CALCULATIONS OF KNOCK SUPPRESSION IN HIGHLY TURBOCHARGED GASOLINE/ETHANOL ENGINES USING DIRECT ETHANOL INJECTION

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Abstract

Calculations are described of knock suppression using direct ethanol injection in spark ignition gasoline/ethanol engines. The calculations show that evaporative cooling from direct ethanol injection, coupled with the high octane rating of ethanol, can be highly effective in inhibiting knock, thereby allowing use of small turbocharged engines with substantially increased efficiency. The calculations indicate that the enhanced knock suppression can allow for more than a factor of two increase in manifold pressure relative to conventional, naturally aspirated engines while also allowing for increased compression ratio. This increased pressure could enable substantial engine downsizing resulting in a part-load efficiency increase of 30% relative to conventional port fueled injected engine operation. Less than one gallon of ethanol for twenty gallons of gasoline could be sufficient to allow this engine downsizing and efficiency increase. Direct ethanol injection could provide a new opportunity to use ethanol more effectively to both displace gasoline and, more importantly, to increase gasoline utilization efficiency.

I. Introduction

The need to reduce gasoline consumption is increasing due to concerns about global warming from CO_2 emissions and the rising price of oil. Gasoline consumption can be reduced by increased engine efficiency and by expanded use of renewable fuels. Gasoline engine efficiency can be improved by use of turbocharged pressure boosting which allows the use of smaller engines. However, this approach is limited by the occurrence of knock (autoignition of the in-cylinder unburned end gas). We have described a concept where direct ethanol injection (DI) greatly increases knock resistance, allows highly turbocharged operation and substantially increases the part-load efficiency of a gasoline engine [1]. The concept could also facilitate expanded use of ethanol, a renewable fuel whose use is growing worldwide.

This DI ethanol boosted gasoline engine concept could provide an economically attractive way to increase gasoline engine fuel economy and correspondingly reduce CO_2 greenhouse gas emissions. This approach would be compatible with the anticipated production of ethanol from biomass. It could offer a substantially lower cost alternative than gasoline/electric hybrid or turbo diesel vehicles. Only a small amount of ethanol (*i.e.* less than one gallon of ethanol for every twenty gallons of gasoline) may be required to achieve a large increase in efficiency. The DI ethanol boosted gasoline engine concept could also enable high efficiency, flexible fuel use of ethanol. The direct injection turbocharged engine can be operated at high efficiency over a range of fuel use between close to 100% gasoline and 100% ethanol. The driver would have the freedom to determine the amount of ethanol use depending upon its price and availability.

Determination of the improvement in knock suppression is a fundamental issue in the consideration of this approach. The purpose of this paper is to describe exploratory calculations of the effect of direct ethanol injection upon knock suppression over a range of engine operating conditions. These calculations provide guidance regarding the amount of turbocharging, engine downsizing, and efficiency gains that can be realized and also about the required amount of ethanol. Section II describes the DI ethanol boosted gasoline engine concept. Section III describes the model used to determine the onset of knock. Section IV describes the results of engine calculations, determining the ethanol requirement for knock avoidance as a function of inlet manifold pressure, engine speed and the effect of injection timing. Section V describes the results for variations in the knock suppression approach, including the use of stratified ethanol addition and the use of other antiknock fuel additives. Conclusions are given in Section VI.

II. DI Ethanol Boosted Gasoline Engine Concept

The DI ethanol boosted gasoline engine concept employs separately controlled direct injection of ethanol into the cylinders of a gasoline engine .The direct ethanol injection provides on-demand enhancement of the octane rating of the gasoline up to very high levels (*e.g.* an octane rating of 130 or more). The on-demand octane enhancement allows pressure boosted engine operation at much higher levels of turbocharging, specific torque and specific power than would otherwise be possible. This makes it feasible for a small,

highly turbocharged engine to be used to attain the same peak performance as a much larger engine while operating much more efficiently at part load. For example, a 3.0 liter engine could potentially be replaced by an engine of about half its size, which could result in a 30% increase in fuel efficiency over a typical driving cycle. Through this ethanol knock suppression mechanism, the highly turbocharged engine may also be able to use a higher compression ratio than a conventional engine.

The ethanol injection is carried out so as to maximize evaporative cooling which occurs when it is directly injected into the engine cylinders. The gasoline can be introduced into the intake port in conventional port-fueled injection. The reduction in temperature of the fuel/air charge from the ethanol evaporative cooling is the major factor in enhancing the fuel octane rating and suppressing knock. The knock suppression allows the highly turbocharged, high torque engine operation which would otherwise not be permissible. Consequently, a small, highly turbocharged engine could provide the same maximum torque and power as a much larger naturally aspirated engine. The engine could also produce more torque in the lower rpm range than the naturally aspirated engine and thus provide a more responsive engine performance. A knock sensor can be used to determine when ethanol is needed to prevent knock. During the brief periods of high torque operation, high fuel fractions of up to 100% ethanol could be used to prevent knock. For much of the drive cycle, vehicles are operated at low torque and there is no need for the use of ethanol to suppress knock.

