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Estimates of DI Hydrous Ethanol Utilization for Knock Avoidance and Comparison to a Measured and Simulated DI E85 Baseline

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Abstract

The use of hydrous ethanol DI fuel for knock avoidance in conjunction with PFI gasoline is investigated. The properties of the hydrous ethanol are described and constraints on the ethanol-water-hydrocarbon mixtures quantified. After a selection of the appropriate water-ethanol blends, calculations are performed using an engine simulation coupled to a kinetic calculation to determine the required hydrous ethanol for knock-avoidance. The volume requirements of hydrous ethanol at two levels of water concentration are then compared to measured and simulated values for DI E85.

I. Introduction

In this report, the advantages of using hydrous ethanol as a directly-injected antiknock second fuel in conjunction with port-injected gasoline is discussed. The advantages of using directly-injected E85 as a secondary antiknock fuel has been described recently [Agarwal]. By using hydrous ethanol, having a higher heat of vaporization than E85, the possibility of decreasing the rate of consumption of the antiknock DI fuel is explored. Decreased rate of consumption will result in longer refill intervals for a given size tank for the antiknock fuel or will decrease the required tank size for a given refill interval.

Hydrous ethanol is being used in Brazil and elsewhere in dedicated alternative fuel vehicles, as well as in flex fuel vehicles which experience only moderately cold conditions (~-10C). The water-ethanol blend of choice in these fuels correspond closely to the distillation azeotrope containing approximately 5% water.

Blends of water-ethanol-gasoline [HE Blends] are being proposed as means of decreasing the cost and energy requirements of using pure ethanol. Blends with water concentration higher than that of the azeotrope are also being investigated in fleets. [Renergie]

For the purpose of decreasing the consumption of the alcohol blends, an antiknock fuel with increased heat of vaporization is desired, achievable through increased water content. In section II, the properties of ethanol-water-hydrocarbon blends are described. A selection of the blend that satisfies the freezing and phase stability requirements is chosen. The use of this blend as a DI antiknock agent is investigated under conditions conducive to knock, i.e., relatively low rpm and high torque. The model to describe the engine is presented, as well as the results of chemical kinetics calculations.

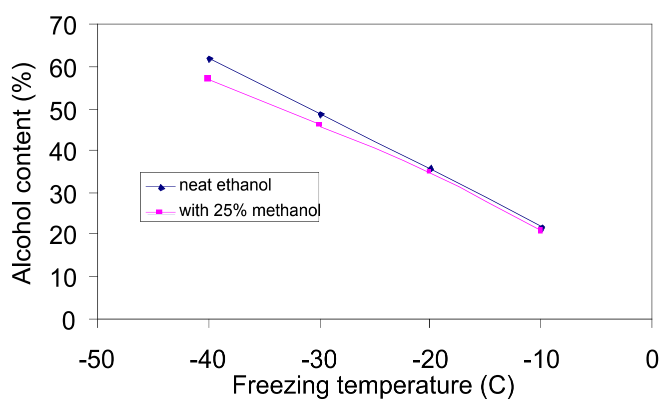


Figure 1. Freezing temperature of ethanol-methanol-water blends

II. Hydrous ethanol properties.

Two important characteristics of hydrous ethanol are the freezing point and the maximum allowable content of hydrocarbons, such as gasoline, prior to the onset of phase separation. Both constrain and limit the selection of possible alcohol blends that can be used as primary fuels in their own right or as knock-suppressing DI fuels.

In the case of ethanol water mixtures, the freezing point as a function of the alcohol content (by volume) is shown in Figure 1. Neat ethanol has a low freezing temperature, of approximately 160 K (not shown). However, the freezing temperature increases rapidly with water addition. To satisfy the constraint of remaining a liquid at -40 C, blends of less than about 40% water are needed.

For general use in the North America market, a fuel is required to remain liquid at temperatures as low as –40C. Thus, ethanol-water blends with ethanol fraction of 60% or greater (by volume) are required, with a 60-40 mix being the minimum. By mass, this mix is about 55-45 ethanol-water.

Methanol helps decrease the total alcohol content at a given freezing temperature slightly. Figure 1 also shows the freezing point vs. alcohol percentage (by volume) for a 75-25 ethanol-methanol mixture.

The phase stability of water-ethanol-hydrocarbon mixtures has been studied recently [Johanes]. Their results are shown in Figure 2. They explored a limited temperature range, with a minimum temperature of -25 C. Even at this moderately cold temperature there is phase separation in the ethanol-water-gasoline system. The maximum water concentration at –25 C for 6% gasoline in the blend is about 20%. The maximum water level will decrease even further at more extreme lower temperatures.

