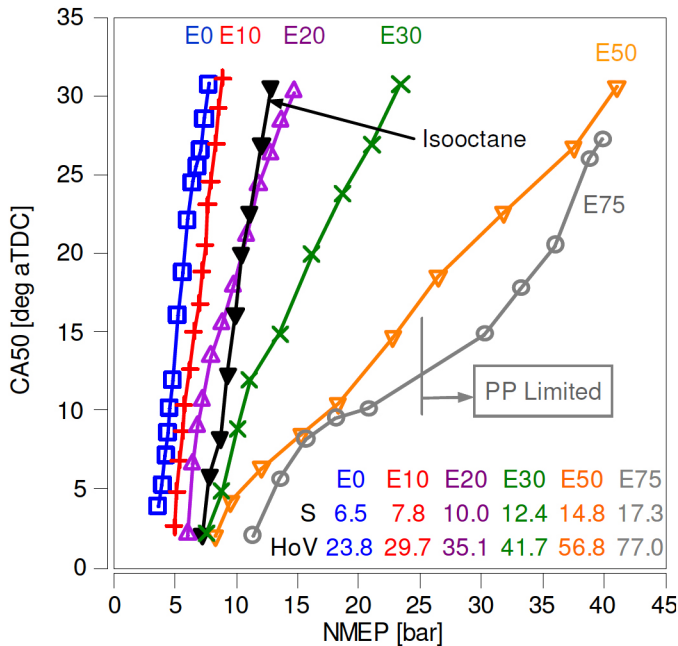


Figure 10. CA50 vs. NMEP for 88 RON blendstock ethanol blends at 10:1 CR and 1500 rpm with DI.

As shown in Figure 10, the low ethanol content fuels exhibit a very steep slope of CA50 vs. NMEP. As ethanol content increases, the slope of CA50 vs. NMEP tends to decrease. For example, NMEP increases only 4 bar as CA50 is retarded from 4° aTDC to 30° aTDC with B88E0-R88 fuel. B88E10-R93 and isooctane have a similar slope. However, NMEP increases by 32 bar for the same change in CA50 with B88E50-R105 fuel. This change in slope is a consequence of increasing HoV and sensitivity as ethanol content is increased. The HoV in kJ/kg of air and sensitivity as determined by RON minus MON for this series of fuels are shown in Figures 3 and 4, respectively, and tabulated in Figure 10.

As spark timing and combustion phasing are retarded, the unburned gas temperature decreases even though the inlet pressure and knock-limited NMEP increase, as illustrated by the model results shown in Figure 11. These results were calculated using AVL's gas exchange and combustion analysis (GCA) model [13,14], which uses the crank angle resolved intake, exhaust, and cylinder pressure measurements as input to a one-dimensional simulation.

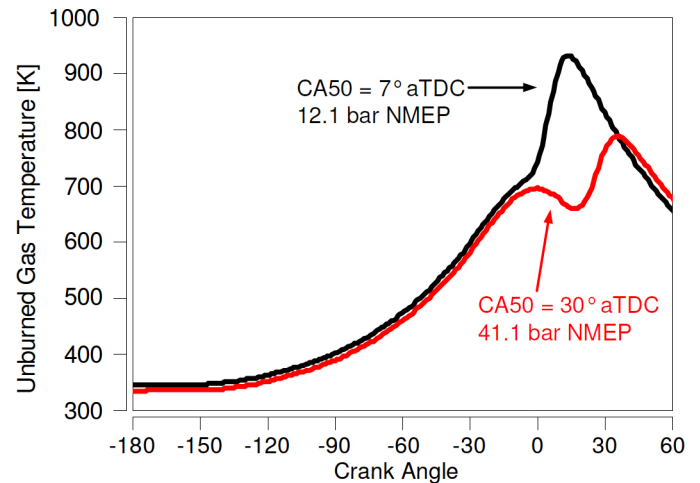


Figure 11. Calculated unburned gas temperature comparing CA50 = 7° aTDC at 12.1 bar NMEP and CA50 = 30° aTDC at 41.1 bar NMEP for B88E50-R105 fuel.

The unburned end gas is adiabatically compressed as the cylinder pressure increases during combustion. The increase in temperature due to this adiabatic compression is a function of the pressure ratio according to the polytropic relationship given in Equation 1, where conditions 1 and 2 correspond to the temperature and pressure of the end gas before and after adiabatic compression, respectively, and γ is the polytropic exponent.

$$T_2 = T_1 \cdot \left(\frac{P_2}{P_1} \right)^{(\gamma-1)/\gamma} \quad (1)$$

Note that it is the pressure ratio and not the absolute pressure which affects the unburned gas temperature. Retarding combustion phasing causes combustion to occur later in the expansion stroke, and consequently the cylinder volume during combustion is larger. Because of this, the pressure rise is reduced compared to the pressure rise that would have occurred for the same heat release in a smaller cylinder volume. As a result, the pressure ratio and temperature of the end gas are reduced as combustion phasing is retarded.

As fuel sensitivity increases, the reduction in unburned gas temperature due to later combustion phasing has an increased effect on the autoignition kinetics of the fuel [4], as shown in Figure 5. The reduction in unburned gas temperature is further enhanced by the charge cooling of DI, with a consequent additional effect on the autoignition kinetics. These factors result in a greater increase in knock-limited NMEP as CA50 is retarded. This is discussed further in the next section.