The ethanol is stored in a separate tank from the gasoline. The two tanks could be formed by dividing a single tank into two compartments. For example, a 20 gallon tank could be divided into a 15 gallon gasoline tank and a 5 gallon ethanol tank. Use of a 5 gallon ethanol tank could make it possible for the ethanol refueling to be required as infrequently as once every two to six months. The vehicle range would not be adversely affected by the reduced size of the gasoline tank because of the higher efficiency of gasoline use.

The fuel management system would have the capability of minimizing the ethanol consumption by employing it only when needed to prevent engine knock and providing only the amount needed to prevent knock at a given level of torque. The percentage of ethanol required would be dependent upon the amount of high torque operation used during the drive cycle.

The high efficiency turbocharged engine could be operated with a wide range of ethanol consumption from the minimum required for knock suppression (less than 5%) to use of 100% ethanol. This flexible use of more ethanol would further reduce gasoline consumption and CO_2 greenhouse gas production. The driver would have the freedom to decide on the amount of ethanol to be used based upon availability, convenience, and the price of ethanol relative to gasoline.

Emissions of air pollutants such as nitrogen oxides (NO_x), carbon monoxide and hydrocarbons would be similar to the low levels from state of the art gasoline engine vehicles and would meet stringent US standards. As in the case with state of the art

gasoline engine vehicles, highly effective emissions control would be obtained by the use of catalytic converters. In addition, ethanol generated from biomass is considered to be carbon neutral.

III. Chemical and Thermal Model of Knock

In order to provide useful predictions of knock suppression throughout the engine operating map, the end-gas conditions were modeled using a volumetric compression of the unburned end-gas mixture through a factor of 21 to represent the combination of piston compression (with a compression ratio of 10) and combustion pressure rise compression up to maximum pressure point, from the initial end-of-intake unburned mixture condition. The timing of this compression was scaled to the intake valve close angle (~50° ABC) to peak pressure angle (15-20° ATC) at the chosen engine speed. The end gas is the air/fuel mixture remaining after about 75% (by mass) of the fuel has combusted, the situation in the cylinder at crank angle of maximum pressure. It is the end gas that is most prone to autoignition (knock). At this point, the end gas attains its maximum temperature. The results for this volumetric compression ratio match the experimental pressure range determined in a single cylinder engine with a stoichiometric gasoline/air mixture at the MIT Sloan Automotive Laboratory [2]. Thus the calculations are performed for conditions close to wide open throttle throughout the engine speed range, the engine conditions where knock is a constraint.

The chemical kinetics code CHEMKIN 4.0.1 [3] was used for the chemical calculations. The CHEMKIN code is a software tool for solving complex chemical kinetics problems. This model uses the chemical model and reaction rate information based upon the Primary Reference gasoline Fuel (PRF) mechanism from Curran et al. [4] to represent the autoignition of the fuel. The mechanism includes an ethanol chemical model [5].

The effect of in-cylinder ethanol vaporization on unburned mixture temperature was calculated from the heat of vaporization of ethanol assuming the ethanol/in-cylinder air system undergoes an adiabatic mixing and vaporization process, at time of injection. The properties of gasoline and ethanol are shown in Table 1. Ethanol has a high latent heat of vaporization, about 3 times that of gasoline. The difference between the ratio of heat of vaporization to the heat of combustion is even higher, due to the lower heat of combustion of ethanol relative to gasoline. Several cases have been considered. The first one is when the ethanol is port fuel injected in the manifold. In this case, the cooling effect from the vaporization of the ethanol is small, as the ethanol is vaporized off the intake valve and manifold walls with minimal impact on the charge temperature. In the present calculations, the heat of vaporization is neglected for ethanol port fuel injection.

The second case described the direct injection of ethanol while the inlet valve is open. In this case, the effect of cooling of the charge results in drawing additional air into the cylinder. Here, the charge cooling process can be analyzed as an adiabatic constant pressure process.

The third case examined is ethanol injection after the inlet valve is closed. Thus, cooling of the charge for this case does not result in additional gas flow into the cylinder, and can be analyzed as an adiabatic constant volume process.

Table 1. Physical properties of ethanol and gasoline

		Gasoline	Ethanol
Density	(kg/m^3)	720	790
c_p	(J/kg-K)	2420	2470
Thermal conductivity	(W/m-K)	0.147	0.182
Viscosity	(kg/m-s)	0.00054	0.0012
Molecular weight	(kg/kmol)	~ 97	41
Latent heat	(kJ/kg)	306	855
Boiling temperature	(K)	399	351
Lower heating value	(MJ/kg)	44	26.9
Octane Number (ON)		87-95	115