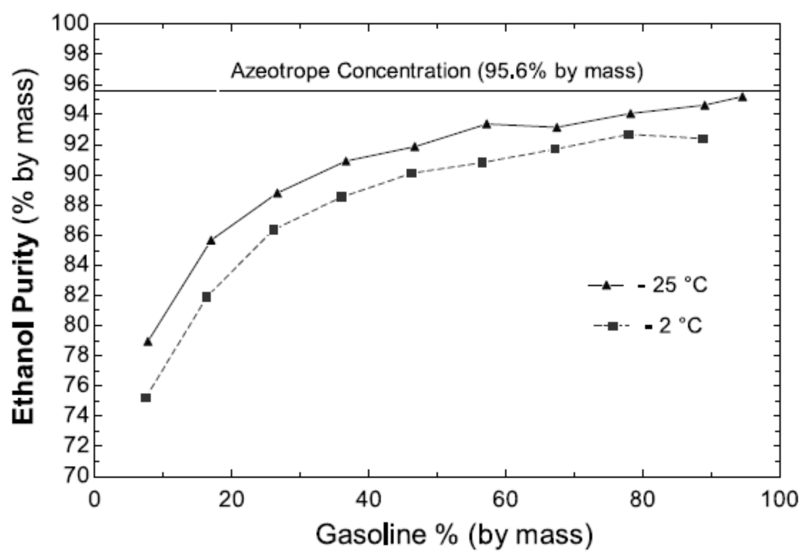


Figure 2. Ethanol purity (ethanol concentration in ethanol-water blends) required to avoid phase separation as a function of the gasoline concentration at two different temperatures.

Based upon these requirements, it was decided to use a 60-40 blend of ethanol-water, h40EtOH, with about 1% gasoline (mainly as a denaturant).

In order to study the implications of relaxed requirements on the hydrous ethanol on knock, a second mixture was investigated. The second mixture was a 30-70 ethanol-water mixture (about 25%-75% water-ethanol by mass), h70EtOH. This mixture freezes at about –15 C, good for a large fraction, but not all of the US, even in winter. With respect to phase separation, Figure 2 indicates that a 10% gasoline, 90% hydrous ethanol (25% water, 75% ethanol by mass) experiences phase separation at –2C. Because of the limited gasoline blending capability, as in the previous case, it will be assumed in this study that the hydrous ethanol contains no gasoline. Concentrations of approximately 1% gasoline in an actual blend of hydrous ethanol for denaturing purposes would have little or no effect on the results or conclusions of this work.

III. Engine performance when using DI E85

In this section, the results of the engine calculations for the parameters that result in borderline knock with E85 are presented and also compared with measured data. A speed-load point at 2000 rpm and 25.7 bar NMEP (IMEP720) is used throughout.

The p-V diagram comparison between the model and the data from a single cylinder engine is shown in Figure 3. Similarly, Figure 4 shows the cylinder pressure as a function of the CA (crank angle) for both the measured data and the simulation. Figure 5 shows the pressure slightly downstream of the exhaust port and upstream of an orifice restriction inserted to represent the backpressure of a turbine. Figures 3, 4 and 5 indicate good agreement between the model developed by Blumberg using GT-Power [Blumberg 2009] for a single cylinder EBS-type engine and the experimental data. The experimental results were provided by a Ford/AVL team from data obtained from a single cylinder engine (SCE) using E85 as the directly injected antiknock agent and port-injected gasoline as the primary fuel.