Figure 1 shows the effect on the cylinder charge temperature due to injection of ethanol into the cylinder for injection prior to closing of the inlet valve (early injection) and injection after the valve closes (late injection). The ordinate is the ethanol fraction (by energy), the rest of the fuel being port-fuel injected gasoline, for a stoichiometric air-fuel mixture. A substantial drop in charge temperature, $\Delta T_{ethanol}$ can be achieved even with relatively small ethanol direct injection fraction.
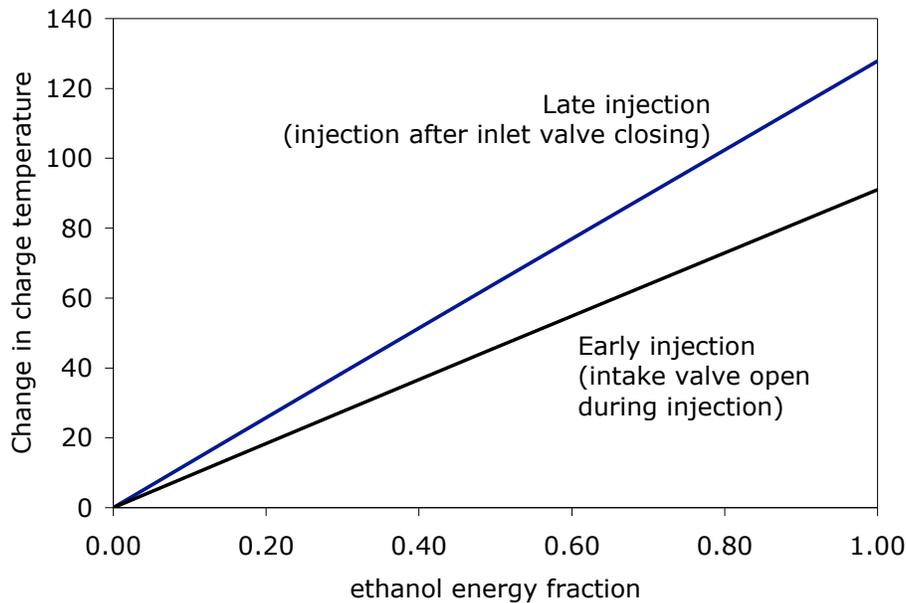

Figure 1. Change in air temperature due to ethanol direct injection, $\Delta T_{ethanol}$, as a function of the direct injected ethanol fraction (by energy) for both early ethanol injection (before the inlet valve closes, resulting in adiabatic constant pressure process) and late ethanol injection (after the inlet valve closes, resulting in adiabatic constant volume process)

We have included the effect of temperature increase due to turbocharging as follows. The increase in air temperature with turbocharging was calculated using an adiabatic reversible compression. Heat transfer in the ducting or in an intercooler decreases this temperature rise. These combined effects are modeled by assuming that the increase in temperature of the air charge into the cylinder, ΔT_{charge}, is

$$\Delta T_{charge} = \beta \, \Delta T_{turbo,ideal}$$

where $\Delta T_{turbo,ideal}$ is the air temperature increase after reversible compression due to boosting, and β is a constant. β represents the multiple processes of irreversibility of the compression (which increases ΔT_{charge}), as well as cooling or the charge due to thermal exchange in the inlet manifold and the presence of an intercooler. Values of β of 0.3, 0.4 and 0.6 have been used in the modeling. Finally, it is assumed that the temperature of the charge at start of compression (air, fuel vapor, residual burned gas) is 380 K for a naturally aspirated engine with gasoline port fuel injection. The initial in-cylinder unburned mixture temperature of the process is thus

$$T_{init} = 380 \text{ K} - \Delta T_{ethanol} + \Delta T_{charge}$$

For simplicity, in the case of late injection (after the intake valve closes), it is assumed that the ethanol is injected immediately after the valve closes and is vaporized rapidly. In practice, injection may occur after the compression cycle has already increased the temperature in the in-cylinder mixture. This increased charge temperature would facilitate ethanol evaporation but not significantly change the magnitude of the evaporative cooling drop in temperature.

The use of an effective intercooler would decrease the temperature substantially more than what correspond to $\beta \sim 0.3$. For example, in the lean-boost concept of Stokes *et al.* [6], the knock constraints demanded the use of very aggressive intercooling. Their calculated inlet charge temperature for their turbocharged engine corresponds to $\beta \sim 0.1$.

The model follows 0.7 crank revolutions, starting at beginning of compression. The amount of ethanol (and the resulting initial temperature) is varied to determine the boundary between knocking and not knocking operation. The knock chemistry is stiff; small perturbations in the initial temperature can result in large changes in behavior. Figure 2 shows the results of the model for wide open throttle, 900 rpm operation for 85 ON and 86 ON gasoline (no ethanol injection). It should be noted that knocking occurred for the 85 ON fuel after the end gas reached maximum pressure. It has been determined that small initial temperature changes result in substantial changes in the timing of the autoignition. Autoignition onset varies by 5 crank angle degrees for one degree of change of the initial temperature (corresponding to 1% change in ethanol energy fraction). Thus the ethanol required to avoid knock is not very sensitive to the timing of autoignition.

It is assumed that the cylinder charge is composed of the fuel and air, with 1% humidity. No composition correction was made for residual burned gas (a few percent) present in

the cylinder. However, the initial temperature of 380 K accounts for the thermal content of the internally recycled combustion products.
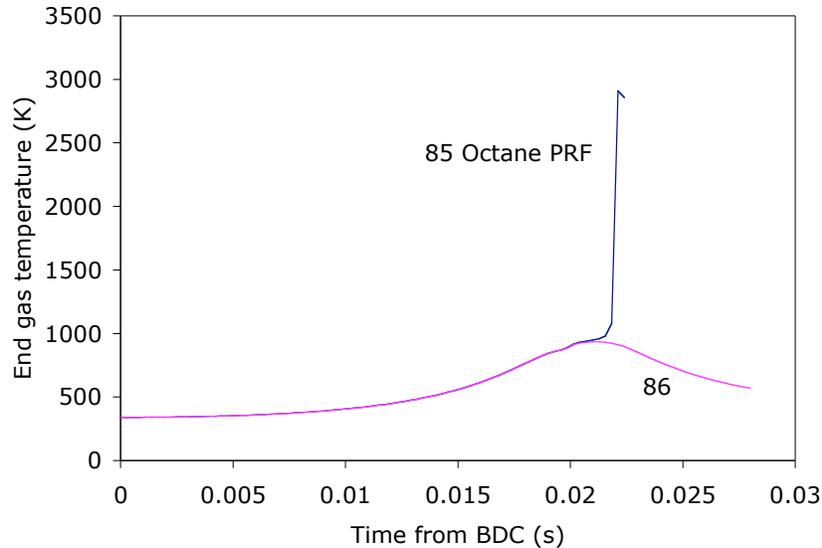

Figure 2. End gas temperature as a function of crank angle, for gasoline injection, 1 bar inlet manifold pressure, (no spark retard), for two grades of gasoline, 85 ON and 86 ON, for initial temperature of 340 K.

IV. Knock Suppression Requirements

In this section, the calculation model is used to determine the required ethanol energy fraction for knock suppression for different inlet manifold pressure, compression ratio and engine speed. Two cases are considered. The first case assumes that the ethanol is homogeneously distributed throughout the cylinder. Results for this case are presented below. The second case investigates the effect of non-uniform or stratified ethanol distribution.

Effects of Injection Timing.

To investigate the effect of early (prior to closing of the inlet valve) and late (after closing of the inlet valve) injection of ethanol, the maximum non-knocking inlet manifold pressure for 100% ethanol is calculated, for an engine compression ratio of 10 and a value of β ~ 0.4. The results are shown in Table 2.

In the "No Evaporative Cooling" column in Table 2, ethanol is port-fuel injected, so the ethanol vaporizes off the inlet valve and the intake manifold walls and thus does not cool the air charge. Use of port-fuel injected (PFI) ethanol allows slight turbocharging (1.05 bar) due to increased octane number of ethanol with respect to gasoline (with a slight increase in charge temperature). The third column corresponds to early injection of ethanol (with inlet valve open, resulting in constant pressure cooling of the charge). The

fourth column is for late injection (after inlet valve closes, with constant volume cooling). The net effect is that the use of port-fuel-injected (PFI) ethanol allows only modest increases in boosting pressure. When the ethanol in-cylinder evaporative cooling is included, the manifold pressure that just avoids knock is substantially raised. In the case of early injection, the initial pressure in the cylinder and the pressure in the inlet manifold are the same (2.4 bar), but the charge temperature is lower than the baseline (380 K), even after the effect of boosting is included. In case of late injection, the manifold pressure can be increased to 4 bar prior to engine knock onset. The larger boosting in the case of late injection is due to the increased cooling of the charge due to the constant volume process (with a constant volume heat capacity about 2/3 that of the constant pressure case).

In the case of late injection (after the inlet valve closes) the cooling of the charge at constant volume decreases the pressure after the injection of the ethanol to about 3 bar (assumed to happen immediately after the inlet valve closes). It is interesting to note that even though the after cooling cylinder pressure (3.0 bar) is reduced relative to the manifold pressure, the in-cylinder pressure is still higher than that with early injection in the case of early injection (2.4 bar). The net effect is that the maximum torque in the case of late injection is higher than that of early injection.

Table 2.
Maximum inlet manifold pressure without knock for 95% ethanol fraction for PFI and early and late direct injection of ethanol.

	No Evaporative Cooling	Evaporative cooling	
		Before Valve Closing	After Valve Closing
Ethanol fraction (by energy)	1	1	1
Max manifold pressure (bar)	1.05	2.4	4.0
Charge pressure after cooling (bar)	1.05	2.4	3.0
Charge temperature after cooling (K)	383	360	355

In practice, injection after the valve has closed and some compression has occurred has the advantage of injecting into hotter gas which helps to insure complete vaporization of the ethanol and prevents or minimizes wall wetting. The calculations in the rest of the paper will be performed for late injection (immediately after the valve closes).

It should also be noted that the temperature of the charge after the injection of the ethanol is comparable for both early and late injection. This is because the greater evaporative cooling effect at constant volume allows a higher manifold pressure which results in a higher engine intake air temperature. The knock onset is closely related to the charge temperature, and thus it is expected that the cases in Table 2 for early and late direct

injection have comparable knocking onset T_{init}. We will come back to this point in the section VI.

Homogeneous Distribution of Ethanol.