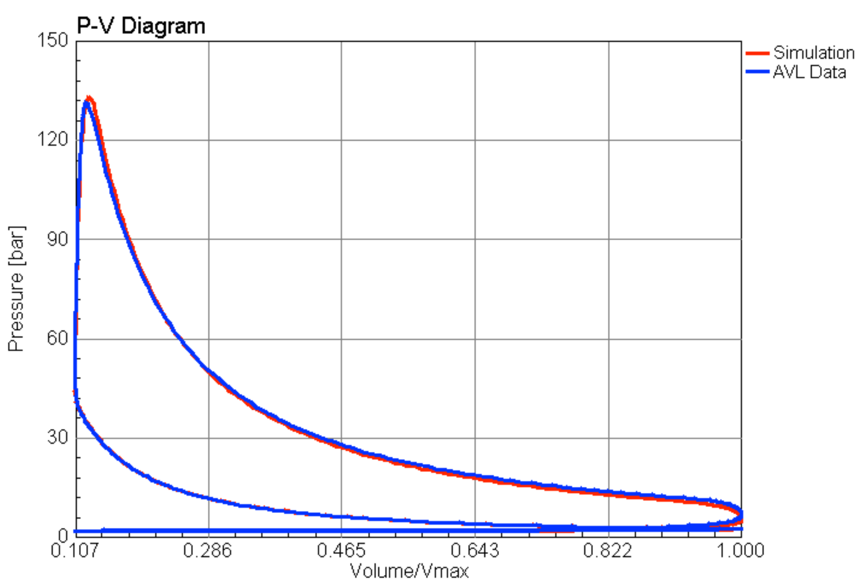


Figure 3. p-V diagram for the engine conditions in the SCE, experimentally determined by AVL/Ford, and the values from the model developed by Blumberg.

The figures show that the model developed by Blumberg closely reflects the conditions of the engine. There are minor discrepancies in the exhaust pressure, which shows some wave phenomena that are not reproduced by the model, although the amplitude and phasing of the peak exhaust pressure match the measured data very well.

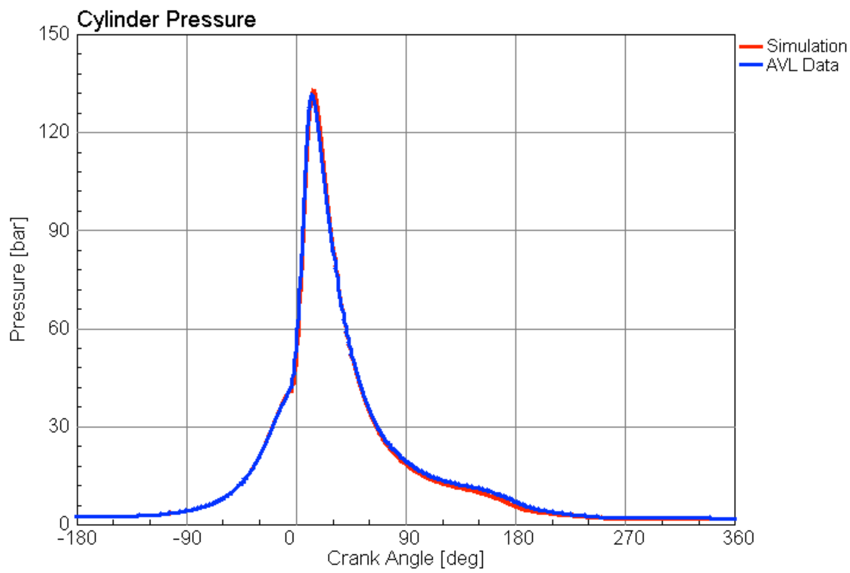


Figure 4. In-cylinder pressure for the cylinder conditions in the SCE, experimentally determined by AVL/Ford, and the values from the model developed by Blumberg.

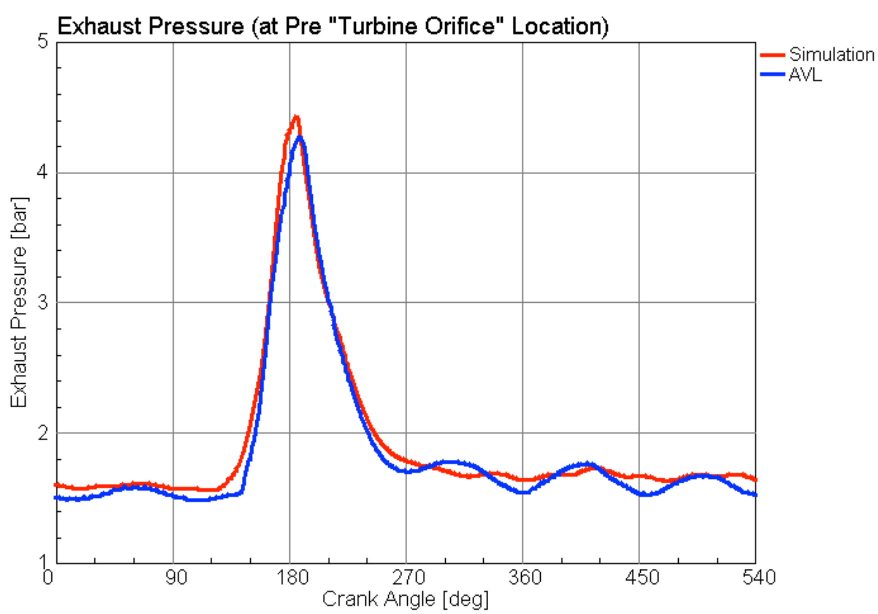


Figure 5. Exhaust pressure for the engine conditions in the SCE, experimentally determined by AVL/Ford, and the values from the model developed by Blumberg.