Here, we examine the ethanol requirements for knock prevention for late ethanol injection as a function of manifold pressure, compression ratio and engine speed.
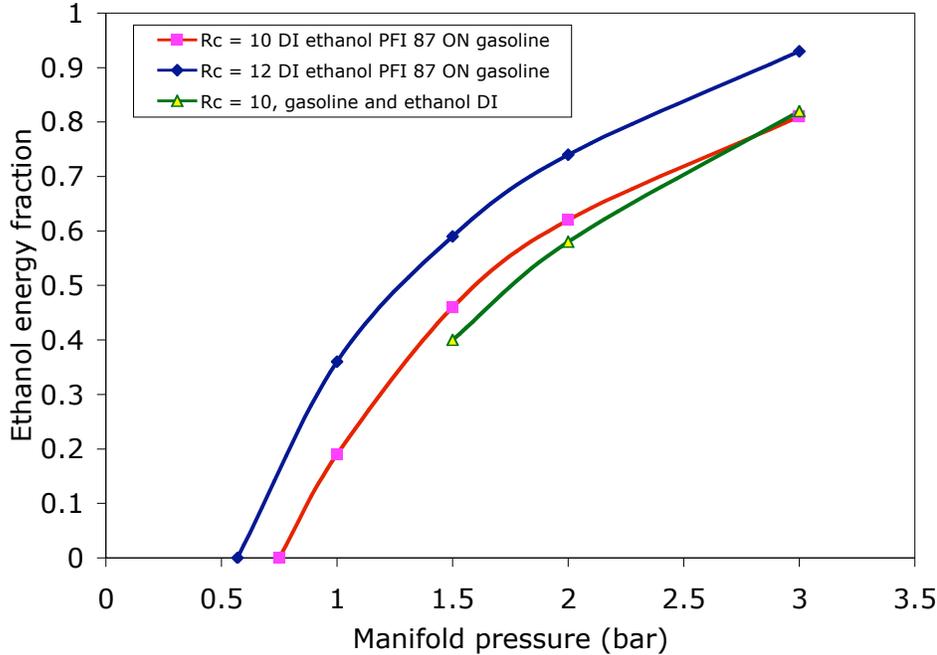

Figure 3. Ethanol fraction (by energy) required to avoid knock; 900 rpm, β = 0.4, homogeneous stoichiometric air/fuel charge.

The ethanol requirements are highest at the lowest engine speeds, since there is more time for the autoignition chemistry to occur. In this paper, it is assumed that spark retard is not used to avoid knock. In practice, it could be used with some loss in torque.

Figure 3 shows the result of the calculations at engine speed of 900 rpm and β = 0.4 for different engine compression ratios, as a function of the inlet manifold pressure. The top two curves are for port injection of gasoline. The case of direct injection of both ethanol and gasoline is shown for comparison. The location of zero ethanol fraction corresponds to the maximum inlet manifold pressure where PRF fuel (87 ON) would just avoid knock in the absence of spark retard. It is assumed that the air/fuel charge is homogeneous.

The same calculations have been performed for increased engine speeds. The results for the case of $R_c = 10$ and β = 0.4 are shown in Figure 4. Contours of constant ethanol energy fraction as a function of inlet manifold pressure and engine speed are shown. The color bar to the right of the graph indicates the ethanol energy fraction at a given point.

As noted above, the highest energy fraction required is at low engine speeds. The boundary where the engine can operate without knock with only gasoline is also shown, and corresponds to the upper region with the darkest blue color. Although the maximum ethanol fraction is high, about 0.6, it occurs at the lowest rpm and highest manifold pressure. It is not clear whether the engine/turbocharger system can satisfactorily operate in this region; even if it did, the fraction of the time in this region would be small. For higher engine speeds (e.g. above 2500 rpm), where the engine would operate more frequently at high torque, the maximum ethanol fraction is closer to about 0.3. Little ethanol is required for inlet manifold pressures less than about 1 bar.
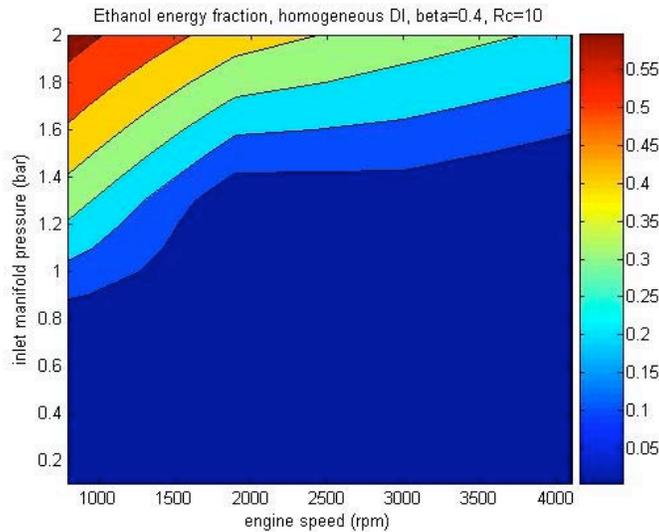
Figure 4. Contours of constant ethanol energy fraction as a function of manifold pressure and engine speed, for β = 0.4, for a compression ratio of 10.

Similar information has been generated for maximum inlet pressures of 2.5 and 3 bar.