The model has been extended to the use of hydrous ethanol. The complete properties of a "fuel" that contains a 60-40 ethanol and water mix (by volume), h40EtOH, were developed separately and subsequently built into GT-Power using appropriate objects available in the software. Key properties included liquid density, heat of vaporization and heat capacities in both the liquid and vapor states. In the next section, comparison between the models for DI E85 and DI h40EtOH hydrous ethanol are compared.

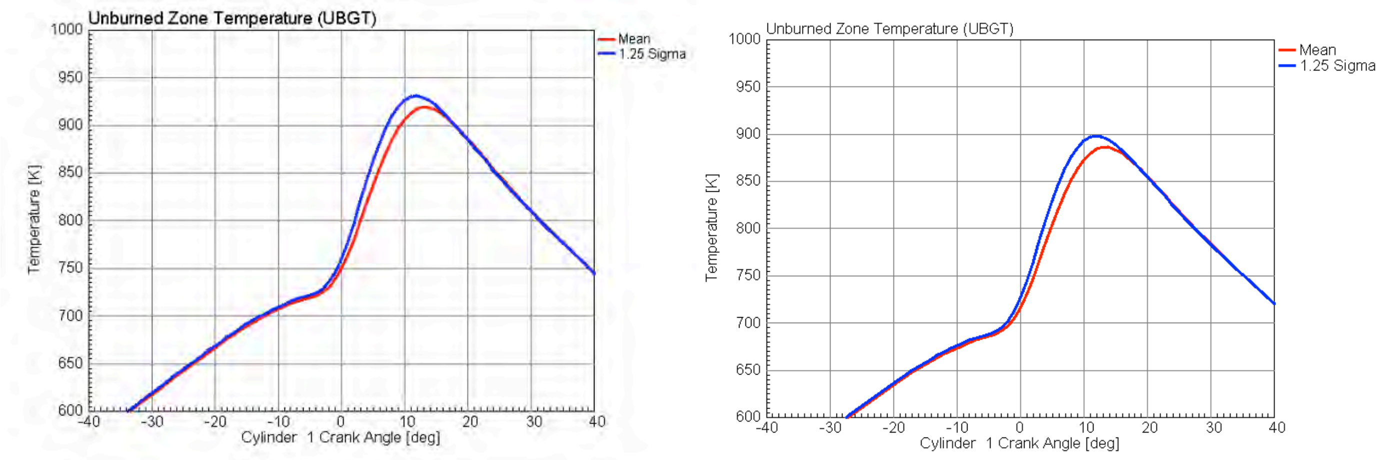
IV. Engine conditions when operating with a 60-40 hydrous ethanol blend

The amount of hydrous ethanol required to suppress knock to a borderline condition was determined using the model described above. For this purpose, a cycle with combustion parameters at 1.25 standard deviations from the mean (i.e., the crank angle at 50% fuel fraction burned advanced and the 10%-90% burn duration shortened with respect to the mean) was employed to represent the fraction of cycles that exhibit knock . In this section, the comparison between the engine conditions using DI E85 and DI h40EtOH hydrous ethanol at borderline knock are discussed. In the next section, the knock calculations are described.

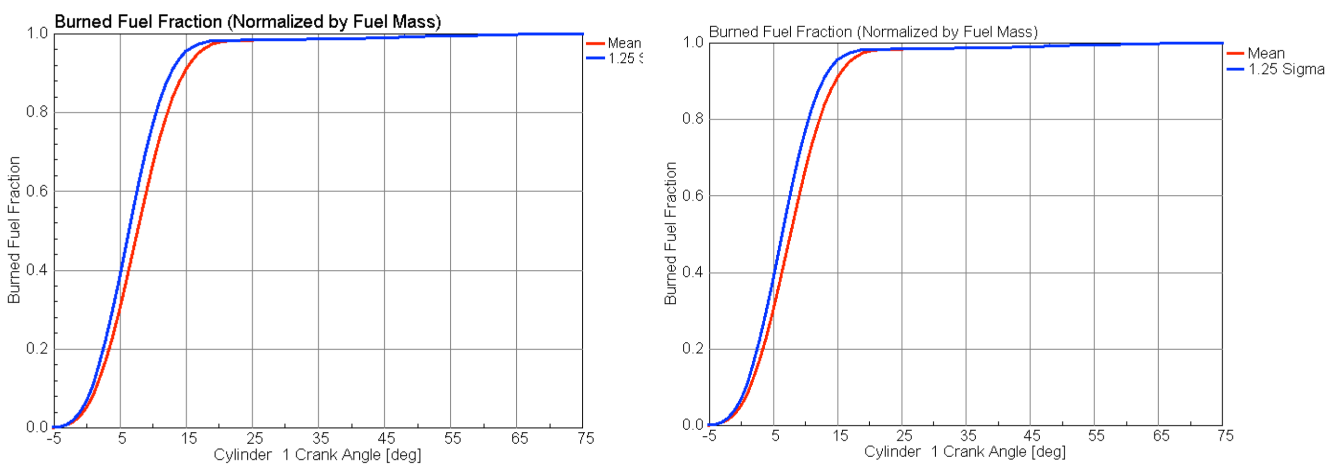
The results are shown in Figure 6. At the left of each picture, the conditions with DI E85 are shown, while at the right the similar conditions with DI h40EtOH hydrous ethanol are displayed. The conditions for the average cycle as well the 1.25σ cycle are shown in each graph.

It is difficult to distinguish between the E85 and hydrous ethanol curves for the cylinder pressure and the unburned fuel fraction vs. crank angle (Figures 6(b) and 6(c)). As the output power level (NMEP) r and the combustion characteristics are kept constant, this is to be expected.

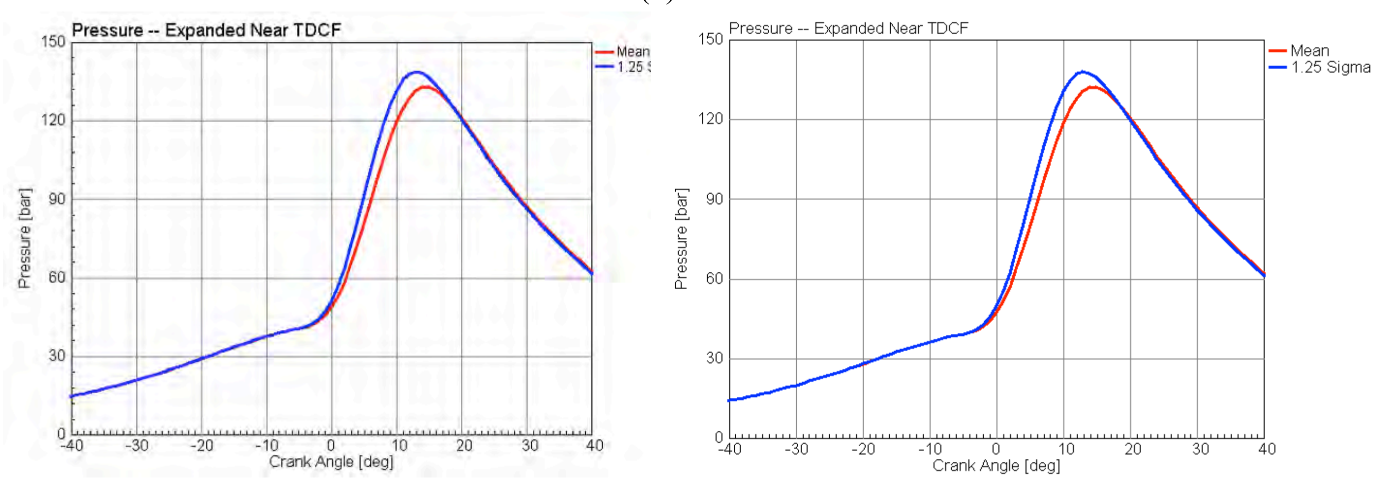
On the other hand, the unburned gas temperatures (UBGT) are substantially different, as shown in Figure 6(a). The peak UBGT is about 50K lower for the case of h40EtOH hydrous ethanol. This is a result of the difference in chemical composition of the overall fuel-air mixtures with hydrous ethanol vs. those of E85 and will be described more fully in the next section. It is interesting to note that the temperature difference between hydrous ethanol and E85 is relatively constant through the precombustion, combustion and post combustion phases that are shown in Figure 6.



(a)



(b)



(c)

Figure 6. Engine conditions at borderline knock for DI E85 (left) and h40EtOH hydrous ethanol (right); (a) unburned gas temperature; (b) burned fuel fraction; and (c) cylinder pressure.