Based on a previous evaluation of the effects of engine downsizing on efficiency [7], the increase in allowed boost pressure and resulting downsizing could increase drive cycle efficiency by about 30% relative to a conventional port fueled engine. We estimate that the required amount of ethanol could be less than 5% of the amount of gasoline used over a drive cycle. Detailed studies of the effects of downsizing and higher compression ratio on various engine maps are needed to more precisely determine the range of potential efficiency benefits and ethanol requirements

Stratified Ethanol Injection

The previous section analyzed the case of homogeneous charge. In this section, the use of stratified (non-uniform) charge is examined as a means to reduce the ethanol requirement.

The end gas is at the farthest distance from the spark, and is thus located in the periphery of the combustion chamber. If the ethanol is injected and remains in the outer regions, the maximum knock impact due to ethanol vaporization cooling can be achieved. Not only is effect of the ethanol maximized (by cooling the end gas), but the rest of the charge that is not end gas is not cooled, and as a consequence the flame propagation speed in the central region is faster than in the case when the ethanol is uniformly distributed throughout the charge and with uniform cooling.

The ethanol calculations are performed by assuming centrally located spark plug, and that the ethanol is injected in a region with a volume fraction given by Ψ. $\Psi = 1$ represent uniform distribution, while $\Psi = 0.5$ represents the case where the ethanol is in the outer half of the volume, corresponding to ethanol in a region with a radius larger than 0.707 times the cylinder radius. It should be noted that after ethanol injection, the boundary between the ethanol containing cooled region and the remaining hotter region varies, as the cooled section contracts and the hotter section expands. This effect is included in the calculations.
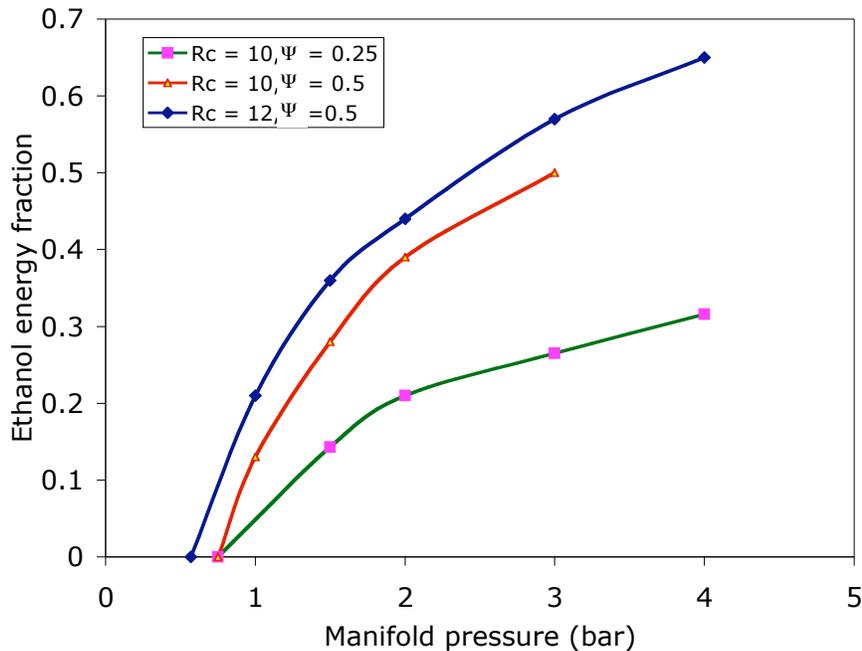

Figure 5. Ethanol energy fraction as a function of the manifold pressure, for the case of non-uniform injection of the ethanol; engine speed of 900 rpm, β = 0.4

The amount of ethanol is then determined assuming that the gasoline is uniformly distributed in the cylinder and the overall air/fuel mixture is stoichiometric (for operation with a three way catalyst). This means that the central hotter region with only gasoline, is leaner than stoichiometric, while the outer colder region, with gasoline and ethanol, is fuel rich.

The resulting temperature stratification could be used to maintain the charge stratification. If the cylinder charge has a strong swirl, centrifugal acceleration in the cylinder can be large, as high as 100 g. Thus the cooler region, with its higher density, will be pushed outward to the periphery, while the lower density region will remain in the central region of the cylinder.

Results of the calculations for the case of stratified ethanol as shown in Figure 5, for several values of Ψ. Stratification could be used to decrease the required ethanol fraction. $\Psi = 0.5$ decreases the required ethanol fraction by about 1/3, while $\Psi = 0.25$ decreases the required ethanol fraction by about 2/3. The reason that the ethanol fraction is not linear with Ψ is due to the fact that the colder region compresses (and therefore, its temperature rises), and thus a given amount of ethanol results in a smaller than expected cooling effect. The case of $\Psi = 0.5$ requires ethanol injection in the outer ~30% of the radius of the cylinder, while the case of $\Psi = 0.25$ required injection in the outer 15% of the radius. The case with $\Psi = 0.25$ is interesting because the ethanol is primarily injected in the end gas region, and thus the ethanol consumption is minimized. However, it may be difficult to inject into this small region around the periphery and avoid wall wetting.