V. Knock calculations with h40EtOH

The chemical kinetics model employed for evaluating autoignition (knock) has been described elsewhere [Blumberg, Bromberg]. The chemical mechanism of Curran *et al* [Curran] has been used. It includes the Marinov mechanism for ethanol [Marinov].

The kinetics follow the conditions in the unburned gas mixture obtained from the GT-Power simulation. The computation is carried out starting at 25 CA BTDC, before which precombustion kinetics are not active. Using the pressure vs. CA values from GT-Power, adiabatic conditions are assumed to calculate the unburned gas-air mixture temperature during compression and combustion.

It has been shown in the E85 studies that the combined temperature and kinetic calculations underestimate the conditions for knock in comparison with the measured results. Indeed, it has been necessary to increase the initial temperature in the chemical kinetic calculations by about 25K to have knock occur with a substantial amount of unburned fuel remaining (> 10%).

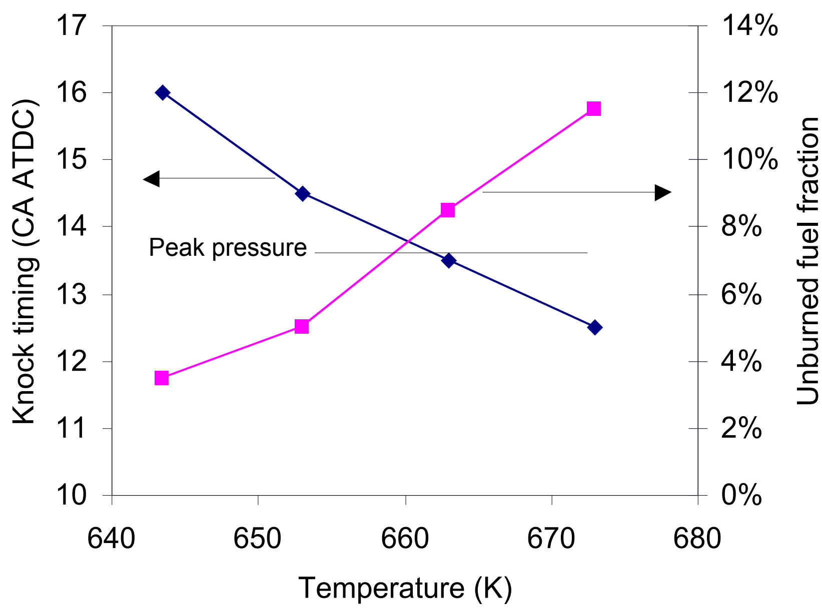


Figure 7. Knocking conditions for 2000 rpm/25.7 bar (DI E85) as a function of the initial temperature of the calculations at 25 CA BTDC.

As shown in Figure 7, the initial temperature of 643 K calculated using GT-Power results in knock timing (*i.e.*, autoignition of the unburned fuel-air mixture) of 16 CA ATDC with only about 4% of unburned air-fuel mixture remaining. To obtain knock at conditions of peak pressure, with 10% of unburned fuel mixture, it is necessary to increase the initial temperature by about 25K.

The engine conditions for borderline knock with E85 are shown in Table 1.

Table 1
GT-Power conditions for borderline knock with DI E85 at low rpm/high NMEP when simulating the SCE.

rpm	2000
Inlet Press. Expt'l (bar)	1.96
Inlet Press. Adjusted (bar)	2.05
NMEP (bar)	25.44
Mass Fraction E85	0.787
Volume Fraction E85	0.781
Volume Ratio (E85/Indol)	3.558
A/F (Stoich)	10.899
Trapped F/A	0.092
Trapped A/F	10.898
Airflow (kg/hr)	82.466
Total Fuel Flow (kg/hr)	7.566
E85 Flow(kg/hr)	5.955
Indolene Flow (kg/hr)	1.610
Indicated Thermal Eff.	39.246
Residual mass (%)	2.758
CA50	6.38
CA1090	11.52

The procedure used to determine the required h40EtOH hydrous ethanol at borderline knock reproduces the methodology and output shown in Figure 7 as employed for gasoline and DI E85. The point chosen for the match has been the one without the increase in temperature to predict knock with 10% of the fuel unburned, that is, it is assumed that an engine with gasoline + DI hydrous ethanol will knock when the unburned fuel air mixture autoignites at 16 CA ATDC, with about 4% remaining unburned-fuel mixture. The amount of DI h40EtOH hydrous ethanol was varied in GT-Power, and the resulting pressure/temperature were used in the chemical kinetics calculations, until this set of conditions was met.