V. Alternative Antiknock Agents.

Our calculations show that for direct injection of ethanol, the larger impact of knock suppression is not the intrinsic knock-resistance of ethanol, but rather its high latent heat of vaporization. This is true for other alcohols. To assess possible alternatives to ethanol, the properties of various hydrocarbons/alternative fuels are listed in Table 3. Although some of these compounds have higher octane numbers than gasoline, some of them have a much larger effect on knock resistance because of their impact on the cylinder charge temperature (Table 3 assumes injection after the inlet valve has closed). Some of these additives (mostly the ethers) have a comparable charge temperature effect to that of gasoline direct injection. The alcohols have optimal properties for use with direct injection, with evaporative cooling temperature changes that are a factor of 3 or more larger than the temperature change due to gasoline direct injection (for 100% or near 100% operation with the anti-knock agent). For ethanol, the change in temperature is a factor of more than 4 larger than that of gasoline, and for methanol the change is about 9 times larger.

Also shown in Table 3 are the ratios of the heat of vaporization to the heat of combustion, a measure of the potential effects when used as antiknock agents. The last entry, ΔT_{air}, indicates the decrease in air temperature for a stoichiometric mixture with 100% antiknock agent energy fraction DI after the inlet valve closes.

The model has been used to calculate the methanol energy fraction required to avoid knock, and it has been determined that it is about half that of ethanol. Although its effect clearly is maximized by the use of methanol, other considerations (including toxicity and corrosivity of the methanol) weigh in favor of ethanol.

Table 3
Antiknock properties of various fuels (calculated from data obtained from reference [8])

Fuel type	RON	MON	(R+M)/2	Net heat of Combustion MJ/kg	Latent heat of vaporization MJ/kg	Vaporization energy/ heat of combustion	Stoic air/fuel ratio	Equiv. Latent heat of vaporization MJ/kg air	ΔT air K
Gasoline				42.8	0.30	0.007	14.6	0.020	-28
Ethyl t-Butyl Ether	118	102	110	36.3	0.31	0.009	12.1	0.026	-35
t-Amyl Methyl Ether	111	98	105	36.3	0.32	0.009	12.1	0.027	-36
Toluene	111	95	103	40.5	0.36	0.009	13.5	0.027	-37
Methyl t-Butil Ether	116	103	110	35.2	0.32	0.009	11.7	0.028	-37
Diisopropyl Ether	110	97	103	38.2	0.34	0.009	12.1	0.028	-39
t-Butyl Alcohol	103	91	97	32.9	0.60	0.018	11.1	0.054	-74
Isopropanol	118	98	108	30.4	0.74	0.024	10.4	0.071	-97
Methanol with cosolvent	114	96	105	26.5	0.88	0.033	8.8	0.100	-137
Ethanol	129	102	115	26.7	0.91	0.034	9	0.102	-138
Methanol	133	105	119	20.0	1.16	0.058	6.4	0.181	-246

VI. Effect of Cooling on Knock-Resistance

It has been mentioned previously that the effect of charge cooling is more important than
the relatively high octane number of the ethanol. In this section the effect of cooling of
the air from the turbocharger by heat transfer (in the ducting and by an intercooler) is
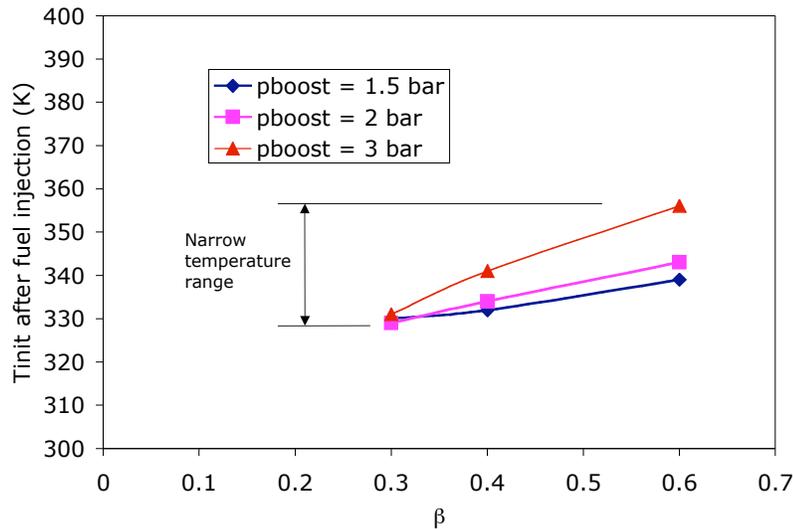discussed.

Figure 6. Initial temperature resulting for direct injection of ethanol as a
function of β for several inlet manifold pressures. The amount of ethanol
directly injected is that which is needed to prevent knock. β = ΔT$_{charge}$/ΔT$_{turbo}$

The ethanol fraction required to suppress knock for several inlet manifold pressures as
well as for different values of β are shown in Figure 6. This figure is calculated for the
case when both ethanol and gasoline are directly injected. The temperature of the charge,
prior to the ethanol/gasoline injection, varies over a wide range, from ~ 400 K to ~ 500
K. This temperature is mainly driven by the change in the inlet manifold pressure.