Table 2
The conditions that result in knock with DI h40EtOH

rpm	2000
Inlet Press. Expt'l (bar)	1.96
Inlet Press. Adjusted (bar)	1.96
NMEP (bar)	25.452
Mass Fraction EHY	0.500
Volue Fraction EHY	0.453
Volume Ratio (EHY/Indol)	0.830
A/F (Stoich)	9.691
Trapped F/A	0.103
Trapped A/F	9.691
Airflow (kg/hr)	81.290
Total Fuel Flow (kg/hr)	8.392
EHY Flow(kg/hr)	4.199
Indolene Flow (kg/hr)	4.190
Indicated Thermal Eff.	39.533
Residual mass (%)	2.909
CA50	6.38
CA1090	11.52

Table 2 shows the resulting conditions that result in the autoignition of gasoline + DI h40EtOH hydrous ethanol at 16 CA ATDC. As indicated in the Tables 1 and 2, the combustion parameters were not changed. It has been determined experimentally [Brewster] that ethanol-water (80-20) mixtures decreases the flame speed (and increases the combustion time), but this is when ALL the fuel is alcohol-water, and it is injected directly. In the present case, as only 50% of the total fuel is being directly injected, combustion parameters have not been adjusted from the E85 baseline.

There is a slight increase in efficiency for hydrous ethanol (0.25% absolute). This is a result of the lower combustion temperatures which reduce heat transfer from the burned gases and decrease the extent of gas dissociation at peak thermal conditions. The effect is small.

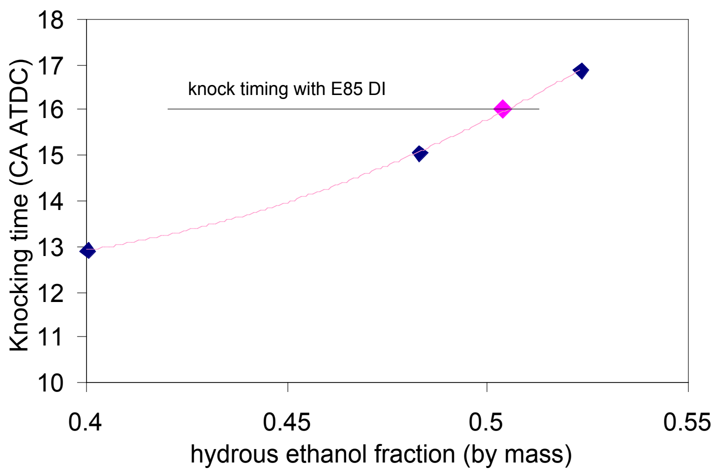


Figure 8. Dependence of knocking time on h40EtOH hydrous ethanol fraction (by mass)

Figure 8 shows the dependence of the knock timing with the fraction of DI h40EtOH. With increasing fraction of DI h40EtOH, the time of knock is delayed as the air/fuel mixture is less prone to autoignite. Also shown in Figure 8 are conditions at which the code predicted autoignition and knock was observed experimentally in the SCE with DI E85. It corresponds to autoignition at 16 CA ATDC. These conditions were chosen to identify the onset of knock with h40EtOH. Thus, it is expected that the engine would be at borderline knock with a mass fraction of approximately 50% h40EtOH.

The rates of consumption of the different fuels (indolene, E85 and h40EtOH) are shown in Table 3. The refill time for the DI E85 case was normalized to 1. For the same tank volume, using h40EtOH would result in over a 40% longer time interval between refills.

VI. Knock calculations with h70EtOH

In this section, the effects and results of higher eater content in the hydrous ethanol blend are explored. As the output power and combustion characteristics have been kept constant, both the cylinder pressure and the fraction of unburned fuel mixture are about constant as a function of the hydrous ethanol directly injected.

As part of this work we evaluated the temperature at 25 CA BTDC as a function of the amount of h70EtOH injected. This value is the starting temperature for the calculations.