The primary purpose of the addition of liquid ethanol is to cool the charge to an initial temperature of $T_{init} \sim 340$ K. This result is consisted with the data in Table 2, where T_{init} is relatively independent of whether the liquid evaporation process occurs at constant pressure or constant volume. In addition, the calculations for methanol addition, described in the previous section, indicate that the temperature after methanol late injection for the case that just avoids knock is similar to that of the ethanol case. Because the methanol has a factor of 2 higher latent heat of vaporization, the required amount of methanol is about half. Note that the octane value of ethanol and methanol are comparable. Thus, the comparison between methanol and ethanol reinforce the importance of the cooling effect for knock avoidance.
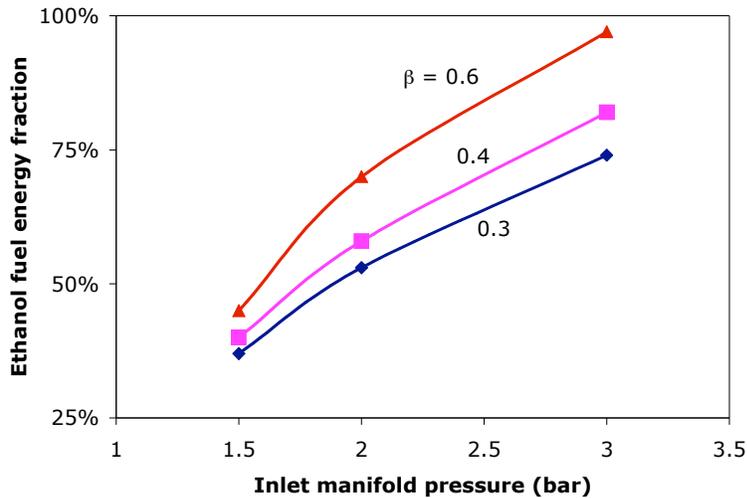

Figure 7. Ethanol fuel energy fraction as a function of the inlet manifold pressure for various value of β for the case of direct injection of ethanol and gasoline.

The ethanol fraction as a function of inlet manifold pressure for the cases illustrated in Figure 6 are shown in Figure 7. The ethanol fraction varies from about 30% at the lowest manifold pressure, to about 100% at the highest pressure.

The 30 K variation of T_{init} in Figure 6 for higher values of β and pressures (which correspond to higher fractions of ethanol), results from the higher octane value of ethanol. However, the main effect is the cooling due to the direct injection of ethanol, corresponding to about 120 K change of the charge temperature by evaporative cooling.

If the ethanol is stored on board in a separate tank, water can be present with the ethanol without affecting the fuel handling system. Hydrous ethanol which contains water has the advantage of lower cost than pure (neat) ethanol. Removing the last 10% to 15% water from ethanol has significant expense and consumes considerable energy. Manufacturing facilities typically produce ethanol with about 10% water by volume unless there is a need for essentially pure (anhydrous) ethanol. The latent heat of

vaporization of water is substantially higher than that of ethanol. 2260 kJ/kg for water, vs 850 kJ/kg for ethanol.

To investigate the effect of the ethanol/water mixtures, the knocking calculations were repeated for 3 bar manifold pressure and $\beta = 0.3$, 0.4 and 0.6 for the case water-ethanol mixtures with 7% weight water (16% molar). This water concentration corresponds to an increase in the latent heat of vaporization of about 14% per kg of mixture, 20% per J delivered by the antiknock agent. The knocking results indicate that the amount of ethanol required is decreased by about 0.04, or about 5%. The effect is thus about a third of that which would be expected from the mixture if the temperature change due to evaporative cooling were the only consideration.

VII. Conclusions

The calculations presented here show that direct ethanol injection could greatly alleviate the knock constraint in boosted spark-ignition gasoline engines. The knock suppression results from both the higher octane rating of ethanol and the effect of the evaporative cooling from the direct injection. Evaporative cooling has a much larger effect than the higher octane rating. The increased knock resistance could be used to allow an increase in the manifold pressure by more than a factor of two. It could also be used to increase the compression ratio. The increased knock resistance could allow engine operation at much higher levels of turbocharging, specific torque and power than would otherwise be possible. Engines could potentially be downsized by a factor of two and the drive cycle efficiency could thereby be increased by approximately 30%. The amount of ethanol that is required could be less than one gallon for every 20 gallons of gasoline.

In addition, the calculations show that it should be possible to substantially reduce the spark retard required at lower engine speeds and high torque. Although a large ethanol energy fraction is required to avoid knock, engines generally operate in this region for only a small fraction of the time and this need for additional ethanol would not increase the overall ethanol utilization significantly. Thus, the engine could provide substantially higher torque at low engine speeds, with the possibility of performance closer to that of diesel engines in the low to mid engine speed range.

The use of direct ethanol injection could provide a new opportunity for enabling high efficiency gasoline engine operation at a low cost. It could also enable high efficiency flexible fuel use of ethanol over the full range from 100% ethanol to close to 100% gasoline. The driver would have the benefit of a high efficiency engine with the freedom to determine the amount of ethanol use depending on its price and availability.

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