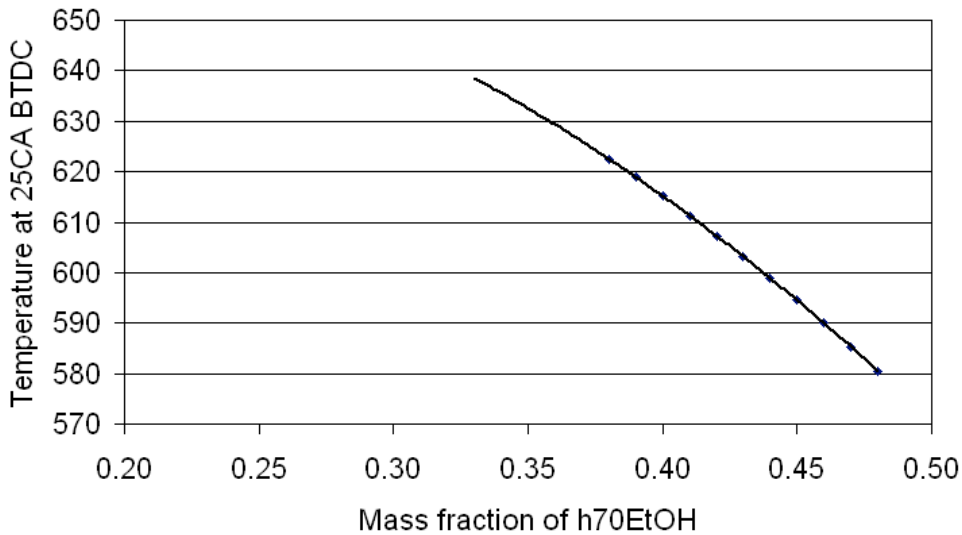


Figure 8. Self-consistent temperatures (for +1.25 s) calculated as a function of the ratio of h70EtoH directly injected into the engine (by mass).

The knock model has been used to determine knocking conditions similar to those of the code when using E85, as in the previous section. It is determined that the ratio of h70EtOH to total fuel flow (by mass) that results in comparable knocking conditions as those of E85 is ~ 44%.

Table 3

Ratios of rates of consumption (by mass and volume) and refill time for antiknock fluid consisting of E85, h40EtOH or h70EtOH

	Antiknock heat of vaporization kJ/kg	Antiknock mass fraction	Antiknock Mass flow rate ratio	Antiknock Volume flow rate ratio	Antiknock refill interval
E85	745	0.78	1	1	1
h40EtOH	1480	0.5	0.72	0.62	1.60
h70EtOH	1900	0.44	0.68	0.55	1.82

Table 3 summarizes the results for E85, h40EtOH and h70EtOH. The third column refers to the mass fraction of antiknock agent divided by total mass of the fuel to the engine. Column 4 gives the antiknock mass flow rate ratio, normalized to the required mass flow of E85, when E85 is used as the antiknock agent. Column 5 shows the flow ratio, again normalized to the E85 flow rate. The use of hydrous ethanol decreases the ratio of the required antiknock fuel. This column indicates the rate of consumption (by volume), normalized to the rate of consumption of E85 if E85 is the antiknock agent. Thus, the flow rate of h40EtOH is about 2/3 and h70EtOH is about 1/2 that of E85, clearly indicating the reduced volumnetric consumption of these antiknock agents compared to E85.

The impact of the water at the higher water concentration is decreased because substantial total consumption rates of fluid (gasoline plus antiknock fluid) are required, as water has no heating value. Also, because ethanol has a lower heating value per unit volume than gasoline and water has none, the total amount of the fuel is higher. Table 3 also shows the normalized value of the antiknock volume flow requirement. For a given size tank, the refill time is inversely proportional to the normalized antiknock requirement. The use of hydrous ethanol decreases the refill requirement by about a factor of 2.

VII. Summary

The use of DI hydrous ethanol as a knock-suppressing fuel was investigated. It was determined that for conditions under the harshest conditions in the North American market, ethanol-water blends with ethanol composition greater than 60% (by volume) were required to prevent freezing. Similarly, at these conditions in order to maintain phase stability, the allowable hydrocarbon concentration would be small, at most a few percent.

Using this composition it was possible to determine (at 2000 rpm, ~26 bar) the utilization requirements of DI hydrous ethanol as a knock suppressant under the knock-prone engine conditions of relatively low engine speed and high output NMEP. It was determined that the volume requirement of the secondary fuel, relative to an E85 baseline, was decreased by about 40% and that the range/refueling interval was increased by about 40%.

Somewhat higher increases of the range and refueling interval can be achieved if higher concentration of water are allowed, either during warmer months or at less northerly latitudes. Increasing the water fraction to 70 percent by volume decreases the ratio of antiknock fuel requirement but, at the same time, slightly increases the total volume requirement. The net effect is to decrease the antiknock fuel requirement by another 10%.

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